Solving Elliptic Control Problems with Interior Point and SQP Methods: Control and State Constraints

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Abstract

We study optimal control problems for semilinear elliptic equations subject to control and state inequality constraints. Both boundary control and distributed control problems are considered with boundary conditions of Dirichlet or Neumann type. By introducing suitable discretization schemes, the control problem is transcribed into a nonlinear programming problem. Necessary conditions of optimality are discussed both for the continuous and the discretized control problem. It is shown that the recently developed interior point method LOQO of [35] is capable of solving these problems even for high discretizations. Four 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 controls.

Key words: Elliptic control problems, boundary and distributed control, control and state constraints, discretization techniques, interior point optimization methods

1 Introduction

Discretization techniques are well established and as will be demonstrated they provide efficient methods for solving optimal control problems with control and state constraints. Through discretization the optimal control problem is transcribed into a finite-dimensional nonlinear programming problem.
Optimal control problems have thus been a stimulus to develop optimization codes for large-scale NLP-problems. Several discretization approaches for solving control problems with ODE's may be found e.g. in [1,5,6,11,23,33]. In most approaches, the underlying NLP-method is either an SQP-method or an Interior Point Method.

In this paper, we study discretization techniques for solving nonlinear optimal control problems with control and state constraints. A combination of both Neumann and Dirichlet boundary conditions is admitted while the control enters the system either as boundary or distributed control. For this rather general class of elliptic control problems, the theory of necessary conditions has not yet been fully developed. For special classes necessary optimality conditions have been derived in [4,14–16,21,22,24,26,27] for boundary controls and in [3,7–9,12,13,20,21,25–27,34] for distributed controls. In section 2 we present a formal statement of first order necessary conditions for the general elliptic problem. In particular, a more detailed discussion is given for bang-bang and singular controls. These conditions turn out to be consistent with their counterparts for the discretized problem obtained from the Kuhn–Tucker conditions (section 3). The main focus is on the numerical solution of control and state constrained problems and on the verification of the optimality conditions. Further numerical examples may be found in [28,29].

In section 3, we discuss a full discretization approach in which both control and state variables are discretized. The resulting large-scale NLP-problem solved subsequently may contain up to 80,000 variables. Two applications are considered in section 4, one to a heat-conduction problem with boundary control and mixed boundary conditions. This example was also chosen such that it yields a convex quadratic programming (QP) problem in its discretized form permitting comparison to a pure QP solver in addition to more classical approaches as SQP and augmented Lagrangian techniques. The second application is from population dynamics. It leads to a quadratically constrained nonconvex QP. A distributed control function is sought which maximizes the profit of harvesting a biological species. The problems are formulated as AMPL [18] scripts and several optimization codes were applied. In particular, the interior point code LOQO [35] successfully and efficiently solved all problems. In both applications also a case with bang–bang control is solved which is especially remarkable in the distributed control example for which we are not aware of another instance in the literature. It needs to be stressed that more nonlinear formulations of these or other applications can be treated in the same way. The code LOQO was designed to solve general nonconvex NLP problems. For a comparison with other codes on several classes of optimization problems, see the benchmarks of [31].
2 Necessary conditions for elliptic control problems with control and state constraints

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with piecewise smooth boundary $\Gamma = \partial \Omega$. The derivative in the direction of the outward unit normal $\nu$ of $\Gamma$ will be denoted by $\partial_{\nu}$. Suppose that the boundary is partitioned as $\Gamma = \Gamma_1 \cup \Gamma_2$ with disjoint sets $\Gamma_1, \Gamma_2 \subset \Gamma$ that consist of finitely many connected components.

2.1 Boundary control problem

We consider the problem of determining a boundary control function $u \in L^\infty(\Gamma)$ which minimizes the functional

$$ F(y, u) = \int_\Omega f(x, y(x)) \, dx + \int_{\Gamma_1} g(x, y(x), u(x)) \, dx + \int_{\Gamma_2} k(x, u(x)) \, dx \quad (2.1) $$

subject to the elliptic state equation,

$$ -\Delta y(x) + d(x, y(x)) = 0, \quad \text{for } x \in \Omega, \quad (2.2) $$

boundary conditions of Neumann or Dirichlet type,

$$ \partial_{\nu} y(x) = b(x, y(x), u(x)), \quad \text{for } x \in \Gamma_1, \quad (2.3) $$

$$ y(x) = a(x, u(x)), \quad \text{for } x \in \Gamma_2, \quad (2.4) $$

and control and state inequality constraints,

$$ C(x, u(x)) \leq 0, \quad \text{for } x \in \Gamma, \quad (2.5) $$

$$ S(x, y(x)) \leq 0, \quad \text{for } x \in \Omega. \quad (2.6) $$

The functions $f : \Omega \times \mathbb{R} \to \mathbb{R}$, $g : \Gamma_1 \times \mathbb{R}^2 \to \mathbb{R}$, $k : \Gamma_2 \times \mathbb{R} \to \mathbb{R}$, $b : \Gamma_1 \times \mathbb{R}^2 \to \mathbb{R}$, $a : \Gamma_2 \times \mathbb{R} \to \mathbb{R}$, $d : \Omega \times \mathbb{R} \to \mathbb{R}$, $C : \Gamma \times \mathbb{R} \to \mathbb{R}$, and $S : \Omega \times \mathbb{R} \to \mathbb{R}$ are assumed to be $C^2$-functions. It is straightforward to include more than one inequality constraint in (2.5) or (2.6). 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.

The Laplacian $\Delta$ in (2.2) can be replaced by any elliptic operator

$$ Ay(x) = \sum_{k,j=1}^2 \partial_{x_k} (a_{kj}(\cdot) \partial_{x_j} y)(x), $$
where the coefficients \( a_{kj} \in C^2(\bar{\Omega}) \) satisfy the following coercivity condition with some \( c > 0 \):

\[
\sum_{k,j=1}^2 a_{kj}(x)v_kv_j \geq c(v_1^2 + v_2^2) \quad \forall x \in \bar{\Omega}, \ v \in \mathbb{R}^2.
\]

However, in the sequel we restrict the discussion to the operator \( A = \Delta \) which simplifies the form of the necessary conditions and the numerical analysis.

An optimal solution of problem (2.1)–(2.6) will be denoted by \( \bar{u} \) and \( \bar{y} \). The active sets for the inequality constraints (2.5), (2.6) are defined by

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

(2.7)

The following regularity conditions are supposed to hold,

\[
C_u(x, \bar{u}(x)) \neq 0 \quad \forall x \in J(C),
\]

\[
S_y(x, \bar{y}(x)) \neq 0 \quad \forall x \in J(S).
\]  

(2.8)

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

First order necessary conditions for the rather general problem (2.1)–(2.6) are not yet available in the literature. The main difficulty results from the Dirichlet condition (2.4) which prevents solution from being sufficiently regular. First order necessary conditions for problems with linear elliptic equations \(-\Delta y(x) + y(x) = 0\) and pure Neumann conditions may be found in Casas [14], Casas et al. [15,16]. A weak formulation for linear elliptic equations and Dirichlet conditions is due to Bergounioux, Kunisch [4].

We shall present first order conditions in a form that can be derived at least in a purely formal way. This form will turn out to be consistent with the first order conditions of Kuhn–Tucker for the discretized elliptic control problem in section 3.1. We assume that there exists an adjoint state \( \tilde{q} \in W^{1,1}(\bar{\Omega}) \), a multiplier \( \tilde{\lambda} \in L^\infty(\Gamma) \), and a regular Borel measure \( \tilde{\mu} \) on \( \Omega \) such that the following conditions hold:

adjoint equation and boundary conditions:

\[
-\Delta \tilde{q}(x) + \tilde{q}(x)d_y(x, \bar{y}(x)) + f_y(x, \bar{y}(x)) + S_y(x, \bar{y}(x)) \tilde{\mu} = 0 \quad \text{on } \Omega,
\]  

(2.9)

\[
\partial_v \tilde{q}(x) - \tilde{q}(x)b_y(x, \bar{y}(x), \bar{u}(x)) + g_y(x, \bar{y}(x), \bar{u}(x)) = 0 \quad \text{on } \Gamma_1,
\]  

(2.10)

\[
\tilde{q}(x) = 0 \quad \text{on } \Gamma_2,
\]  

(2.11)
minimum condition for \( x \in \Gamma_1 \):

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

(2.12)

minimum condition for \( x \in \Gamma_2 \):

\[
k_u(x, \bar{u}(x)) + \partial_q q(x) a_u(x, \bar{u}(x)) + \bar{\lambda}(x) C_u(x, \bar{u}(x)) = 0 ,
\]  

(2.13)

complementarity conditions:

\[
\bar{\lambda}(x) \geq 0 \quad \text{on} \quad J(C), \quad \bar{\lambda}(x) = 0 \quad \text{on} \quad \Gamma \setminus J(C),
\]  

(2.14)

\[
d\bar{\mu} \geq 0 \quad \text{in} \quad J(S), \quad d\bar{\mu} = 0 \quad \text{in} \quad \Omega \setminus J(S).
\]

The adjoint equations (2.9)–(2.11) are understood in the weak sense, cf. Casas et al. [16]. According to Bourbaki [10], Chapter 9, the regular Borel measure \( \bar{\mu} \) appearing in the adjoint equation (2.9) has the decomposition

\[
\bar{\mu} = \bar{\nu} \cdot dx + \bar{\nu}_s \cdot \bar{\mu}_s ,
\]  

(2.15)

where \( dx \) represents the Lebesgue measure and \( \bar{\mu}_s \) is singular with respect to \( dx \); the functions \( \bar{\nu}, \bar{\nu}_s \) are measurable on \( \Omega \). The problem of obtaining the decomposition (2.15) explicitly is related to the difficulty of determining the structure of the active set \( J(S) \). In section 3, we shall make an attempt to approximate the measure by the multipliers of the discretized control problem.

In many applications, the cost functional (2.1) is of tracking type, cf. [2,4,22,24],

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

(2.16)

with given functions \( y_d \in C(\bar{\Omega}), u_d \in L^\infty(\Gamma) \), and nonnegative weight \( \alpha \geq 0 \). The control and state constraints (2.5) and (2.6) are taken to be box constraints of the simple type

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

(2.17)

with functions \( \psi \in C(\bar{\Omega}) \) and \( u_1, u_2 \in L^\infty(\Gamma) \). Here, in particular we assume that the functions \( g \) and \( k \) in (2.1) coincide. For these data the adjoint
equations (2.9)-(2.11) become

\[-\Delta \bar{q}(x) + \bar{q}(x) d_y(x, \bar{y}(x)) + \bar{y}(x) - y_d(x) + \bar{\mu} = 0 \quad \text{in } \Omega,\]

\[\partial_\nu \bar{q}(x) - \bar{q}(x) b_\nu(x, \bar{y}(x), \bar{u}(x)) = 0 \quad \text{on } \Gamma_1, \quad (2.18)\]

\[\bar{q}(x) = 0 \quad \text{on } \Gamma_2.\]

If the function $b$ in the Neumann condition (2.3) has the special form $b(x, y, u) = b_0(x, y) + u$, then the minimum condition (2.12) reduces to

\[[\alpha(\bar{u}(x) - u_d(x)) - \bar{q}(x)] (u - \bar{u}(x)) \geq 0 \quad \forall x \in \Gamma_1, \ u \in [u_1(x), u_2(x)]. \quad (2.19)\]

Likewise, if the function $a$ in (2.4) is given by $a(x, u) = a_0(x) + u$, the minimum condition (2.13) yields

\[[\alpha(\bar{u}(x) - u_d(x)) + \partial_\nu \bar{q}(x)] (u - \bar{u}(x)) \geq 0 \quad \forall x \in \Gamma_2, \ u \in [u_1(x), u_2(x)]. \quad (2.20)\]

**Case** $\alpha > 0$ : The previous conditions determine the following control laws:

for $x \in \Gamma_1$,

\[\bar{u}(x) = \begin{cases} 
  u_d(x) + \bar{q}(x)/\alpha, & \text{if } u_d(x) + \bar{q}(x)/\alpha \in (u_1(x), u_2(x)), \\
  u_1(x), & \text{if } u_d(x) + \bar{q}(x)/\alpha \leq u_1(x), \\
  u_2(x), & \text{if } u_d(x) + \bar{q}(x)/\alpha \geq u_2(x).
\end{cases} \quad (2.21)\]

for $x \in \Gamma_2$,

\[\bar{u}(x) = \begin{cases} 
  u_d(x) - \partial_\nu \bar{q}(x)/\alpha, & \text{if } u_d(x) - \partial_\nu \bar{q}(x)/\alpha \in (u_1(x), u_2(x)), \\
  u_1(x), & \text{if } u_d(x) - \partial_\nu \bar{q}(x)/\alpha \leq u_1(x), \\
  u_2(x), & \text{if } u_d(x) - \partial_\nu \bar{q}(x)/\alpha \geq u_2(x).
\end{cases} \quad (2.22)\]

**Case** $\alpha = 0$ : We obtain an optimal control of *bang-bang* or *singular* type:

for $x \in \Gamma_1$,

\[\bar{u}(x) = \begin{cases} 
  u_1(x), & \text{if } \bar{q}(x) < 0, \\
  u_2(x), & \text{if } \bar{q}(x) > 0, \\
  \text{singular}, & \text{if } \bar{q}(x) = 0 \quad \text{on } \Gamma_{s_1} \subset \Gamma_1, \ \text{meas}(\Gamma_{s_1}) > 0.
\end{cases} \quad (2.23)\]
for \( x \in \Gamma_2 \),
\[
\bar{u}(x) = \begin{cases} 
    u_1(x) & \text{if } \partial_{\nu}\bar{q}(x) > 0, \\
    u_2(x) & \text{if } \partial_{\nu}\bar{q}(x) < 0, \\
    \text{singular} & \text{if } \partial_{\nu}\bar{q}(x) = 0 \text{ on } \Gamma_{s2} \subset \Gamma_2, \text{meas}(\Gamma_{s2}) > 0.
\end{cases}
\] (2.24)

Hence in case \( \alpha = 0 \), the so-called \textit{switching function} is given by the adjoint function \( \bar{q}(x) \) on the boundary \( \Gamma_1 \) resp. by the outward normal derivative \( \partial_{\nu}\bar{q}(x) \) on the boundary \( \Gamma_2 \). The isolated zeros of the switching function are the \textit{switching points} of a bang–bang control; cf. the example in section 4.1.

2.2 Distributed Control Problem

Here the problem is to determine a distributed control function \( u \in L^\infty(\Omega) \) that minimizes the functional
\[
F(y, u) = \int_{\Omega} f(x, y(x), u(x)) \, dx + \int_{\Gamma_1} g(x, y(x)) \, dx
\] (2.25)

subject to the elliptic state equation,
\[
-\Delta y(x) + d(x, y(x), u(x)) = 0, \quad \text{for } x \in \Omega,
\] (2.26)

Neumann and Dirichlet boundary conditions,
\[
\partial_{\nu} y(x) = b(x, y(x)), \quad \text{for } x \in \Gamma_1,
\] (2.27)
\[
y(x) = y_2(x), \quad \text{for } x \in \Gamma_2,
\] (2.28)

and mixed control–state inequality constraints resp. \textit{pure} state inequality constraints,
\[
C(x, y(x), u(x)) \leq 0, \quad \text{for } x \in \Omega,
\] (2.29)
\[
S(x, y(x)) \leq 0, \quad \text{for } x \in \Omega.
\] (2.30)

The functions \( f : \Omega \times \mathbb{R}^2 \to \mathbb{R}, \quad g : \Gamma_1 \times \mathbb{R}^2 \to \mathbb{R}, \quad b : \Gamma_1 \times \mathbb{R}^2 \to \mathbb{R}, \quad d : \Omega \times \mathbb{R} \to \mathbb{R}, \quad C : \Omega \times \mathbb{R}^2 \to \mathbb{R}, \quad \text{and } S : \Omega \times \mathbb{R} \to \mathbb{R} \) are assumed to be \( C^2 \)-functions, while the Dirichlet condition (2.28) holds with \( y_2 \in C^1(\Gamma_2) \).

The above distributed control problem is slightly more general than the one considered in Bonnans and Casas [9] where first order conditions have been
given in terms of a weak and strong Pontryagin principle. For linear elliptic equations, first order conditions may also be found in Bergounioux et al. [3], Bonnans and Casas [8]. Nonlinear elliptic equations of Lotka–Volterra type have been treated in Canada et al. [12] and Leung, Stojanovic [25,34].

Denote an optimal solution of problem (2.25)–(2.30) by \( \bar{u} \) and \( \bar{y} \). The active sets corresponding to the inequality constraints (2.29), (2.30) are given by

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

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

It is required that the following regularity conditions analogous to (2.8) hold:

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

\[
S_y(x, \bar{y}(x)) \neq 0 \quad \forall x \in J(S).
\]

Then first order necessary conditions can be stated in the following form. There exist an adjoint state \( \bar{q} \in W^{1,1}(\bar{\Omega}) \), a multiplier \( \bar{\lambda} \in L^{\infty}(\Omega) \) and a regular Borel measure \( \bar{\mu} \) in \( \Omega \) such that the following conditions hold:

**adjoint equation and boundary conditions:**

\[-\Delta \bar{q}(x) + \bar{q}(x) \frac{\partial y}{\partial x} (x, \bar{y}(x), \bar{u}(x)) + f_y(x, \bar{y}(x), \bar{u}(x)) + \]

\[+ \bar{\lambda}(x) C_y(x, \bar{y}(x), \bar{u}(x)) + S_y(x, \bar{y}(x)) \bar{\mu} = 0 \quad \text{in} \quad \Omega, \quad (2.33)\]

\[\partial_n \bar{q}(x) - \bar{q}(x) b_y(x, \bar{y}(x)) + g_y(x, \bar{y}(x)) = 0 \quad \text{on} \quad \Gamma_1, \quad (2.34)\]

\[\bar{q}(x) = 0 \quad \text{on} \quad \Gamma_2, \quad (2.35)\]

**minimum condition for** \( x \in \Omega \):

\[f_u(x, \bar{y}(x), \bar{u}(x)) + \bar{q}(x) \frac{\partial u}{\partial x} (x, \bar{y}(x), \bar{u}(x)) + \bar{\lambda}(x) C_u(x, \bar{y}(x), \bar{u}(x)) = 0, \quad (2.36)\]

**complementarity conditions:**

\[\bar{\lambda}(x) \geq 0 \quad \text{in} \quad J(C), \quad \bar{\lambda}(x) = 0 \quad \text{in} \quad \Omega \setminus J(C), \]

\[d\bar{\mu} \geq 0 \quad \text{in} \quad J(S), \quad d\bar{\mu} = 0 \quad \text{in} \quad \Omega \setminus S(S). \]

The adjoint equations (2.33)–(2.35) are understood in the weak sense. The regular Borel measure in the adjoint equation (2.33) has a decomposition
similar to that in (2.15),
\[
\bar{\mu} = \bar{\nu} \cdot dx + \bar{\nu}_s \cdot \bar{\mu}_s, 
\]  
(2.38)

where \( dx \) represents the Lebesgue measure and the measure \( \bar{\mu}_s \) is singular with respect to \( dx \).

With regard to Example 4.2 in section 4 we shall discuss the minimum condition (2.36) in case that the control and state constraints (2.29) and (2.30) are box constraints
\[
y(x) \leq \psi(x), \quad u_1(x) \leq u(x) \leq u_2(x) \quad \forall \ x \in \Omega, 
\]  
(2.39)

with functions \( \psi \in C(\bar{\Omega}) \) and \( u_1, u_2 \in L^\infty(\Omega) \). We immediately derive from (2.36) the control law
\[
\left[ f_u(x, \bar{y}(x), \bar{u}(x)) + q(x) d_u(x, \bar{y}(x), \bar{u}(x)) \right] (u - \bar{u}(x)) \geq 0 
\]
\[
\forall \ u \in [u_1(x), u_2(x)], \ x \in \Omega. 
\]  
(2.40)

It is straightforward to obtain analogous control laws for tracking functionals similar to (2.16).

3 Discretization and optimization techniques

The discussion of discretization schemes is restricted to the standard situation where the domain is the unit square \( \Omega = (0,1) \times (0,1) \). The purpose of this section is to develop discretization techniques by which the boundary control problem (2.1)–(2.6) and the distributed control problem (2.25)–(2.30) are transformed into a nonlinear programming problem (NLP-problem) of the form

\[
\text{Minimize} \quad F^h(z) \quad \text{subject to} \quad G^h(z) = 0, \quad H(z) \leq 0. 
\]  
(3.1)

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

The form (3.1) will be achieved by solving the elliptic equation (2.2) resp. (2.26) with the standard five-point-star discretization scheme. Choose a num-
ber \( N \in \mathbb{N}_+ \) and the stepsize \( h := 1/(N + 1) \). Consider the mesh points
\[
x_{ij} = (i h, j h), \quad 0 \leq i, j \leq N + 1,
\]
and define the following sets of indices \((i, j)\) residing either in the domain \( \Omega \) or on the four edges of the boundary \( \Gamma \):
\[
I(\Omega) := \{ (i, j) \mid 1 \leq i, j \leq N \},
I(\Gamma) := \{ (i, j) \mid i = 1, ..., N, j = 0 \text{ or } j = N + 1, j = 1, ..., N, i = 0 \text{ or } i = N + 1 \}, \quad (3.2)
I(\Gamma_k) := \{ (i, j) \in I(\Gamma) \mid x_{ij} \in \Gamma_k \}, \quad k = 1, 2,
I(\tilde{\Omega}) := I(\Omega) \cup I(\Gamma), \quad I(\Omega \cup \Gamma_1) := I(\Omega) \cup I(\Gamma_1).
\]
Obviously, we have \( \#I(\Omega) = N^2 \), \( \#I(\Gamma) = 4 \times N \); define further \( M_1 := \#I(\Gamma_1) \).

We shall first discuss discretization schemes for the boundary control problem and will then only indicate the necessary modifications to obtain schemes for the distributed control problem.

### 3.1 Discretization of the boundary control problem

Let \( y_{ij} \) denote approximations of the state variables \( y(x_{ij}) \) for \((i, j) \in I(\tilde{\Omega})\) and let \( u_{ij} \) be approximations for the control variables \( u(x_{ij}) \) for \((i, j) \in I(\Gamma)\). We specify the functions \( F^h, G^h, H \) for the optimization problem (3.1) corresponding to problem (2.1)–(2.6) as follows. The optimization variable \( z \) in (3.1) is taken as the vector
\[
z := \left( (y_{ij})_{(i,j) \in I(\Omega \cup \Gamma_1)}, (u_{ij})_{(i,j) \in I(\Gamma)} \right) \in \mathbb{R}^{N^2 + M_1 + 4N}.
\]
Note that we do not consider the variables \( y_{ij}, (i, j) \in I(\Gamma_2) \), explicitly as optimization variables since they are prescribed by the Dirichlet condition (2.4).

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),
\[
G^h_{ij}(z) := 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2 d(x_{ij}, y_{ij}) = 0. \quad (3.3)
\]
In these equations may appear the undefined variables $y_{ij}$ for $(i,j) \in \Gamma_2$. These variables have to be substituted by the Dirichlet conditions (2.4),

$$y_{ij} = a(x_{ij}, u_{ij}) \quad \text{for all } (i,j) \in I(\Gamma_2). \quad (3.4)$$

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

$$y_{ij}^r := \begin{cases} 
  y_{i0} - y_{i1}, & \text{for } j = 0, \quad i = 1, \ldots, N \\
  y_{ij} - y_{ij}, & \text{for } i = 0, \quad j = 1, \ldots, N \\
  y_{N+1,j} - y_{N,j}, & \text{for } i = N+1, \quad j = 1, \ldots, N \\
  y_{i,N+1} - y_{iN}, & \text{for } j = N+1, \quad i = 1, \ldots, N
\end{cases} \quad (3.5)$$

Then the discrete form of the Neumann boundary condition (2.3) leads to the equality constraints

$$B^h(z) := y_{ij}^r - h b(x_{ij}, y_{ij}, u_{ij}) = 0 \quad \text{for } (i,j) \in I(\Gamma_1). \quad (3.6)$$

The control and state inequality constraints (2.5) and (2.6) yield the inequality constraints

$$C(x_{ij}, u_{ij}) \leq 0 \quad \text{for } (i,j) \in I(\Gamma), \quad (3.7)$$

$$S(x_{ij}, y_{ij}) \leq 0 \quad \text{for } (i,j) \in I(\Omega), \quad (3.8)$$

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

$$F^h(z) := h^2 \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma_1)} g(x_{ij}, y_{ij}, u_{ij})$$

$$+ h \sum_{(i,j) \in I(\Gamma_2)} h(x_{ij}, u_{ij}). \quad (3.9)$$

Then the relations (3.2)-(3.8) define an NLP–problem of the form (3.1).

Associate Lagrange multipliers $q = (q_{ij})_{(i,j) \in I(\Omega \cup \Gamma_1)}$, $\lambda = (\lambda_{ij})_{(i,j) \in I(\Gamma)}$ and $\mu = (\mu_{ij})_{(i,j) \in I(\Omega)}$ with the equality constraints (3.3) and (3.6) resp. the inequality constraints (3.7) and (3.8). Then the Lagrangian function for the above NLP–problem becomes:

$$L(z, q, \lambda, \mu) := h^2 \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma_1)} g(x_{ij}, y_{ij}, u_{ij})$$

$$+ \sum_{(i,j) \in I(\Gamma_2)} h(x_{ij}, u_{ij}). \quad (3.10)$$

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\[ + \frac{h}{2} \sum_{(i,j) \in \Gamma_2} k(x_{ij}, y_{ij}) + \sum_{(i,j) \in \Omega} \left[ q_{ij} C_{ij}^h(z) + \mu_{ij} S(x_{ij}, y_{ij}) \right] \\
+ \sum_{(i,j) \in \Omega_{11}} q_{ij} B_{ij}^h(z) + \sum_{(i,j) \in \Omega} \lambda_{ij} C(x_{ij}, u_{ij}) \].

The multipliers $\lambda$ and $\mu$ satisfy complementarity conditions corresponding to (2.14):

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

Now we discuss the necessary conditions of optimality

\[ 0 = L_z = \left( (L_{y_{ij}})_{(i,j) \in \Omega \cup \Gamma_1}, (L_{u_{ij}})_{(i,j) \in \Omega} \right) \]

for state and control variables assuming different combinations of indices $(i, j)$. For state variables with indices $(i, j) \in \Omega$ we obtain the relations

\[ 0 = L_{y_{ij}} = 4q_{ij} - q_{i+1,j} - q_{i,j+1} - q_{i,j-1} - q_{i,j+1} + h^2 q_{ij} d_y(x_{ij}, y_{ij}) \]
\[ + h^2 f_y(x_{ij}, y_{ij}) + \mu_{ij} S_y(x_{ij}, y_{ij}). \] (3.11)

These equations contain multipliers $q_{ij}$ for $(i, j) \in \Gamma_2$ that do not appear in the Lagrangian (3.10). To make equations and definitions consistent, we put

\[ q_{ij} = 0 \quad \text{for} \quad (i, j) \in \Gamma_2. \] (3.12)

This substitution corresponds to the Dirichlet condition (2.11). Relations (3.11) then reveal that the Lagrange multipliers $q = (q_{ij})$ satisfy the five-point-star difference equations for the adjoint equation $-\Delta q + \dot{q} d_y + f_y + S_y \dot{\mu} = 0$ in (2.9) if we use the following approximation for the Borel measure $\tilde{\mu}$,

\[ \int_{sq(h^2)} d\tilde{\mu} \sim \mu_{ij}, \] (3.13)

where $sq(h^2)$ denotes a square centered at $x_{ij}$ with area $h^2$. Recall the decomposition (2.15) of the measure $\tilde{\mu} = \bar{\nu} \cdot dx + \bar{\nu}_s \cdot \bar{\nu}_s$. If the singular part of the measure vanishes, i.e. $\bar{\nu}_s \cdot \bar{\nu}_s = 0$, then (3.13) yields the following approximation for the density $\bar{\nu}$,

\[ \bar{\nu}(x_{ij}) \sim \mu_{ij}/h^2. \] (3.14)
In case that the measure $\bar{\nu} = \nu_\delta \cdot \delta(x - x_{ij})$ is a delta distribution, we obtain from (3.13) the relation

$$\bar{\nu}_s \sim \mu_{ij}.$$ (3.15)

On the boundary part $\Gamma_1$ we get for indices $(i, j) \in I(\Gamma_1)$ assuming, e.g., $j = 0, i \in \{1, ..., N\}$:

$$0 = L_{y_{i0}} = -q_{i1} + q_{i0} \ h \ b_y(x_{i0}, y_{i0}) + h \ g_y(x_{i0}, y_{i0}, u_{i0})$$
$$= h \left[ \frac{q_{i0} - q_{i1}}{h} - q_{i0} \ b_y(x_{i0}, y_{i0}) + g_y(x_{i0}, y_{i0}, u_{i0}) \right].$$

Recalling (3.5) this represents the discrete version of the Neumann boundary condition (2.10).

Finally, necessary conditions with respect to the control variables $u_{ij}$ for indices $(i, j) \in I(\Gamma)$ are determined by the following two relations. For $(i, j) \in \Gamma_1$ with, e.g., $j = 0, i \in \{1, ..., N\}$, we get

$$0 = L_{u_{i0}} = h \ g_u(x_{i0}, y_{i0}, u_{i0}) - q_{i0} \ h \ b_u(x_{i0}, y_{i0}, u_{i0}) + \lambda_{i0} C_u(x_{i0}, u_{i0})$$
$$= h \left[ g_u(x_{i0}, y_{i0}, u_{i0}) - q_{i0} \ b_u(x_{i0}, y_{i0}, u_{i0}) + \frac{\lambda_{i0}}{h} C_u(x_{i0}, u_{i0}) \right].$$

This equation yields the discrete version of the optimality condition (2.12) for the control, if we use the identification

$$\tilde{\lambda}(x_{i0}) \sim \frac{\lambda_{i0}}{h}.$$ (3.16)

For indices $(i, j) \in \Gamma_2$ with, e.g., $j = 0, i \in \{1, ..., N\}$, we find

$$0 = L_{u_{i0}} = h \ k_u(x_{i0}, u_{i0}) - q_{i1} \ a_u(x_{i0}, u_{i0}) + \lambda_{i0} C_u(x_{i0}, u_{i0})$$
$$= h \left[ k_u(x_{i0}, u_{i0}) - \frac{q_{i1}}{h} \ a_u(x_{i0}, u_{i0}) + \frac{\lambda_{i0}}{h} C_u(x_{i0}, u_{i0}) \right].$$

Observing $q_{i0} = 0$ and the approximation (3.5) of the normal derivative, the minimum condition (2.13) holds with the substitutions

$$\partial_\nu \bar{q}(x_{i0}) \sim -q_{i1}/h, \quad \tilde{\lambda}(x_{i0}) \sim \frac{\lambda_{i0}}{h}.$$ (3.17)
3.2 Discretization of the distributed control problem

The optimization variable $z$ in (3.1) is now taken as the vector

$$ z := ((y_{ij})_{(i,j)\in I(\Omega \times \Gamma_1)}, (u_{ij})_{(i,j)\in I(\Omega)}) \in \mathbb{R}^{2nN^2 + M_1}. $$

Due to the Dirichlet conditions (2.28), the variables $y_{ij}$ for $(i,j) \in I(\Gamma_2)$ can be eliminated from the optimization process.

The application of the five-point-star to the elliptic equation $-\Delta y(x) + d(x, y(x), u(x)) = 0$ in (2.26) yields the following equations for all $(i,j) \in I(\Omega)$:

$$ G^h_{ij}(z) := 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2 d(x_{ij}, y_{ij}, u_{ij}) = 0. \quad (3.18) $$

The Dirichlet condition (2.28) is incorporated by fixing the values $y_{ij}$ on $\Gamma_2$:

$$ y_{ij} = y_2(x_{ij}) \quad \forall \ (i,j) \in I(\Gamma_2). \quad (3.19) $$

Observing the approximation (3.5) of the outward normal derivative, the discrete form of the Neumann boundary condition in (2.27) leads to the equality constraints

$$ B^h(x_{ij}, y_{ij}) := y^\nu_{ij} - h b(x_{ij}, y_{ij}) = 0 \quad \text{for} \quad (i,j) \in I(\Gamma_1). \quad (3.20) $$

The control and state inequality constraints (2.29) and (2.30) yield the inequality constraints

$$ C(x_{ij}, y_{ij}, u_{ij}) \leq 0, \quad \forall \ (i,j) \in I(\Omega). \quad (3.21) $$

$$ S(x_{ij}, y_{ij}) \leq 0, \quad \forall \ (i,j) \in I(\Omega). \quad (3.22) $$

Note again that these inequality constraints do not depend on the meshsize $h$. The discretized form of the cost function (2.25) is

$$ F^h(z) := h^2 \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}, u_{ij}) + h \sum_{(i,j)\in I(\Gamma_1)} g(x_{ij}, y_{ij}). \quad (3.23) $$

Hence, for distributed control problems the NLP–problem (3.1) is given by the relations (3.18)–(3.23). The corresponding Lagrangian function is

$$ L(z, q, \lambda, \mu) := h^2 \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}, u_{ij}) + h \sum_{(i,j)\in I(\Gamma_1)} g(x_{ij}, y_{ij}) \quad (3.24) $$
\[
+ \sum_{(i,j) \in I(\Omega)} [q_{ij} C(x_{ij}, y_{ij}, u_{ij}) + \lambda_{ij} C(x_{ij}, y_{ij}, u_{ij}) + \mu_{ij} S(x_{ij}, y_{ij})]
\]

\[
+ \sum_{(i,j) \in \Gamma_1} q_{ij} B^h(z),
\]

where the Lagrange multipliers \( q = (q_{ij})_{(i,j) \in I(\Omega \cup \Gamma_1)}, \lambda = (\lambda_{ij})_{(i,j) \in I(\Omega)} \) and \( \mu = (\mu_{ij})_{(i,j) \in I(\Omega)} \) are associated with the equality constraints (3.18) and (3.20), resp. the inequality constraints (3.21) and (3.22). The multipliers \( \lambda \) and \( \mu \) satisfy complementarity conditions corresponding to (2.37):

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

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

The discussion of the necessary conditions of optimality

\[
0 = L_z = ((L_{y_{ij}})_{(i,j) \in I(\Omega \cup \Gamma_1)}, (L_{u_{ij}})_{(i,j) \in I(\Omega)})
\]

is similar to that for boundary control problems. For state variables \( y_{ij} \) with indices \( (i, j) \in I(\Omega) \) we obtain the relations

\[
0 = L_{y_{ij}} = 4q_{ij} - q_{i+1,j} - q_{i-1,j} - q_{i,j+1} - q_{i,j-1} + h^2 q_{ij} d_y(x_{ij}, y_{ij}, u_{ij}) + h^2 f_y(x_{ij}, y_{ij}, u_{ij}) + \lambda_{ij} C_y(x_{ij}, y_{ij}, u_{ij}) + \mu_{ij} S_y(x_{ij}, y_{ij}). \quad (3.25)
\]

Here as in (3.12), the undefined multipliers are set to

\[
q_{ij} = 0 \quad \forall (i, j) \in \Gamma_2, \quad (3.26)
\]

in accordance with the Dirichlet condition (2.35). We deduce from equations (3.25) that the Lagrange multipliers \( q = (q_{ij}) \) satisfy the five-point-star difference equations for the adjoint equation \(-\Delta \tilde{q} + \tilde{q} d_y + f_y + \lambda C_y + S_y \tilde{\mu} = 0\) in (2.33) if we approximate the measure \( \tilde{\mu} \) and the multiplier function \( \tilde{\lambda} \) in \( \Omega \) by

\[
h^2 \tilde{\lambda}(x_{ij}) \sim \lambda_{ij}, \quad \int_{sq(h^2)} \tilde{d}\tilde{\mu} \sim \mu_{ij}, \quad (3.27)
\]

where \( sq(h^2) \) denotes a square centered at \( x_{ij} \) with area \( h^2 \). Recall again the decomposition (2.38) of the measure \( \tilde{\mu} = \tilde{v} \cdot dx + \tilde{v}_s \cdot \tilde{\mu}_s \). If the singular part of the measure vanishes, then (3.27) yields an approximation for the density \( \tilde{v} \),

\[
\tilde{v}(x_{ij}) \sim \mu_{ij}/h^2. \quad (3.28)
\]
while for a delta distribution $\bar{\mu} = \nu_s \cdot \delta(x - x_{ij})$ we deduce from (3.27) the approximation
\[
\bar{\nu}_s \sim \mu_{ij}.
\]

For indices $(i, j) \in I(\Gamma_1)$ on the boundary $\Gamma_1$ we obtain, e.g., for $j = 0, i \in \{1, \ldots, N\}$,
\[
0 = L_{y_{i0}} = -q_{i1} + q_{i0} h b_y(x_{i0}, y_{i0}) + h g_y(x_{i0}, y_{i0}),
\]
which constitutes the discrete version of the Neumann boundary condition (2.34).

Finally, necessary conditions with respect to the control variables $u_{ij}$ for $(i, j) \in I(\Omega)$ are determined by
\[
0 = L_{u_{ij}} = h^2 f_u(x_{ij}, y_{ij}, u_{ij}) + q_{ij} h^2 d_u(x_{ij}, y_{ij}, u_{ij}) + \lambda_{ij} C_u(x_{ij}, y_{ij}, u_{ij}).
\]
From this equation we can recover the discrete version of the control law (2.12), if we use the identification
\[
\bar{\lambda}(x_{ij}) \sim \lambda_{ij}/h^2 \quad \forall \ (i, j) \in \Omega.
\]

### 3.3 Optimization codes and modeling environment

For the numerical solution of all problems considered in the following section a combination of the AMPL [18] algebraic modeling language and the interior point solver LOQO [35] 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. We used the following codes for our numerical study: LANCELOT [17], MINOS [32], SNOPT [19], the convex QP-solver BPMPD [30], and LOQO [35]. LOQO 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 [31]. It was thus chosen for the following computations. 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.
4 Numerical examples

We consider elliptic problems with the following specifications: the domain is the unit square \( \Omega = (0, 1) \times (0, 1) \), the cost functional is of tracking type (2.16) in the boundary control case, and the control and state constraints are box constraints of the form (2.17) or (2.39).

4.1 A boundary control example

In this section an example from heat conduction is chosen to demonstrate the viability of the proposed approach. It is meant to be typical for practical problems that have to be solved in industrial and other applications. A mathematical description of the problem is as follows. The underlying boundary value problem is Laplace’s equation on the unit square, corresponding to no internal heat sources, coupled with mixed boundary conditions, namely homogeneous Neumann conditions on \( x_2 = 0 \), or no heat flux across this boundary, a heat flux proportional to the temperature at the boundaries \( x_1 = 0 \) and \( x_1 = 1 \), while the solution is controlled on \( x_2 = 1 \). The control function is to be found such that the temperature in the central subsquare of length 0.5 is as close as possible to a given function \( y_d = 1 \) in the \( L_2 \)-norm. In the first version of the problem a multiple \( \alpha \) of a regularizing boundary integral over the control function is added to the objective functional, while without this a bang-bang control may be expected in the second version. To complete the problem definition upper and lower bounds of 10 respectively 0 are imposed on both state and control.

Thus letting \( \Gamma_2 = \{ (x_1, 1) \mid 0 \leq x_1 \leq 1 \} \) and \( \Omega_0 = [0.25, 0.75]^2 \), the control problem is to determine a function \( u \in L^\infty(\Gamma_2) \) which minimizes

\[
F(y, u) = \frac{1}{2} \int_{\Omega_0} (y(x) - 1)^2 \, dx + \frac{\alpha}{2} \int_{\Gamma_2} u(x)^2 \, dx
\]

subject to the state equation, Neumann and Dirichlet boundary conditions.
and control and state inequality constraints,

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

\[\partial_{\nu} y(x) = 0 \quad \text{for} \quad x_2 = 0, \quad 0 \leq x_1 \leq 1,\]

\[\partial_{\nu} y(x) = y(x) - 5 \quad \text{for} \quad x_1 \in \{0, 1\}, \quad 0 \leq x_2 \leq 1,\]

\[y(x) = u(x) \quad \text{for} \quad x_2 = 1, \quad 0 \leq x_1 \leq 1, \quad (4.2)\]

\[y(x) \leq 3.15 \quad \text{in} \quad \Omega_0,\]

\[y(x) \leq 10 \quad \text{in} \quad \Omega \setminus \Omega_0,\]

\[0 \leq u(x) \leq 10 \quad \text{for} \quad x_2 = 1, \quad 0 \leq x_1 \leq 1.\]

The NLP–problem to be solved is given by (3.3)–(3.9). It is a linearly constrained convex quadratic program.

**Case \(\alpha > 0\):** The following table lists the results for four different optimization packages with an AMPL interface and one, BPMPD, which was applied after translating the AMPL file into extended MPS format. For a reference to AMPL, the codes, and the MPS format as well as for other benchmarks, see [31]. An asterisk denotes failure, while otherwise the CPU seconds on a Linux-PC with 450MHz PII and 512 MB are listed. The optimization problem of the largest instance has 32, 757 variables and 32, 578 constraints. A probable reason for the failures of SNOPT and MINOS is the near linear independence of the equality constraints which causes an increasing ill-conditioning with growing \(N\).

**Table 1**

**Results for Example 4.1, \(\alpha = 0.005\)**

<table>
<thead>
<tr>
<th>(N)</th>
<th>LOQO</th>
<th>SNOPT</th>
<th>LANC</th>
<th>MINOS</th>
<th>BPMPD</th>
<th>(F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>13</td>
<td>41</td>
<td>1126</td>
<td>18</td>
<td>4</td>
<td>.2789728</td>
</tr>
<tr>
<td>120</td>
<td>203</td>
<td>*</td>
<td>29561</td>
<td>369</td>
<td>*</td>
<td>.2590819</td>
</tr>
<tr>
<td>180</td>
<td>722</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>186</td>
<td>.2530543</td>
</tr>
</tbody>
</table>

The optimal control and adjoint variable for the weight \(\alpha = 0.005\) are shown in Figure 1. It is instructive to discuss the necessary conditions (2.19)–(2.23) that apply in this case. The state constraint \(y(x) \leq 3.15\) for \(x \in \Omega_0\) becomes active at two points \(x^1 = (1/4, 3/4), x^2 = (3/4, 3/4)\), while the state constraint \(y(x) \leq 10\) in \(\Omega \setminus \Omega_0\) does not become active. Hence, the adjoint
Fig. 1. Example 4.1, $\alpha = 0.005$ : Optimal control on $\Gamma_2$ and adjoint variable $q_{iN}$.

Fig. 2. Example 4.1, $\alpha = 0.005$ : Optimal state and adjoint variable on $\Omega$.

equations (2.19) are

$$\begin{align*}
-\Delta q(x) + \tilde{y}(x) - 1 + \rho &= 0 \quad \text{in} \quad \Omega_0 = [0.25, 0.75]^2, \\
-\Delta \tilde{q}(x) &= 0 \quad \text{in} \quad \Omega \setminus \Omega_0, \\
\partial_{\nu} \tilde{q}(x) &= 0 \quad \text{on} \quad \Gamma_1 = \partial \Omega \setminus \Gamma_2, \\
\tilde{q}(x) &= 0 \quad \text{on} \quad \Gamma_2,
\end{align*}$$

(4.3)

where the measure is given by $\bar{\mu} = \bar{p}_s^1 \delta(x - x^1) + \bar{p}_s^2 \delta(x - x^2)$. The approxi-
mation (3.15) yields the values \( \tilde{\nu}_s^1 = \tilde{\nu}_s^2 = -0.198746 \). The optimal state and adjoint variable on \( \Omega \) are displayed in Figure 2.

The minimum condition reduces to the case (2.22) with \( x \in \Gamma_2 \) since no control is applied on the Neumann boundary \( \Gamma_1 \). In view of \( u_d(x) = 0 \) we get from (2.22) for all \( x = (x_1, 1) \), \( 0 \leq x_1 \leq 1 \):

\[
\bar{u}(x) = \begin{cases} 
-\partial_v \tilde{q}(x)/\alpha, & \text{if } -\partial_v \tilde{q}(x)/\alpha \in (0,10), \\
0, & \text{if } -\partial_v \tilde{q}(x)/\alpha \leq 0, \\
10, & \text{if } -\partial_v \tilde{q}(x)/\alpha \geq 10, 
\end{cases}
\]  

(4.4)

In order to evaluate its discrete analogon, we recall definition (3.5) and relation (3.17) which give

\[
\partial_v \tilde{q}(x_{i,N+1}) \sim -q_{iN}/h, \quad i = 1, \ldots, N.
\]

Hence, the discrete version of the minimum condition (4.4) requires to check the conditions

\[
u_{i,N+1} = \begin{cases} 
q_{iN}/(\alpha * h), & \text{if } q_{iN}/(\alpha * h) \in (0,10), \\
0, & \text{if } q_{iN} \leq 0, \\
10, & \text{if } q_{iN}/(\alpha * h) \geq 10 
\end{cases}, \quad i = 1, \ldots, N.
\]  

(4.5)

By inspecting Figure 1, the reader may verify this condition for the value \( \alpha = 0.005 \).

**Case** \( \alpha = 0 \): Table 2 lists the results for the five optimization packages used in Table 1.

**Table 2**
Results for Example 4.1, \( \alpha = 0 \)

<table>
<thead>
<tr>
<th>N</th>
<th>LOQO</th>
<th>SNOPT</th>
<th>LANC</th>
<th>MINOS</th>
<th>BPMPD</th>
<th>( F )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>149</td>
<td>1516</td>
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</tr>
<tr>
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<td>939</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>243</td>
<td>.1512835</td>
</tr>
</tbody>
</table>

The adjoint equation agrees with equation (4.3). The optimal control shown in Figure 4 is bang–bang. Accordingly, the minimum condition (2.24) yields
Fig. 3. Example 4.1, \( \alpha = 0 \) : Optimal state and control.

Fig. 4. Example 4.1, \( \alpha = 0 \) : Optimal control on \( \Gamma_2 \) and switching function \( q_{iN} \).

\[ \bar{u}(x) = \begin{cases} 
    u_1(x), & \text{if } \partial_v q(x) > 0 \\
    u_2(x), & \text{if } \partial_v q(x) < 0
\end{cases}. \]  \hspace{1cm} (4.6)

Its discrete variant yields in analogy to (4.5),

\[ u_{i,N+1} = \begin{cases} 
    0, & \text{if } q_{iN} < 0 \\
    10, & \text{if } q_{iN} > 0
\end{cases}, \quad i = 1, \ldots, N, \]  \hspace{1cm} (4.7)
Fig. 5. Example 4.1, $\alpha = 0$ : Adjoint variable on $\Omega$.

which is confirmed by Figure 4.

4.2 A distributed control example

In this section we consider an optimal control problem for a semilinear elliptic equation of logistic type which was studied in Leung, Stojanovic [25,34]. The problem is to determine a distributed control $u \in L^\infty(\Omega)$ that minimizes the functional

$$F(y,u) = \int_\Omega (Mu(x)^2 - Ku(x)y(x)) \, dx$$

subject to the elliptic state equation

$$-\Delta y(x) = y(x)(a(x) - u(x) - by(x)), \quad \text{for} \quad x \in \Omega,$$

homogeneous Neumann boundary conditions,

$$\partial_\nu y(x) = 0, \quad \text{for} \quad x \in \Gamma,$$

and control and state inequality constraints

$$u_1 \leq u(x) \leq u_2 \quad y(x) \leq \psi(x), \quad \text{for} \quad x \in \Omega.$$
Here, \( y(x) \) denotes the population of a biological species, \( a(x) \) a spatially dependent intrinsic growth rate, \( b \) the crowding effect, while \( F \) denotes the difference between economic cost and revenue, with nonnegative constants \( M, K \). The goal is to find a control function which maximizes profit. A similar control problem with Dirichlet boundary conditions was recently studied by Canada et al. [12]. Three numerical methods, two of interior point type, were compared in [2] for linear problems and homogeneous Dirichlet conditions.

The adjoint equations (2.33), (2.34) applied to problem (4.8)–(4.11) lead to

\[
-\Delta \tilde{q}(x) + \tilde{q}(x) \ast \left[ 2b\tilde{g}(x) + \tilde{u}(x) - a(x) \right] - K\tilde{u}(x) + \rho = 0, \quad \text{in } \Omega, \\
\partial_b \tilde{q}(x) = 0, \quad \text{on } \Gamma.
\]

The minimum condition (2.40) gives the following two control laws. For \( M > 0 \) we get

\[
\tilde{u}(x) = P_{[u_1, u_2]} \left( \frac{1}{2M} \left[ (K - \tilde{q}(x)) \tilde{g}(x) \right] \right) , \quad (4.12)
\]

where \( P_{[u_1, u_2]} \) denotes the projection operator on the interval \([u_1, u_2]\). In case \( M = 0 \) we can put \( K = 1 \) and obtain

\[
\tilde{u}(x) = \begin{cases} 
  u_1, & \text{if } \tilde{q}(x) - 1 > 0 \\
  u_2, & \text{if } \tilde{q}(x) - 1 < 0 \\
  \text{singular}, & \text{if } \tilde{q}(x) - 1 = 0 \quad \text{in } \Omega \subset \Omega, \text{meas}(\Omega_s) > 0
\end{cases} . \quad (4.13)
\]

For the sake of reference the data were chosen as in [25], Example 5.2:

\[
a(x) = 7 + 4\sin(2\pi x_1 x_2), \quad b = 1, \quad M = 1, \quad K = 0.8.
\]

For this case the computational approach of [25] is not valid. Additionally, bound and state constraints were chosen: \( u_1 = 1.7, u_2 = 2, \phi(x) = 7.1 \). Both types of bounds become active. The optimal control and state are shown in Figure 6. The reader may verify that the control law (4.12) is satisfied. The state variable attains its upper bound at the two points \( x^1 = (0.21, 0.99), x^2 = (0.99, 0.21) \) near the boundary. It has to be noted that this example leads to a difficult nonlinear optimization problem which is not a QP anymore but a quadratically constrained quadratic program. Thus, the QP solver BPMPD is not applicable. For testing the local optimality of the computed solution, second–order sufficient conditions would need to be evaluated. To the best of our knowledge for this class of elliptic problems the literature does not provide a verifiable set of such conditions. A practical test could be devised by checking

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Fig. 6. Optimal control and state for Example 4.2, $M = 1, K = 0.8$.

the positive definiteness of the projected Hessian of the Lagrangian. This test will be part of our future work.

In the following tables an asterisk denotes failure and an "m" that the available memory was exceeded. The fact that made the previous problem and those in [28,29] difficult for SQP–based methods, namely the near linear dependence of the constraints, here the discretized boundary value problem, which exhibits increasing ill−conditioning for growing $N$, is even more pronounced through the homogeneous Neumann conditions resulting in singular constraints. The largest instance has 79,998 variables and 40,397 constraints in the NLP problem. These results were obtained on a HP9000-K260 with 256MB.

Table 3
Results for Example 4.2, $M = 1, K = 0.8$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>LOQO</th>
<th>SNOPT</th>
<th>LANC</th>
<th>MINOS</th>
<th>$F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>218</td>
<td>3281</td>
<td>2356</td>
<td>289</td>
<td>-6.485781</td>
</tr>
<tr>
<td>100</td>
<td>2141</td>
<td>m</td>
<td>103794</td>
<td>5331</td>
<td>-6.576428</td>
</tr>
<tr>
<td>200</td>
<td>28517</td>
<td>m</td>
<td>*</td>
<td>*</td>
<td>-6.620092</td>
</tr>
</tbody>
</table>

To confirm that a bang-bang control can occur in this problem the case $M = 0$, $K = 1$, $u_1 = 2$, $u_2 = 6$, $\psi(x) = 4.8$ was solved. The optimal control and state are shown in Figure 7. Both the control and the state constraints become active. The adjoint variable and the switching curves $\bar{q}(x) = 1$ displayed in Figure 8 admit a verification of the control law (4.13). While the CPU times for $N = 200$ are excessive, the accuracy for $N = 100$ should be sufficient and the times are acceptable. To avoid the trivial solution $y = 0$ of the state
Table 4
Results for Example 4.2, $M = 0, K = 1$.

<table>
<thead>
<tr>
<th>N</th>
<th>LOQO</th>
<th>SNOPT</th>
<th>LANC</th>
<th>MINOS</th>
<th>$F$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>3704</td>
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<tr>
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<td>116328</td>
<td>*</td>
<td>-18.73615</td>
</tr>
<tr>
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<td>57264</td>
<td>m</td>
<td>*</td>
<td>*</td>
<td>-18.86331</td>
</tr>
</tbody>
</table>

Fig. 7. Optimal control and state for Example 4.2, $M = 0, K = 1$.
equation nonzero starting values for the state were chosen in this example.
As in the case $M = 1$, the local optimality of the solution shown in Figure 7
would need to be verified.

References

[1] A. Barclay, P.E. Gill, and J. B. Rosen, SQP methods and their applications
to numerical optimal control, in Variational Calculus, Optimal Control and

of interior point methods and a Moreau–Yosida based active set strategy for


Fig. 8. Optimal adjoint variable and switching curves for Example 4.2, $M=0, K=1$.


