A Collection of Optimal Control Problems with Control and State Constraints *

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Introduction

In the last years, the nonlinear programming techniques have shown to be an effective approach to the numerical solution of optimal control problems ([15], [16], [17], [11]). Indeed, by applying a convenient discretization technique to the optimal control problem, we can obtain a finite dimensional nonlinear programming (NLP) problem, which, under suitable assumptions, is consistent with the continuous formulation ([15],[16]).

Furthermore, the Newton interior point algorithms developed in the last ten years, have shown to be very reliable in finding the solution of such NLP problems.

In this work, a collection of elliptic and parabolic control problems with control and state constraints is described. In particular, we focus on the discretization techniques which yield to NLP problems having large, sparse and structured Hessian and Jacobian matrices.

The paper is organized as follows: in the section 1 the general class of the elliptic boundary control problems is considered, with Neumann or Dirichlet boundary condition, paying a special attention to the discretization and optimization techniques.

Furthermore, we focus on a special case of such elliptic problem, with a particular tracking type objective functional.

Then we describe in detail ten different boundary control problems, reporting the sparsity pattern of the Hessian and Jacobian matrices and the minimum value of the discrete cost functional for a given meshsize.

The section 2 is concerned with the distributed elliptic control problems. Also in this case, we describe in detail the discretization and optimization techniques and we consider the special case of a tracking type cost functional.

^{*}This research was supported by the Italian Ministry for Education, University and Research (MIUR), FIRB Project RBAU01JYPN.

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In the section 3 we consider a class of parabolic control problem, and the related dicretization and optimizazion techniques. It follows the description of seven NLP problems arising from parabolic control problems devised from the literature, for which we show the sparsity pattern of the Jacobian and Hessian matrices.

1 Elliptic boundary control problems

1.1 Statement of the problem

We consider the following elliptic boundary control problem with Neumann boundary conditions: given a bounded domain $\Omega \subset \mathbb{R}^2$ with piecewise smooth boundary Γ , determine a boundary control function $u \in L^{\infty}(\Gamma)$ which minimizes the cost functional

$$F(y,u) = \int_{\Omega} f(x,y(x))dx + \int_{\Gamma} g(x,y(x),u(x))dx, \qquad (1)$$

subject to the elliptic state equation

$$-\Delta y(x) + d(x, y(x)) = 0 \qquad \text{for } x \in \Omega,$$
(2)

and to the Neumann boundary conditions

$$\partial_{\nu} y(x) = b(x, y(x), u(x)) \quad \text{for } x \in \Gamma.$$
 (3)

Here ∂_{ν} denotes the derivative in the direction of the outward unit normal ν of Γ . We introduce also control and state inequality constraints

$$C(x, y(x), u(x)) \leq 0 \qquad x \in \Gamma, S(x, y(x)) \leq 0 \qquad x \in \overline{\Omega}.$$
(4)

Here $\overline{\Omega} = \Omega \cup \Gamma$. The functions $f : \Omega \times \mathbb{R} \to \mathbb{R}, g : \Gamma \times \mathbb{R}^2 \to \mathbb{R}, d : \Omega \times \mathbb{R} \to \mathbb{R}, b : \Gamma \times \mathbb{R}^2 \to \mathbb{R}, C : \Gamma \times \mathbb{R}^2 \to \mathbb{R}, S : \overline{\Omega} \times \mathbb{R} \to \mathbb{R}$ are assumed to be C^2 functions.

When the elliptic boundary problem has Dirichlet conditions, the problem (1)-(4) becomes: determine a boundary control function $u \in L^{\infty}(\Gamma)$ which minimizes the cost functional

$$F(y,u) = \int_{\Omega} f(x,y(x))dx + \int_{\Gamma} g(x,u(x))dx, \qquad (5)$$

subject to the state equation (2), the Dirichlet conditions

$$y(x) = b(x, u(x))$$
 for $x \in \Gamma$, (6)

and the inequality constraints on control and state

$$C(x, u(x)) \leq 0 \qquad x \in \Gamma, S(x, y(x)) \leq 0 \qquad x \in \Omega.$$

$$(7)$$

Here $f: \Omega \times \mathbb{R} \to \mathbb{R}, g: \Gamma \times \mathbb{R} \to \mathbb{R}, d: \Omega \times \mathbb{R} \to \mathbb{R}, b: \Gamma \times \mathbb{R} \to \mathbb{R}, C: \Gamma \times \mathbb{R} \to \mathbb{R}, S: \Omega \times \mathbb{R} \to \mathbb{R}, and f, g, d, b, C, S are C² functions.$

A third version of an elliptic control problem is the following: determine a boundary control function $u \in L^{\infty}(\Gamma)$ which minimizes the cost functional

$$F(y,u) = \int_{\Omega} f(x,y(x))dx + \int_{\Gamma_{\alpha}} g(x,y(x),u(x))dx + \int_{\Gamma_{\beta}} K(x,u(x))dx,$$
(8)

where $\Gamma = \Gamma_{\alpha} \cup \Gamma_{\beta}$ with disjoint sets $\Gamma_{\alpha}, \Gamma_{\beta} \subset \Gamma$ that consist of finitely many connected components, subject to the state equation (2), to the boundary conditions of Neumann and Dirichlet type:

$$\partial_{\nu} y(x) = b_1(x, y(x), u(x)) \quad \text{for } x \in \Gamma_{\alpha},$$
(9)

$$y(x) = b_2(x, u(x)) \qquad \text{for } x \in \Gamma_\beta, \tag{10}$$

and the inequality constraints on control and state

$$C(x, u(x)) \leq 0 \qquad x \in \Gamma, S(x, y(x)) \leq 0 \qquad x \in \Omega.$$
(11)

Here $f: \Omega \times \mathbb{R} \to \mathbb{R}, g: \Gamma_{\alpha} \times \mathbb{R}^2 \to \mathbb{R}, d: \Omega \times \mathbb{R} \to \mathbb{R}, K: \Gamma_{\beta} \times \mathbb{R} \to \mathbb{R}, b_1: \Gamma_{\alpha} \times \mathbb{R}^2 \to \mathbb{R}, b_2: \Gamma_{\beta} \times \mathbb{R} \to \mathbb{R}, C: \Gamma \times \mathbb{R} \to \mathbb{R}, S: \Omega \times \mathbb{R} \to \mathbb{R}, and f, g, K, d, b_1, b_2, C, S are C^2 functions.$

For the general class of elliptic control problems, the theory of necessary conditions has not been yet fully developed. First order necessary optimality conditions for linear elliptic equations $-\Delta y(x)+y(x) = 0$ and pure Neumann conditions may be found in [8], [9], [10]. Problem (1)–(4) is considered as a mathematical programming problem in Banach spaces to which the first order Karush Kuhn Tucker conditions are applicable. For this approach, see [15].

For Dirichlet boundary conditions, a weak formulation of first order necessary conditions for linear elliptic equations may be found in [2]. Furthermore, first order conditions are derived in [15] in a purely formal way. This form of conditions is justified by its analogy in the first order necessary conditions for the discretized version of elliptic problem.

Also in the case of the problem (8)–(11), first order conditions are derived in a purely formal way in [17].

1.2 Discretization and optimization techniques

In the application of nonlinear programming techniques to optimal control, we use a full discretization approach [7], [3], [13], where both the control and

the state variables are discretized and the integration method is incorporated as an explicit equality constraint at each gridpoint. This technique leads to a large scale nonlinear programming problem (NLP) with a sparse structure of the Jacobian of the constraints. We consider the standard situation where the elliptic operator is the laplacian and $\Omega = (0, 1) \times (0, 1)$. Given a positive integer N, we define the stepsize h as

$$h = \frac{1}{N+1}$$

and we consider the mesh points

$$x_{ij} = (ih, jh), \quad 0 \le i, j \le N+1$$

In particular, denoting the following subsets of indices as follows

$$\begin{split} I(\Omega) &\doteq \{(i,j): 1 \le i, j, \le N\}, \\ I_1(\Gamma) &\doteq \{(i,0): 1 \le i \le N\}, \\ I_2(\Gamma) &\doteq \{(0,j): 1 \le j \le N\}, \\ I_3(\Gamma) &\doteq \{(N+1,j): 1 \le j \le N\}, \\ I_4(\Gamma) &\doteq \{(i,N+1): 1 \le i \le N\}, \\ I(\Gamma) &\doteq \cup_{k=1}^4 I_k(\Gamma), \\ I(\overline{\Omega}) &\doteq I(\Omega) \cup I(\Gamma), \\ I(\Gamma_{\alpha}) &\doteq \{(i,j): x_{ij} \in \Gamma_{\alpha}\}, \\ I(\Gamma_{\beta}) &= I(\Gamma) - I(\Gamma_{\alpha}), \end{split}$$

we have $x_{ij} \in \Omega$ for $(i, j) \in I(\Omega)$, $x_{ij} \in \Gamma$ for $(i, j) \in I(\Gamma)$, $x_{ij} \in \Gamma_{\alpha}$ for $(i, j) \in I(\Gamma_{\alpha})$ and $x_{ij} \in \Gamma_{\beta}$ for $(i, j) \in I(\Gamma_{\beta})$. As usual, we denote the approximations of the state and control variables in the mesh points as

$$\begin{array}{lll} y(x_{ij}) &\approx & y_{ij} & (i,j) \in I(\Omega), \\ u(x_{ij}) &\approx & u_{ij} & (i,j) \in I(\Gamma). \end{array}$$

Now, we define the vector z as the vector whose entries are the approximations of the control and state variables.

When the Neumann boundary conditions (3) hold, z is given by

$$z \doteq \left((y_{ij})_{(i,j)\in I(\bar{\Omega})}, (u_{ij})_{(i,j)\in I(\Gamma)} \right) \in \mathbb{R}^{N^2 + 8N}.$$

$$(12)$$

The laplacian operator $\Delta y(x)$ is approximated by using the standard five points formula for each $x_{ij}, (i, j) \in I(\Omega)$; so, according to the previous notations, we have

$$-\Delta y(x_{ij}) \approx \frac{1}{h^2} \{ 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} \}.$$
 (13)

The values of the normal derivative, needed for the Neumann boundary conditions, are approximated in the mesh points by y_{ij}^{ν}/h , where

$$y_{ij}^{\nu} \doteq \begin{cases} y_{i0} - y_{i1}, & \text{for } j = 0 & i = 1, \dots, N \\ y_{0j} - y_{1j}, & \text{for } i = 0 & j = 1, \dots, N \\ y_{N+1,j} - y_{N,j}, & \text{for } i = N+1 & j = 1, \dots, N \\ y_{i,N+1} - y_{i,N}, & \text{for } j = N+1 & i = 1, \dots, N \end{cases}$$
(14)

Then, the discrete form of the elliptic equation and the discrete Neumann boundary conditions lead to the equality constraints

$$G_{ij}^{h}(z) \doteq 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2 d(x_{ij}, y_{ij}) = 0, \quad (15)$$

for $(i, j) \in I(\Omega)$ and

$$B_{ij}^{h}(z) \doteq y_{ij}^{\nu} - hb(x_{ij}, y_{ij}, u_{ij}) = 0 \qquad \text{for } (i, j) \in I(\Gamma).$$
(16)

The control and state inequality constraints (4) lead to the inequality constraints on the variable z

$$C_{ij}(x_{ij}, y_{ij}, u_{ij}) \leq 0 \quad (i, j) \in I(\Gamma),$$

$$(17)$$

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

$$(18)$$

When Dirichlet boundary conditions (6) are given, they are incorporated by the discrete relations

$$y_{ij} = b(x_{ij}, u_{ij}) \qquad \text{for } (i, j) \in I(\Gamma).$$
(19)

Then, the number of the optimization variables is reduced, so that we define

$$z \doteq \left((y_{ij})_{(i,j) \in I(\Omega)}, (u_{ij})_{(i,j) \in I(\Gamma)} \right) \in \mathbb{R}^{N^2 + 4N}.$$
 (20)

The equality constraints are given by (15) where y_{i0} , y_{iN+1} , y_{0j} , y_{N+1j} are replaced by $b(x_{i0}, u_{i0})$, $b(x_{iN+1}, u_{iN+1})$, $b(x_{0j}, u_{0j})$, $b(x_{N+1j}, u_{N+1j})$ respectively. The control and state inequality constraints (7) give rise to the inequality constraints

$$\begin{array}{rcl}
C_{ij}(x_{ij}, u_{ij}) &\leq & 0 & (i, j) \in I(\Gamma), \\
S_{ij}(x_{ij}, y_{ij}) &\leq & 0 & (i, j) \in I(\Omega).
\end{array}$$
(21)

When Dirichlet and Neumann boundary conditions (9) and (10) are given, these conditions are incorporated by the discrete relations

$$B_{ij}^{h}(z) = y_{ij}^{\nu} - hb_1(x_{ij}, y_{ij}, u_{ij}) \qquad (i, j) \in I(\Gamma_{\alpha}),$$
(22)

$$y_{ij} = b_2(x_{ij}, u_{ij}) \qquad (i, j) \in I(\Gamma_\beta).$$

$$(23)$$

Then the number of variables is reduced, so that we define

$$z \doteq \left((y_{ij})_{(i,j)\in I(\Omega)\cup\in I(\Gamma_{\alpha})}, (u_{ij})_{(i,j)\in I(\Gamma)} \right) \in \mathbb{R}^{N^2 + \tau(N)}.$$

$$(24)$$

Here $\tau(N)$ is the number of variables related to the meshpoints on the edges of Γ , where we have to compute y_{ij} (meshpoints on Γ_{α}) and u_{ij} (meshpoints on Γ). Then, the equality constraints are given by

$$G_{ij}^h(z) = 0 \qquad (i,j) \in I(\Omega), \tag{25}$$

$$B_{ij}^h(z) = 0 \qquad (i,j) \in I(\Gamma_\alpha).$$

$$(26)$$

The control and state inequality constraints agree with those in (21). The approximations of the functionals (1), (5) and (8) are obtained by the rectangular rule and they are given by

$$F^{h}(z) \doteq h^{2} \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j)\in I(\Gamma)} g(x_{ij}, y_{ij}, u_{ij})$$
(27)

for Neumann boundary conditions, by

$$F^{h}(z) \doteq h^{2} \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j)\in I(\Gamma)} g(x_{ij}, u_{ij})$$
(28)

for Dirichlet boundary conditions, or by

$$F^{h}(z) \doteq h^{2} \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j)\in I(\Gamma_{\alpha})} g(x_{ij}, y_{ij}, u_{ij}) + h \sum_{(i,j)\in I(\Gamma_{\beta})} K(x_{ij}, u_{ij})$$
(29)

for mixed Neumann and Dirichlet boundary conditions.

So, for every N, we obtain a NLP problem; if we state Neumann conditions, the optimization variable z belongs to \mathbb{R}^{N^2+8N} and the discrete boundary conditions (16) are included in the equality constraints:

$$\begin{array}{ll}
\min & F^{h}(z) \\
G^{h}_{ij}(z) = 0 & (i,j) \in I(\Omega), \\
B^{h}_{ij}(z) = 0 & (i,j) \in I(\Gamma), \\
C_{ij}(z) \leq 0 & (i,j) \in I(\Gamma), \\
S_{ij}(z) \leq 0 & (i,j) \in I(\overline{\Omega}).
\end{array}$$
(30)

With Dirichlet conditions, the problem becomes

$$\begin{array}{ll}
\min & F^h(z) \\
G^h_{ij}(z) = 0 & (i,j) \in I(\Omega), \\
C_{ij}(z) \le 0 & (i,j) \in I(\Gamma), \\
S_{ij}(z) \le 0 & (i,j) \in I(\Omega).
\end{array}$$
(31)

with $z \in \mathbb{R}^{N^2+4N}$. With mixed boundary conditions, the NLP problem is as follows:

$$\begin{array}{ll}
\min & F^{h}(z) \\
G^{h}_{ij}(z) = 0 & (i,j) \in I(\Omega), \\
B^{h}_{ij}(z) = 0 & (i,j) \in I(\Gamma_{\alpha}), \\
C_{ij}(z) \leq 0 & (i,j) \in I(\Gamma), \\
S_{ij}(z) \leq 0 & (i,j) \in I(\Omega).
\end{array}$$
(32)

with $z \in \mathbb{R}^{N^2 + \tau(N)}$. The lagrangian functions of (30), (31) and (32) are respectively given by

$$L(z, q, \mu, \lambda) = h^{2} \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma)} g(x_{ij}, y_{ij}, u_{ij}) + \sum_{(i,j) \in I(\Omega)} q_{ij} G_{ij}^{h}(z) + \sum_{(i,j) \in I(\bar{\Omega})} \mu_{ij} S(x_{ij}, y_{ij}) + \sum_{(i,j) \in I(\Gamma)} [q_{ij} B_{ij}^{h}(z) + \lambda_{ij} C(x_{ij}, y_{ij}, u_{ij})],$$
(33)

$$L(z, q, \mu, \lambda) = h^{2} \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma)} g(x_{ij}, u_{ij}) + \sum_{(i,j) \in I(\Omega)} [q_{ij}G_{ij}^{h}(z) + \mu_{ij}S(x_{ij}, y_{ij})] + \sum_{(i,j) \in I(\Gamma)} \lambda_{ij}C(x_{ij}, u_{ij}),$$
(34)

$$L(z, q, \mu, \lambda) = h^{2} \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma_{\alpha})} g(x_{ij}, y_{ij}, u_{ij}) + + h \sum_{(i,j) \in I(\Gamma_{\beta})} K(x_{ij}, u_{ij}) + + \sum_{(i,j) \in I(\Omega)} [q_{ij}G_{ij}^{h}(z) + \mu_{ij}S(x_{ij}, y_{ij})] + + \sum_{(i,j) \in I(\Gamma_{\alpha})} q_{ij}B_{ij}^{h}(z) + \sum_{(i,j) \in I(\Gamma)} \lambda_{ij}C(x_{ij}, u_{ij}),$$
(35)

where the Lagrange multipliers $q = (q_{ij})_{(i,j)\in I(\bar{\Omega})}$ for (33), $q = (q_{ij})_{(i,j)\in I(\Omega)}$ for (34), $q = (q_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma_{\alpha})}$ for (35) are associated with the equality constraints and $\mu = (\mu_{ij})_{(i,j)\in I(\bar{\Omega})}$ (or $(i,j)\in I(\Omega)$) and $\lambda = (\lambda_{ij})_{(i,j)\in I(\Gamma)}$ are related to the inequality constraints $S_{ij}(z) \leq 0$ and $C_{ij}(z) \leq 0$ respectively. The ordering of the discrete variables y_{ij} and u_{ij} in the array z determines the structure of the Jacobian matrix of the equality constraints and of the



Figure 1: Ordering of the discrete variables

Hessian matrix of the lagrangian function. The Figure 1 depicts the strategy chosen here: the first entries of z are the y_{ij} , $(i, j) \in I(\Omega)$ in lexicographic order from (i, j) = (1, 1) to (i, j) = (N, N). Then, when we have boundary Neumann conditions, we store in the array z the boundary values y_{ij} , where $(i, j) \in I_k(\Gamma)$, for k = 1, 2, 3, 4. Finally, we store in the array z the discrete control variables u_{ij} in the same order of the boundary entries y_{ij} . For the problems (31) and (32), we use the same strategy.

1.3 Test problems: general description

In the following, we consider elliptic problems where the cost functional is of tracking type

$$F(y,u) = \frac{1}{2} \int_{\Omega} (y(x) - y_d(x))^2 dx + \frac{\alpha}{2} \int_{\Gamma} (u(x) - u_d(x))^2 dx, \qquad (36)$$

with given function $y_d \in C(\overline{\Omega})$, $u_d \in L^{\infty}(\Gamma)$ and a nonnegative weight $\alpha \geq 0$. We assume that the control and state constraints are box constraints of the simple type

$$y(x) \le \psi(x)$$
 on Ω or $\overline{\Omega}$, (37)

$$u_1(x) \le u(x) \le u_2(x)$$
 on Γ , (38)

with functions $\psi \in C(\overline{\Omega})$ and $u_1, u_2 \in L^{\infty}(\Gamma)$.

We assume that an optimal solution of the considered optimal control problem exists and we denote by $\bar{y}(x)$ and $\bar{u}(x)$ the optimal state function and the optimal control function respectively. If the function b in (3) is such that $b_u = 1^1$ (or respectively b in (6) is such that $b_u = 1$ or b_1 in (9) is such that $b_{1u} = 1$), the optimal control $\bar{u}(x)$ is completely determined.

In the case of Neumann boundary condition, if we denote by $\bar{q}(x)$ the adjoint state corresponding to $\bar{y}(x)$ and $\bar{u}(x)$, we have:

• case
$$\alpha > 0$$
:

$$\bar{u}(x) = \begin{cases} u_d(x) + \bar{q}(x)/\alpha & \text{if } u_d(x) + \bar{q}(x)/\alpha \in (u_1(x), u_2(x)), \\ u_1(x) & \text{if } u_d(x) + \bar{q}(x)/\alpha \le u_1(x), \\ u_2(x) & \text{if } u_d(x) + \bar{q}(x)/\alpha \ge u_2(x), \end{cases}$$
(39)

• case $\alpha = 0$: we obtain an optimal control of bang-bang or singular type:

$$\bar{u}(x) = \begin{cases} u_1(x) & \text{if } \bar{q}(x) < 0, \\ u_2(x) & \text{if } \bar{q}(x) > 0, \\ \text{singular} & \text{if } \bar{q}(x) = 0 \text{ on } \Gamma_S \subset \Gamma, \quad \int_{\Gamma_S} dx > 0. \end{cases}$$
(40)

For $\alpha = 0$, the adjoint state function $\bar{q}(x)$ on the boundary plays the role of a switching function. The isolated zeros of $\bar{q}(x)$ are switching points of a bang-bang control.

For Dirichlet boundary conditions, we obtain the same results if we replace $\bar{q}(x)$ formally by $-\partial_{\nu}\bar{q}(x)$. For $\alpha = 0$, the outward normal derivatives $-\partial_{\nu}\bar{q}(x)$ plays the role of a switching function. The isolated zeros of $-\partial_{\nu}\bar{q}(x)$ are the switching points of a bang-bang control.

For mixed boundary conditions, if $b_{1u} = 1$ and $\bar{q}(x)$ denotes the adjoint state, we have:

• case $\alpha > 0$: for $x \in \Gamma(\alpha)$, $\bar{u}(x)$ is as in (39), while for $x \in \Gamma_{\beta}$, $\bar{u}(x)$ is as in (39) with $\bar{q}(x)$ replaced by $-\partial_{\nu}\bar{q}(x)$;

¹Here and in the following we denote $b_u = \partial b / \partial u$

• case $\alpha = 0$: we obtain an optimal control of bang-bang or singular type; for $x \in \Gamma_{\alpha}$, $\bar{u}(x)$ is as in (40) while for $x \in \Gamma_{\beta}$, $\bar{u}(x)$ is as in (40) with $\bar{q}(x)$ replaced by $-\partial_{\nu}\bar{q}(x)$; here Γ is replaced by Γ_{α} or Γ_{β} .

Then, for $\alpha = 0$, the switching function is given by $\bar{q}(x)$ on Γ_{α} and by $-\partial_{\nu}\bar{q}(x)$ on Γ_{β} . The isolated zeros of the switching function are the switching points of a bang-bang control.

The discrete counterpart of $\bar{q}(x)$ is the vector of the Lagrange multipliers $q = q_{ij}$. For Dirichlet boundary conditions, $\partial_{\nu}\bar{q}(x)|_{\Gamma}$ is replaced by q_{ij}^{ν}/h , where q_{ij}^{ν} is given by the finite differences of (14). In this case, we assume that q_{ij} are equal to zero on Γ ($q_{i0} = q_{iN+1} = q_{0j} = q_{N+1j} = 0$). For mixed boundary conditions, $\bar{q}(x)$ is replaced by the Lagrange multipliers on Γ_{α} and $\partial_{\nu}\bar{q}(x)$ is replaced by q_{ij}^{ν}/h on Γ_{β} with q_{ij}^{ν} as in (14). Furthermore, $q_{ij} = 0$ for $(i, j) \in I(\Gamma_{\beta})$.

In all the described test problems, 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 Γ .

1.4 Test problems: discretization technique.

When the discretization techniques described in section 1.2 are applied to a cost functional of tracking type (36), $F^h(z)$ can be written as follows:

$$F^{h}(z) = \frac{1}{2}h^{2} \sum_{(i,j)\in I(\Omega)} (y_{ij} - y_{d}(x_{ij}))^{2} + \frac{\alpha}{2}h \sum_{(i,j)\in I(\Gamma)} (u_{ij} - u_{d}(x_{ij}))^{2}.$$

The Hessian matrix H of $F^{h}(z)$ is a diagonal matrix, given by

$$H = diag(h^2 I_{n_1}, 0_{n_2}, h\alpha I_{n_3}), \tag{41}$$

where $n_1 = N^2$, $n_2 = 0$, $n_3 = 4N$ for Dirichlet boundary conditions, $n_1 = N^2, n_2 = 4N, n_3 = 4N$ for Neumann boundary conditions. For mixed boundary conditions, n_1, n_2, n_3 depend on the choice of Γ_{α} and Γ_{β} (see problems 1.9 and 1.10).

Now, we determine the Jacobian matrix J of the equality constraints. For Dirichlet boundary conditions, J is an $N^2 \times (N^2 + 4N)$ matrix, given by

$$J = [Y + D, E], \tag{42}$$

where the $N^2 \times N^2$ matrix D is

$$D = h^2 diag\left(\frac{\partial d(x_{ij}, y_{ij})}{\partial y_{ij}}\right)$$

the $N^2 \times 4N$ matrix E is a sparse matrix with non null entries equal to $-\frac{\partial b(x_{ij}, u_{ij})}{\partial u_{ij}}$, so that

$$e_{kl} = \begin{cases} -\frac{\partial b(x_{i0}, u_{i0})}{\partial u_{i0}} & l, k, i = 1, \dots, N \\ -\frac{\partial b(x_{0j}, u_{0j})}{\partial u_{0j}} & j = 1, \dots, N \quad k = (j-1)N + 1, l = N + j \\ -\frac{\partial b(x_{N+1j}, u_{N+1j})}{\partial u_{N+1j}} & j = 1, \dots, N \quad k = jN, l = 2N + j \\ -\frac{\partial b(x_{iN+1}, u_{iN+1})}{\partial u_{iN+1}} & i = 1, \dots, N \quad k = N^2 - N + i, l = 4N - N + i \end{cases}$$
(43)

and, finally, Y is an $N\times N$ block tridiagonal matrix with $N\times N$ diagonal blocks given by

$$\begin{pmatrix}
4 & -1 & & \\
-1 & 4 & -1 & & \\
& \ddots & \ddots & \ddots & \\
& & -1 & 4 & -1 \\
& & & -1 & 4
\end{pmatrix}$$
(44)

and off diagonal blocks equal to $-I_N$.

For Neumann boundary conditions, J is an $(N^2 + 4N) \times (N^2 + 8N)$ matrix, that can be written as follows

$$J = \begin{bmatrix} Y + D & B^t & 0_{4N} \\ B & T & S \end{bmatrix},$$
(45)

where Y and D are $N^2 \times N^2$ matrices as in (42) and S, T are the following $4N \times 4N$ diagonal matrices:

$$S = diag\left(-h\frac{\partial b(x_{ij}, y_{ij}, u_{ij})}{\partial u_{ij}}\right), \quad (i, j) \in I(\Gamma)$$
(46)

$$T = diag\left(1 - h\frac{\partial b(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij}}\right), \quad (i, j) \in I(\Gamma)$$
(47)

and B^t is a sparse $N^2 \times 4N$ matrix where the nonzero entries are equal to 1 and whose indices are the same of the nonzero entries of E in (42). We point out that $S = -hI_{4N}$ if $b_u = 1$.

For mixed boundary conditions, the structure of J is similar to (45), but the sizes of B, T and S depend on the choice of Γ_{α} and Γ_{β} (see problems 1.9 and 1.10). The hessian matrix \bar{H} of the lagrangian function is equal to H in (??) for Dirichlet boundary conditions, while for Neumann conditions, \bar{H} is given by

$$\bar{H} = H + \begin{pmatrix} Y & & \\ & \bar{T} & \bar{V} \\ & \bar{V}^t & \bar{S} \end{pmatrix},$$
(48)

where the $N^2 \times N^2$ matrix \bar{Y} , the $4N \times 4N$ matrices \bar{T} , \bar{S} and \bar{V} are given by

$$\bar{Y} = diag\left(h^2 q_{ij} \frac{\partial^2 d(x_{ij}, y_{ij})}{\partial y_{ij}^2}\right), \quad (i, j) \in I(\Omega), \tag{49}$$

$$\bar{T} = diag\left(-hq_{ij}\frac{\partial^2 b(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij}^2}\right), \quad (i, j) \in I(\Gamma),$$
(50)

$$\bar{S} = diag\left(-hq_{ij}\frac{\partial^2 b(x_{ij}, y_{ij}, u_{ij})}{\partial u_{ij}^2}\right), \quad (i, j) \in I(\Gamma),$$
(51)

$$\bar{V} = diag\left(-hq_{ij}\frac{\partial^2 b(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij}u_{ij}}\right), \quad (i, j) \in I(\Gamma).$$
(52)

Note that, if $b_u = 1$, then $\bar{S} = \bar{V} = 0_{4N}$.

For mixed boundary conditions, the Hessian matrix \overline{H} of the lagrangian function is similar to (48), but the size of \overline{T} , \overline{S} , and \overline{V} depends on the choice of Γ_{α} and Γ_{β} (see problems 1.9 and 1.10).

For convenience, the numerical results reported in the following for all the test problems are referred to the fixed stepsize h = 1/(N+1), with N = 99.



Problem 1.1 (Example 5.5 in [15])

We consider the following elliptic control problem with Neumann boundary conditions: minimize the functional

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

subject to

on
$$\Omega$$
: $-\Delta y(x) = 0$, $y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1)))$,
on Γ : $\partial_{\nu} y(x) = u(x) - y(x)^2$, $3.7 \le u(x) \le 4.5$, $u_d(x) \equiv 0, \alpha = 0.01$
on $\overline{\Omega}$: $y(x) \le 2.071$.

This problem leads to a NLP problem. The structure of the Jacobian and Hessian matrices J and H are depicted in figure 2. The pictures, here and in the following, are obtained with N = 5.

The Hessian matrix H of F^h is a positive semidefinite matrix, because the entries related to $y_{ij}, (i, j) \in I(\Gamma)$ are equal to zero, while the Hessian matrix \overline{H} of the lagrangian function is an indefinite diagonal matrix (see figure 3). The minimum of the cost functional is $F(\overline{y}, \overline{u}) = 0.55224597$. The optimal control is a continuous function and, on the bottom edge of Γ , it is such that

• $\bar{u}(x) = 3.7$ for $x = (x_1, 0)$, with $x_1 \in (0, .18) \cup (.82, 1)$

Figure 3: Problem 1.1: Hessian matrix \overline{H}



•
$$\bar{u}(x) = 4.5$$
 for $x = (x_1, 0)$, with $x_1 \in (.36, .64)$.

Since $b_u = 1$, on the edges of Γ , we have

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

The active set for the state constraint $y(x) \leq 2.071$ is given by the midpoints of the edges of Γ . The dual variable for this active inequality constraint is 0.0004478692. At $x_{i0} = (0.5, 0)$, we have $y_{i0} = 2.071$, $q_{i0} = -0.04651456$.

Problem 1.2 (Example 5.6 in [15])

We consider the following elliptic control problem with nonlinear Neumann boundary conditions: minimize the functional (36) subject to

on
$$\Omega$$
: $-\Delta y(x) = 0$, $y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1)))$,
on Γ : $\partial_{\nu} y(x) = u(x) - y(x)^2$, $6 \le u(x) \le 9$, $u_d(x) \equiv 0, \alpha = 0$,
on $\overline{\Omega}$: $y(x) \le 2.835$.

The obtained programming problem is an NLP problem where the Jacobian matrix J and the Hessian matrix H have the same structure of those of the previous problem (see figure 2), but the entries of the Hessian matrix of F^h related to the control variables u_{ij} are equal to zero. These entries are zero



also in H. Furthermore, the nonlinearity of the Neumann conditions leads to nonconstant diagonal entries (the ones related to the y_{ij} , $(i, j) \in I(\Gamma)$) in the Hessian \overline{H} of the Lagrangian, which is an indefinite diagonal matrix (see figure 4). The minimum of the cost functional is $F(\overline{y}, \overline{u}) = 0.015078$. The optimal control is a bang-bang control, that, on the edges of Γ , is given by

$$\bar{u} = \begin{cases} 6 & \text{if } q_{ij} < 0\\ 9 & \text{if } q_{ij} > 0 \end{cases}$$

where j = 1 for the bottom edge, j = N for the top edge, i = 1 for the left edge and i = N for the right edge. The switching points on the bottom edge of Γ are approximately (.33,0) and (.67,0). The optimal state is equal to 2.835 at the midpoints of the edges of Γ . The dual variable for this active inequality constraint is $\mu_{ij} = 0.00002895$.

Problem 1.3 (Example 5.7 in [15])

We consider the following elliptic control problem with Neumann boundary conditions: minimize the functional (36) subject to

on Ω : $-\Delta y(x) - y(x) + y(x)^3 = 0$, $y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1)))$ on Γ : $\partial_{\nu} y(x) = u(x)$, $1.8 \le u(x) \le 2.5$, $u_d(x) \equiv 0, \alpha = 0.01$ on $\overline{\Omega}$: $y(x) \le 2.7$.

By means of the discretization techniques, a NLP problem is obtained again; the structures of the Jacobian matrix J and of the Hessian matrix H of F^h

Figure 5: Problem 1.3: Hessian matrix \overline{H}



are the same of those in problem 1.1 (see figure 2), but the Hessian matrix \overline{H} of the lagrangian function has the form in figure 5. In this case the first N^2 entries of the diagonal depend on the values of y_{ij} , $(i, j) \in I(\Omega)$. The minimum of the cost functional is $F(\overline{y}, \overline{u}) = 0.0.264163$ The optimal control is a continuous function and, on the bottom edge of Γ , it is such that

- $\bar{u}(x) = 1.8$ for the points $x = (x_1, 0), x_1 \in (0, .15) \cup (.85, 1)$
- $\bar{u}(x) = 2.5$ for the points $x = (x_1, 0), x_1 \in (.29, .71)$.

Indeed, on the edges of Γ , we have

$$\bar{u}(x) = \begin{cases} \bar{q}(x) \cdot 100 & \text{if } \bar{q}(x) \cdot 100 \in (1.8, 2.5) \\ 1.8 & \text{if } \bar{q}(x) \cdot 100 \leq 1.8 \\ 2.5 & \text{if } \bar{q}(x) \cdot 100 \geq 2.5 \end{cases}$$

The active set for the state constraint $y(x) \leq 2.7$ is given by the points adjacent to the corners of the domain. The dual variable for this active inequality constraint is $\mu_{ij} = 0.0034573$.

Problem 1.4 (Example 5.8 in [15])

The cost functional and the constraints are the same of problem 1.3, but we choose $\alpha = 0$; so the Jacobian J has the same structure than problem 1.3, while the structures of the Hessian matrix H of F^h and of the Hessian matrix \bar{H} of the Lagrangian are given in figure 6. The minimum of the

Figure 6: Problem 1.4: Hessian matrices H and \overline{H}



cost functional is $F(\bar{y}, \bar{u}) = 0.165531$. The optimal control is a bang-bang control, and, on the bottom edge of Γ , it is given by

$$\bar{u}(x) = \begin{cases} 1.8 & \text{if } q_{ij} < 0\\ 2.5 & \text{if } q_{ij} > 0 \end{cases}$$

where j = 1 for the bottom edge, j = N for the top edge, i = 1 for the left edge and i = N for the right edge of Γ . The switching points on the bottom edge of Γ are approximately (.21,0) and (.79,0). Again, the optimal state is active at the points adjacent to the corners of the domain. The dual variable for this active inequality constraint is $\mu_{ij} = 0.030118$.

Problem 1.5 (Example 5.1 in [15])

We consider the following elliptic control problem with Dirichlet boundary conditions: minimize the functional (36) subject to

on
$$\Omega$$
: $-\Delta y(x) = 20$, $\begin{array}{c} y(x) \leq 3.5, \\ y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1), \\ \text{on } \Gamma$: $y(x) = u(x), \quad 0 \leq u(x) \leq 10, \quad u_d(x) \equiv 0, \alpha = 0.01. \end{array}$

This control problem leads to a strictly convex quadratic programming (QP) problem whose Jacobian and Hessian matrices J and H are structured as shown in figure 7.

Figure 7: Problem 1.5



For N = 99, the minimum of the cost functional is $F(\bar{y}, \bar{u}) = 0.196525$. 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 $\mu_{ij} = 0.24602$. Here $q_{ij} = -0.21312$, $y_{ij} = 3.5$, $y_{ij} - y_d(x_{ij}) = 0.1875$. Furthermore y(.4, .5) = 3.449163 and u(0, .5) = 1.690270.

Problem 1.6 (Example 5.2 in [15])

The cost functional and the constraints are the same of problem 1.5, except that we choose $\alpha = 0$ instead of $\alpha = 0.01$. Then, the Jacobian matrix J has the same structure as in figure 7, while the diagonal entries of the Hessian matrix H related to the variables u_{ij} are equal to 0 (see figure 8). The programming problem is a convex QP problem.

In this case we can expect either a bang-bang or a singular control. We observe the following numerical results (N = 99):

- the minimum of the cost functional is $F(\bar{y}, \bar{u}) = .096695;$
- both the control and state constraint do not become active; the optimal control is totally singular on Γ ; from the numerical point of view, this means that the multipliers q_{i1} , q_{iN} , q_{1j} , q_{Nj} are equal to zero.

Problem 1.7 (Example 5.3 in [15])

Figure 8: Problem 1.6: Hessian matrix $H = \overline{H}$



We consider the following elliptic control problem with Dirichlet boundary conditions: minimize the functional (36) subject to

on
$$\Omega$$
: $-\Delta y(x) = 20$, $\begin{array}{c} y(x) \leq 3.2, \\ y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1), \end{array}$
on Γ : $y(x) = u(x)$, $1.6 \leq u(x) \leq 2.3$, $u_d(x) \equiv 0, \alpha = 0.01$.

The discretized problem is a strictly convex QP problem and the structures of Jacobian and Hessian matrices are the same of problem 1.5 (see figure 7). For N = 99, the minimum of the cost functional is $F(\bar{y}, \bar{u}) = 0.321010$. Furthermore y(x) = 3.2 at the center point $x_{ij} = (0.5, 0.5)$. The corresponding multiplier is $\mu_{ij} = 0.642704$; the optimal control is continuous and, on the bottom edge of Γ , it is such that

- $u_{i0} = 2.3$ for the points on the edge having the x_1 coordinate in $(.002, .18) \cup (.82, .98);$
- $u_{i0} = 1.6$ for the points on the edge having the x_1 coordinate in (.23, .77);

Indeed, in view of $\alpha = h = 0.01$, we have

$$u_{i,0} = \begin{cases} q_{i,1} \cdot 10^4 & \text{if } q_{i,1} \cdot 10^4 \in (1.6, 2.3) \\ 1.6 & \text{if } q_{i,1} \cdot 10^4 \le 1.6 \\ 2.3 & \text{if } q_{i,1} \cdot 10^4 \ge 2.3 \end{cases}$$

The data are the same of problem 1.7, but $\alpha = 0$, so the Hessian matrix H is positive semidefinite with zero entries in correspondence of the variables u_{ij} . We have a convex QP problem. The minimum of the cost functional is $F(\bar{y}, \bar{u}) = 0.249178$. The optimal control is a bang-bang control and

$$u_{i,0} = \begin{cases} 1.6 & \text{if } q_{i,1} < 0\\ 2.3 & \text{if } q_{i,1} > 0 \end{cases}$$

The switching points on the bottom edge of Γ are (.2, 0) and (.8, 0). The optimal state is active at the center point $x_{ij} = (.5, .5)$ and the multiplier related to this active inequality constraint is $\mu_{ij} = 0.73378$.

Problem 1.9 (Example 4.1 in [17])

We consider the following elliptic control problem with mixed Dirichlet and Neumann boundary conditions: given $\Gamma_{\beta} = \{(x_1, 1) : 0 \leq x_1 \leq 1\}$ and $\Omega_0 = [0.25, 0.75]^2$, minimize the cost functional

$$F(y,u) = \frac{1}{2} \int_{\Omega_0} (y(x) - 1)^2 dx + \frac{\alpha}{2} \int_{\Gamma_\beta} u(x)^2 dx$$
(53)

subject to

on
$$\Omega$$
: $-\Delta y(x) = 0$, $0 \le y(x) \le 3.15 \text{ on } \Omega_0$
on Γ_{α} : $\delta_{\nu} y(x) = 0$, $0 \le y(x) \le 10 \text{ on } \Omega - \Omega_0$
on Γ_{α} : $\delta_{\nu} y(x) = y(x) - 5$ for $x_2 = 0, 0 \le x_1 \le 1$
 $\delta_{\nu} y(x) = y(x) - 5$ for $x_1 \in \{0, 1\}, 0 \le x_2 \le 1$
on Γ_{β} : $y(x) = u(x)$ $0 \le u(x) \le 10$
 $\alpha = 0.005$

In this case, $z \equiv ((y_{ij})_{(i,j) \in I(\Omega) \cup I(\Gamma_{\alpha})}, (u_{ij})_{(i,j) \in I(\Gamma_{\beta})}) \in \mathbb{R}^{N^2 + 4N}$. The programming problem is a convex QP problem. The Jacobian matrix J corresponding to the equality constraints is given by

$$J = \left[\begin{array}{ccc} Y & U^t & E \\ U & T & 0_N \end{array} \right]$$

where Y is a block tridiagonal $N^2 \times N^2$ matrix as in (42), $[U^t \quad E] = B^t$ is a $N^2 \times 4N$ matrix as in (45), U is a sparse $3N \times N^2$ matrix, T is a diagonal $3N \times 3N$ matrix as in (47). The Hessian matrix H of $F^h(y, u)$ is a square diagonal matrix of order $N^2 + 4N$. The Hessian matrix \bar{H} of the lagrangian



function is equal to H. The structures of J and H are reported in figure 9 The diagonal entries of H corresponding to the indices of $x_{ij} \in \Omega - \Omega_0$ are equal to zero. In the same way, the diagonal entries of H corresponding to $y_{ij}, (i, j) \in I(\Gamma_\alpha)$ are equal to zero. The entries related to u_{ij} are equal to $h\alpha$. The minimum of the cost functional is $F(\bar{y}, \bar{u}) = 0.26284923$. The state constraint $y \leq 3.15$ for $x \in \Omega_0$ becomes active at the points $(\frac{1}{4}, \frac{3}{4})$ and $(\frac{3}{4}, \frac{3}{4})$ while the state constraint $y \leq 10$ in $\Omega - \Omega_0$ does not become active. Since no control is applied on the boundary Γ_α , we have

$$u_{iN+1} = \begin{cases} q_{iN}/(\alpha h) & \text{if } q_{iN}/(\alpha h) \in (0, 10) \\ 0 & \text{if } q_{iN}/(\alpha h) \le 0 \\ 10 & \text{if } q_{iN}/(\alpha h) \ge 0 \end{cases}$$

Problem 1.10 (Example 4.1 in [17] with $\alpha = 0$)

The cost functional and the constraints are the same of the previous problem, but in this case we choose $\alpha = 0$. The optimal control is a bang–bang control, given by

$$u_{i,N+1} = \begin{cases} 0 & \text{if } q_{iN} \le 0\\ 10 & \text{if } q_{iN} \ge 0 \end{cases}$$

The programming problem is a convex QP problem. The Jacobian matrix of the equality constraints is the same of the problem 1.9 (see figure 9); the Hessian matrix H is a diagonal matrix as that of the problem 1.9, but the entries corresponding to u_{ij} are equal to 0 (see figure 10).

Figure 10: Problem 1.10: Hessian matrix $H=\bar{H}$



2 Elliptic distributed control problems

2.1 Statement of the problem

We consider the following elliptic distributed control problem with mixed Neumann and Dirichlet boundary conditions: given a bounded domain $\Omega \subset \mathbb{R}^2$ with piecewise smooth boundary Γ , where $\Gamma = \Gamma_{\alpha} \cup \Gamma_{\beta}$ with disjoints sets $\Gamma_{\alpha}, \Gamma_{\beta} \subset \Gamma$ that are composed of finitely many smooth and connected components, determine a distributed control function $u \in L^{\infty}(\Omega)$ that minimizes the cost functional

$$F(y,u) = \int_{\Omega} f(x,y(x),u(x))dx + \int_{\Gamma_{\alpha}} g(x,y(x))dx, \qquad (54)$$

subject to the elliptic state equation

$$-\Delta y(x) + d(x, y(x), u(x)) = 0 \text{ for } x \in \Omega,$$
(55)

and to the Neumann and Dirichet boundary conditions

$$\partial_{\nu} y(x) = b_1(x, y(x)) \qquad \text{for } x \in \Gamma_{\alpha}$$

$$\tag{56}$$

$$y(x) = b_2(x) \qquad \text{for } x \in \Gamma_\beta$$
 (57)

and mixed control-state or pure state inequality constraints

$$\begin{array}{rcl}
C(x,y(x),u(x)) &\leq & 0 & x \in \Omega \\
S(x,y(x)) &\leq & 0 & x \in \Omega \cup \Gamma_{\alpha}.
\end{array}$$
(58)

The functions $f : \Omega \times \mathbb{R}^2 \to \mathbb{R}$, $g : \Gamma_{\alpha} \times \mathbb{R} \to \mathbb{R}$, $d : \Omega \times \mathbb{R}^2 \to \mathbb{R}$, $b_1 : \Gamma_{\alpha} \times \mathbb{R} \to \mathbb{R}$, $b_2 : \Gamma_{\beta} \times \mathbb{R} \to \mathbb{R}$, $C : \Omega \times \mathbb{R}^2 \to \mathbb{R}$, and $S : \Omega \cup \Gamma_{\alpha} \times \mathbb{R} \to \mathbb{R}$ are assumed to be C^1 functions. As for boundary control problem, also for the distributed control problem, first order necessary conditions known in literature (see [5] and [4], [1] for linear elliptic equations and [6], [14], [19] for nonlinear elliptic equations of Lotka–Volterra type) have been formally extended in [16]. In this way, the necessary conditions are consistent with their counterparts in the discretized problems, given by the KKT conditions.

2.2 Discretization and optimization techniques

For the distributed control problems, we can use the same discretization and optimization techniques described in section 1.2 for the boundary control.

Also in this case, we consider the standard situation where the elliptic operator is the laplacian and $\Omega = (0,1) \times (0,1)$. Given a positive integer N and $h = \frac{1}{N+1}$, consider the mesh points

$$x_{ij} = (ih, jh), \quad 0 \le i, j \le N+1.$$

Assume the same notations stated in 1.2. We define the vector z as the vector whose entries are the approximations of the state variables y_{ij} , $(i, j) \in I(\Omega) \cup I(\Gamma_{\alpha})$ and of the control variables u_{ij} , $(i, j) \in I(\Omega)$:

$$z \doteq \left((y_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma_{\alpha})}, (u_{ij})_{(i,j)\in I(\Gamma)} \right) \in \mathbb{R}^{2N^2 + \tau(N)}.$$

$$(59)$$

where $\tau(N)$ is the number of index pairs of $I(\Gamma_{\alpha})$. The remaining state variables y_{ij} , $(i, j) \in I(\Gamma_{\beta})$ are determined by the Dirichlet condition (57) as

$$y_{ij} = b_2(x_{ij}) \text{ for } (i,j) \in I(\Gamma_\beta).$$
 (60)

The derivative $\partial_{\nu} y(x_{ij})$ in the direction of the outward normal is approximated by y_{ij}^{ν}/h , where y_{ij}^{ν} is defined in (14). Then the discrete form of the Neumann boundary condition (56) leads to the equality constraints

$$B_{ij}^{h}(z) \doteq y_{ij}^{\nu} - hb_1(x_{ij}, y_{ij}) = 0, \quad \text{for } (i, j) \in I(\Gamma_{\alpha}).$$
(61)

The application of the five points formula to the elliptic equation (55) yields the following equality constraint for all $(i, j) \in I(\Omega)$

$$G_{ij}^{h}(z) \doteq 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2 d(x_{ij}, y_{ij}, u_{ij}) = 0.$$
(62)

Note that the discrete Dirichlet conditions (60) are used in this equation to substitute the variables y_{ij} for $(i.j) \in I(\Gamma_{\beta})$. The control and state inequality constraints (58) yield the inequality constraints

$$C(x_{ij}, y_{ij}, u_{ij}) \le 0 \qquad \text{for } (i, j) \in I(\Omega), \tag{63}$$

$$S(x_{ij}, y_{ij}) \le 0 \qquad \text{for } (i, j) \in I(\Omega) \cup I(\Gamma_{\alpha}).$$
(64)

The discretized form of the cost functional (54) is

$$F^{h}(z) \doteq h^{2} \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}, u_{ij}) + h \sum_{(i,j)\in I(\Gamma_{\alpha})} g(x_{ij}, y_{ij}).$$
(65)

In summary, for any N, we have the following nonlinear programming (NLP) problem:

$$\begin{array}{cccc}
\min & F^{h}(z) \\
G^{h}_{ij}(z) = 0 & (i,j) \in I(\Omega), \\
B^{h}_{ij}(z) = 0 & (i,j) \in I(\Gamma_{\alpha}), \\
C(x_{ij}, y_{ij}, u_{ij}) \leq 0 & (i,j) \in I(\Omega), \\
S(x_{ij}, y_{ij}) \leq 0 & (i,j) \in I(\Omega) \cup I(\Gamma_{\alpha}),
\end{array}$$
(66)

with $z \in \mathbb{R}^{2N^2 + \tau(N)}$. The lagrangian function of the NLP problem (66) is given by

$$L(z,q,\lambda,\mu) = h^{2} \sum_{(i,j)\in I(\Omega)} f(x_{ij}, y_{ij}, u_{ij}) + h \sum_{(i,j)\in I(\Gamma_{\alpha})} g(x_{ij}, y_{ij}) + \sum_{(i,j)\in I(\Omega)} [q_{ij}G^{h}_{ij}(z) + \lambda_{ij}C(x_{ij}, y_{ij}, u_{ij}) + \mu_{ij}S(x_{ij}, y_{ij})] + \sum_{(i,j)\in I(\Gamma_{\alpha})} [\mu_{ij}S(x_{ij}, y_{ij}) + q_{ij}B^{h}_{ij}(z)],$$
(67)

where the Lagrange multipliers $q = (q_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma_{\alpha})}$, $\lambda = (\lambda_{ij})_{(i,j)\in I(\Omega)}$ and $\mu = (\mu_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma_{\alpha})}$ are associated respectively with the equality constraints (62) and (61) and with the inequality constraints (63) and (64). The ordering of the discrete variables y_{ij} and u_{ij} in the array z is described in subsection 1.2 (see figure 1).

2.3 Test problems: general description

In the following, we consider elliptic problems where the cost functional is of tracking type (except for the last problems):

$$F(y,u) = \frac{1}{2} \int_{\Omega} (y(x) - y_d(x))^2 dx + \frac{\alpha}{2} \int_{\Omega} (u(x) - u_d(x))^2 dx, \qquad (68)$$

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

$$y(x) \le \psi(x) \quad \text{on } \Omega,$$
 (69)

$$u_1(x) \le u(x) \le u_2(x) \quad \text{on } \Omega, \tag{70}$$

with functions $\psi \in C(\overline{\Omega})$ and $u_1, u_2 \in L^{\infty}(\Omega)$. We assume that an optimal solution $\overline{y}(x)$ and $\overline{u}(x)$ of the optimal control problems exists. If d(x, y, u) in the state equation (55) is linear in the control variable u, the optimal control $\overline{u}(x)$ is completely determined. If we denote by $\overline{q}(x)$ the adjoint state corresponding to $\overline{y}(x)$ and $\overline{u}(x)$, we have:

• case
$$\alpha \ge 0$$
: for $x \in \Omega$

$$\bar{u}(x) = \begin{cases} u_d(x) + \bar{q}(x)/\alpha & \text{if } u_d(x) + \bar{q}(x)/\alpha \in (u_1(x), u_2(x)), \\ u_1(x) & \text{if } u_d(x) + \bar{q}(x)/\alpha \le u_1(x), \\ u_2(x) & \text{if } u_d(x) + \bar{q}(x)/\alpha \ge u_2(x), \end{cases}$$
(71)

• case $\alpha = 0$: we obtain an optimal control of bang-bang or singular type:

$$\bar{u}(x) = \begin{cases} u_1(x) & \text{if } \bar{q}(x) < 0, \\ u_2(x) & \text{if } \bar{q}(x) > 0, \\ \text{singular} & \text{if } \bar{q}(x) = 0 \text{ on } \Omega_S \subset \Omega, \quad \int_{\Omega_S} dx > 0. \end{cases}$$
(72)

The discrete counterpart of $\bar{q}(x)$ is the vector of the Lagrange multipliers $q = (q_{ij})$, where we set $q_{ij} = 0$ for $(i, j) \in I(\Gamma_{\beta})$.

2.4 Test problems: discretization techniques

When the discretization techniques described in section 2.2 are applied to a cost functional of tracking type (68), $F^h(z)$ can be written as follows:

$$F^{h}(z) = \frac{1}{2}h^{2} \sum_{(i,j)\in I(\Omega)} (y_{ij} - y_{d}(x_{ij}))^{2} + \frac{\alpha}{2}h \sum_{(i,j)\in I(\Omega)} (u_{ij} - u_{d}(x_{ij}))^{2}.$$

The Hessian matrix H of $F^{h}(z)$ is a diagonal matrix, given by

$$H = diag(h^2 I_{n_1}, 0_{n_2}, h\alpha I_{n_3}), \tag{73}$$

where $n_1 = N^2$, $n_2 = \tau(N)$, $n_3 = N^2$. If $\Gamma_{\alpha} = \emptyset$ and $\Gamma_{\beta} = \Gamma$ (Dirichlet boundary conditions only), then $n_2 = 0$. If $\Gamma_{\alpha} = \Gamma$ and $\Gamma_{\beta} = \emptyset$ (Neumann boundary conditions), then $n_2 = 4N$.

Now, we determine the Jacobian matrix J of the equality constraints. J is a sparse $(N^2 + \tau(N)) \times (2N^2 + \tau(N))$ matrix, that can be written as follows:

$$J = \begin{bmatrix} Y + D & \bar{U}^t & \bar{E} \\ \bar{U} & T & 0 \end{bmatrix}$$
(74)

where Y is an $N \times N$ block tridiagonal matrix as in (42), D is a square diagonal matrix of order N^2 with diagonal entries of the form

$$\left(h^2 \frac{\partial d(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij}}\right), \quad (i, j) \in I(\Omega),$$

 \overline{U}^t is a sparse $N^2 \times \tau(N)$ matrix with non null entries equal to -1, \overline{E} is a square diagonal matrix of order N^2 with diagonal entries $h^2 \frac{\partial d(x_{ij}, y_{ij}, u_{ij})}{\partial u_{ij}}$, $(i, j) \in I(\Omega)$ and, finally, T is a square diagonal matrix of order $\tau(N)$ with diagonal entries

$$\left(1 - h \frac{\partial b_1(x_{ij}, y_{ij})}{\partial y_{ij}}\right), \quad (i, j) \in I(\Gamma_\alpha).$$

If $\Gamma_{\alpha} = \emptyset$, $\Gamma_{\beta} = \Gamma$, J becomes equal to the following $N^2 \times 2N^2$ matrix:

$$J = [Y + D, \bar{E}]. \tag{75}$$

If $\Gamma_{\alpha} = \Gamma$, $\Gamma_{\beta} = \emptyset$, J is a $(N^2 + 4N) \times (2N^2 + 4N)$ matrix. The Hessian matrix \overline{H} of the lagrangian function has the following form:

$$\bar{H} = H + \begin{pmatrix} \bar{Y} & \bar{Z} \\ & \bar{T} \\ \bar{Z}^t & \bar{S} \end{pmatrix},$$
(76)

where the $N^2 \times N^2$ matrices \bar{Y} , \bar{Z} , \bar{S} and the $\tau(N) \times \tau(N)$ matrix \bar{T} are given by:

$$\bar{Y} = diag\left(h^2 q_{ij} \frac{\partial^2 d(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij}^2}\right), \quad (i, j) \in I(\Omega), \tag{77}$$

$$\bar{S} = diag\left(-hq_{ij}\frac{\partial^2 d(x_{ij}, y_{ij}, u_{ij})}{\partial u_{ij}^2}\right), \quad (i, j) \in I(\Omega),$$
(78)

$$\bar{Z} = diag\left(h^2 q_{ij} \frac{\partial^2 d(x_{ij}, y_{ij}, u_{ij})}{\partial y_{ij} \partial u_{ij}}\right), \quad (i, j) \in I(\Omega),$$
(79)

$$\bar{T} = diag\left(-hq_{ij}\frac{\partial^2 b_1(x_{ij}, y_{ij})}{\partial y_{ij}^2}\right), \quad (i, j) \in I(\Gamma_\alpha).$$
(80)

If $\Gamma_{\alpha} = \emptyset$, $\Gamma_{\beta} = \Gamma$, \overline{H} becomes a $2N^2 \times 2N^2$ matrix with the following form:

$$\bar{H} = H + \left(\begin{array}{cc} \bar{Y} & \bar{Z} \\ \bar{Z}^t & \bar{S} \end{array} \right)$$

For convenience, the numerical results reported in the following for all the test problems are referred to the fixed stepsize h = 1/(N+1), with N = 99 and in some cases also with N = 199.

Figure 11: Problem 2.1



Problem 2.1 (Example 1 in [16])

We consider the following elliptic control problem with Dirichlet boundary conditions ($\Gamma_{\alpha} = \emptyset$): minimize the cost functional (54) subject to

on
$$\Omega$$
: $-\Delta y(x) - y(x) + y(x)^3 = u$, $\begin{aligned} y(x) &\leq 0.185, \quad 1.5 \leq u(x) \leq 4.5, \\ y_d(x) &= 1 + 2(x_1(x_1 - 1) + x_2(x_2 - 1)), \\ u_d(x) &\equiv 0, \alpha = 0.001. \end{aligned}$

The discretization techniques lead to a NLP problem. In figure 11, the structure of the Jacobian matrix J and that of the Hessian matrix \bar{H} of the lagrangian function are reported (for N = 5). Since $d_u(x, y, u) = 1$ and $\alpha > 0$, we have that

$$u_{ij} = \left\{ \begin{array}{ll} q_{ij} \cdot 10^3 & \text{if } q_{ij} \cdot 10^3 \in (1.5, 4.5) \\ 1.5 & \text{if } q_{ij} \cdot 10^3 \leq 1.5 \\ 4.5 & \text{if } q_{ij} \cdot 10^3 \geq 4.5 \end{array} \right\}$$
(81)

The state constraint is active at the center (0.5, 0.5). For N = 99, $F(\bar{y}, \bar{u}) = 0.0621615$; for N = 199, $F(\bar{y}, \bar{u}) = 0.0644263$.

Problem 2.2 (Example 2 in [16])

Figure 12: Problem 2.2



The data are the same of the previous problem, but in this case $\alpha = 0$. The matrix J has the same structure than in the problem 2.1 (see figure 11); the Hessian matrix \overline{H} of the lagrangian function is a diagonal matrix, but the diagonal entries of \overline{H} corresponding to u_{ij} , $(i, j) \in I(\Omega)$ are equal to 0 (see figure 12). Since $\alpha = 0$, we obtain a bang-bang control, having the following form:

$$\bar{u}(x) = \left\{ \begin{array}{ll} 1.5 & \text{if } \bar{q}(x) < 0\\ 4.5 & \text{if } \bar{q}(x) > 0 \end{array} \right\}$$

For N = 99, $F(\bar{y}, \bar{u}) = 0.0564479$; for N = 199, $F(\bar{y}, \bar{u}) = 0.0586978$.

Problem 2.3 (Example 3 in [16])

We consider the following elliptic control problem with Dirichlet boundary conditions: minimize the functional (54) subject to

on Ω :	$-\Delta y(x) - \exp(y(x)) = u,$	$y(x) \le 0.11, -5 \le u(x) \le 5,$ $u_1(x) = \sin(2\pi x_1)\sin(2\pi x_2)$
on Γ :	y(x) = 0,	$g_d(x) \equiv \sin(2\pi x_1) \sin(2\pi x_2),$ $u_d(x) \equiv 0, \alpha = 0.001.$

The structure of the Jacobian matrix J and of the Hessian matrix \overline{H} for the discretized NLP problem is the same of the problem 2.1 (see figure 11). From (71), we have

$$u_{ij} = \begin{cases} q_{ij} \cdot 1000 & \text{if } q_{ij} \cdot 1000 \in (-5,5) \\ -5 & \text{if } q_{ij} \cdot 1000 \leq -5 \\ 5 & \text{if } q_{ij} \cdot 1000 \geq 5 \end{cases}$$

The state constraint is active at the points (.26, .26), (.74, .74). For N = 99, at the point (.26, .26), we have $q_{ij} = 0.00858$, $y_{ij} = .11$, $y_d(x_{ij}) = 1$, $\mu_{ij} = 0.00251$. Furthermore $q_{i+1j} = 0.00912$, $q_{i-1j} = 0.00926$, $q_{ij+1} = 0.00912$, $q_{ij-1} = 0.00926$. For N = 99, $F(\bar{y}, \bar{u}) = 0.110263$; for N = 199, $F(\bar{y}, \bar{u}) = 0.1102685$.

Problem 2.4 (Example 4 in [16])

We consider the following elliptic control problem with Neumann boundary conditions: minimize the functional (54) subject to

on
$$\Omega$$
: $-\Delta y(x) - \exp(y(x)) = u$, $\begin{aligned} y(x) &\leq 0.371, \quad -8 \leq u(x) \leq 9, \\ y_d(x) &= \sin(2\pi x_1)\sin(2\pi x_2), \end{aligned}$
on Γ : $\partial_{\nu} y(x) + y(x) = 0$, $u_d(x) \equiv 0, \alpha = 0.001. \end{aligned}$

The figure 13 illustrates the structure of the matrices of the NLP problem. In this case $\Gamma_{\alpha} = \Gamma$ and $\Gamma_{\beta} = \emptyset$. Since $\alpha > 0$ and $d_u(x, y, u) = 1$, we have

$$u_{ij} = \begin{cases} q_{ij} \cdot 1000 & \text{if } q_{ij} \cdot 1000 \in (-8,9) \\ -8 & \text{if } q_{ij} \cdot 1000 \leq -8 \\ 9 & \text{if } q_{ij} \cdot 1000 \geq 9 \end{cases}$$

For N = 99, $F(\bar{y}, \bar{u}) = 0.07806389$; for N = 199, $F(\bar{y}, \bar{u}) = 0.07842597$. We report also the values of y and u at the point (.5, .5): $y_{ij} = -0.009152$ (N = 99) and $y_{ij} = -0.008243$ (N = 199) while $u_{ij} = -1.619699$ (N = 99)and $u_{ij} = -1.588730$ (N = 199).

Problem 2.5 (Example 5 in [16])

This problem has the same data as the previous one, except for the choice $\alpha = 0$. The Jacobian matrix J has the same structure of that in figure 13; the Hessian matrix \bar{H} of the lagrangian function has diagonal entries corresponding to the variables u_{ij} equal to zero (see figure 14). In this case, the optimal control is a bang-bang control having the form:

$$\bar{u}(x) = \begin{cases} -8 & \text{if } \bar{q}(x) < 0\\ 9 & \text{if } \bar{q}(x) > 0 \end{cases}$$

For N = 99, $F(\bar{y}, \bar{u}) = 0.0526639$.





Figure 14: Problem 2.2



We consider the following elliptic control problem with Neumann boundary conditions: minimize the functional

$$\int_{\Omega} (Mu(x)^2 - Ku(x)y(x))dx \tag{82}$$

subject to

on
$$\Omega$$
: $-\Delta y(x) = y(x)(a(x) - u(x) - by(x))$ $y(x) \le \psi(x),$
 $u_1 \le u(x) \le u_2,$ (83)
on Γ : $\partial_{\nu} y(x) = 0.$

where

$$a(x) = 7 + 4\sin(2\pi x_1 x_2) \tag{84}$$

$$b = 1$$
, $M = 1$, $K = 0.8$, $u_1 = 1.7$, $u_2 = 2$, $\psi(x) = 7.1$

The discrete Neumann conditions

$$y_{ij}^{\nu} = 0 \qquad (i,j) \in I(\Gamma)$$

suggest to reduce the number of variables y_{ij} , $(i, j) \in I(\Gamma) \cup I(\Omega)$. In other words, from the equality constraints (61), we obtain

$$egin{aligned} y_{0j} &= y_{1j}, \ y_{N+1j} &= y_{Nj}, \ y_{i0} &= y_{i1}, \ y_{iN+1} &= y_{iN}. \end{aligned}$$

Thus the Jacobian matrix J is an $N^2\times 2N^2$ matrix with the form

$$J = \begin{bmatrix} Y + D & \bar{E} \end{bmatrix}$$

where \tilde{Y} is an $N \times N$ block tridiagonal matrix with the off diagonal blocks equal to $-I_N$ and the diagonal block of the form

$$\tilde{Y}_{11} = \tilde{Y}_{NN} = \begin{bmatrix} 2 & -1 & & \\ -1 & 3 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 3 & -1 \\ & & & -1 & 2 \end{bmatrix},$$

Figure 15: Problem 2.6



$$\tilde{Y}_{ii} = \begin{bmatrix} 3 & -1 & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 3 \end{bmatrix}, \qquad i = 2, \dots, N-1.$$

Furthermore, the matrices D and \overline{E} are as in (74). The matrix H has the form

$$\left(\begin{array}{cc} 0_{N^2} & -Kh^2 I_{N^2} \\ -Kh^2 I_{N^2} & 2h^2 M I_{N^2} \end{array}\right)$$

and the matrix \overline{H} is equal to

$$\bar{H} = H + \left(\begin{array}{cc} \bar{Y} & \bar{Z} \\ \bar{Z}^t & \bar{S} \end{array} \right)$$

where \bar{Y} , \bar{Z} , and \bar{S} are as in (??) (in this case $\bar{S}=0$). The structures of matrices J and \bar{H} are depicted in figure 15.

The discretized problem is again a NLP problem.

The state variable attains its upper bound at the two points (0.21, 0.99) and (.99, .21) near the boundary. For N = 99, $F(\bar{y}, \bar{u}) = -6.576428$; for N = 199, $F(\bar{y}, \bar{u}) = -6.620092$.

Figure 16: Problem 2.7



Problem 2.7 Example 4.2 in [17]

The problem has the same data of the previous problem, but in this case we choose

$$b = 1$$
, $M = 0$, $K = 1$, $u_1 = 2$, $u_2 = 6$, $\psi(x) = 4.8$

The structure of the Jacobian matrix J is the same of the previous problem (see figure 15). The matrix \overline{H} has the diagonal entries corresponding to the variables u_{ij} equal to zero (see figure 16).

In this case, the optimal control is a bang–bang control. For N = 99, $F(\bar{y}, \bar{u}) = -18.73615$; for N = 199, $F(\bar{y}, \bar{u}) = -18.86331$.

Problem 2.8 (Example 6 in [17])

We consider the following elliptic control problem with Neumann boundary conditions: minimize the functional (82) subject to

on Ω :	$-\Delta y(x) = y(x)(a(x) - u(x) - by(x))$	$y(x) \leq c$	$\psi(x),$
		$u_1 \leq u($	$x) \leq u_2,$
on Γ :	$\partial_{\nu} y(x) = 0$	$x_1 = 1$	$0 \le x_2 \le 1$
		$x_2 = 1$	$0 \le x_1 \le 1$
	$\partial_{\nu} y(x) + y(x) = 0$	$x_1 = 0$	$0 \le x_2 \le 1$
		$x_2 = 0$	$0 \le x_1 \le 1$

where

$$a(x) = 7 + 4\sin(2\pi x_1 x_2)$$

$$b = 1$$
, $M = 1$, $K = 0.8$, $u_1 = 1.4$, $u_2 = 1.6$, $\psi(x) = 6.09$

In this case we can reduce the number of the discrete variables exploiting the discrete Neumann conditions

$$y_{ij}^{\nu} = 0 \qquad (i,j) \in I_3(\Gamma) \cup I_4(\Gamma),$$

so we obtain

$$y_{N+1j} = y_{Nj},$$

$$y_{iN+1} = y_{iN}.$$

The Jacobian matrix J is given by (74) with $\tau(N) = 2N$ and has the form

$$J = \left[\begin{array}{ccc} \hat{Y} + D & \hat{U}^t & \bar{E} \\ U & I & 0_{2N,N^2} \end{array} \right].$$

The matrix \hat{Y} is an $N^2 \times N^2$ block tridiagonal matrix where the diagonal $N \times N$ blocks are given by

$$\hat{Y}_{ii} = \begin{bmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 3 \end{bmatrix}, \quad i = 1, \dots, N - 1,$$
$$\hat{Y}_{NN} = \begin{bmatrix} 3 & -1 & & & \\ -1 & 3 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 3 & -1 \\ & & & & -1 & 2 \end{bmatrix}$$

and the off diagonal blocks are equal to $-I_N$. The matrix U is a sparse $2N \times N^2$ matrix with nonzero entries with column indices corresponding to the variables y_{i1} and y_{1j} for i, j = 1, ..., N. The diagonal matrices D and \overline{E} are as in (74). The structure of J for N = 5 is depicted in figure 17. The Hessian matrix H of $F^h(z)$ has the form

$$H = \begin{bmatrix} 0_{N^2} & 0_{N^2,2N} & -Kh^2 I_{N^2} \\ 0_{N^2,2N} & 0_{2N} & 0_{N^2,2N} \\ -Kh^2 I_{N^2} & 0_{N^2,2N} & 2h^2 M I_{N^2} \end{bmatrix},$$

Figure 17: Problem 2.8



as shown in figure 17, while the Hessian matrix of the lagrangian function is given by

$$\bar{H} = H + \left(\begin{array}{cc} Y & Z \\ & \bar{T} \\ \bar{Z}^t & \bar{S} \end{array}\right)$$

(see figure 18) where \bar{Y} , \bar{Z} , \bar{S} and \bar{T} are diagonal matrices as in (76). In this case \bar{S} and \bar{T} are equal to zero. For N = 99, $F(\bar{y}, \bar{u}) = -4.27569$; for N = 199, $F(\bar{y}, \bar{u}) = -4.31709$.



Figure 18: Problem 2.8

3 Parabolic control problems

3.1 Statement of the problem

We consider the following optimal control problem: determine a piecewise continuous control function u(x,t), $(x,t) \in [0,1] \times [0,1]$ which minimizes the cost functional

$$F(u) = \int_0^1 \int_0^1 (y^2(x,t) + \alpha u^2(x,t)) dx dt + \int_0^1 y^2(x,1) dx$$
(85)

subject to the diffusion-convection equation

$$y_t = ay_{xx} + by_x - cy + d + \tilde{\sigma}u, \qquad (x,t) \in (0,1) \times [0,1],$$
 (86)

the initial condition

$$y(x,0) = y_0(x), \qquad x \in [0,1],$$
(87)

the boundary conditions

$$y(0,t) = g_0(t), \qquad y(1,t) = g_1(t), \qquad t \in [0,1]$$
(88)

and state constraint and/or control constraints

$$y_{min} \le y(x,t) \le y_{max}$$
 $(x,t) \in [0,1] \times [0,1]$ (89)

$$u_{min} \le u(x,t) \le u_{max}$$
 $(x,t) \in [0,1] \times [0,1].$ (90)

Here y(x,t) is a function of the arguments x (space) and t (time) which characterizes the state of the controlled system and u(x,t) is a function which characterizes the control actions of the system. The parameters a, b,c, are known and constant with a > 0, $c \ge 0$; $\tilde{\sigma}$ is a constant or a given function of the argument y. The function d is the source term and it may be a function of y, while $y_0(x)$, $g_0(t)$, $g_1(t)$ are given functions, satisfying the compatibility conditions

$$y_0(0) = g_0(0), \qquad y_0(1) = g_1(0).$$
 (91)

3.2 Discretization techniques

The technique employed to obtain an NLP problem from the optimal control problem (85)–(90) is described in [11]. For sake of completeness, we report this description, specifying the structure of the involved matrices when d and $\tilde{\sigma}$ depend on the argument y. To obtain finite difference approximations of

the diffusion-convection problem (86), (87), (88), we discretize first only the spatial variable x, leaving the time variable t continuous. The interval $0 \le x \le 1$ is subdivided into N + 1 subintervals of size h, so that $h = \frac{1}{N+1}$. We denote by x_i the point ih, $i = 0, \ldots, N + 1$. If we use the following central difference formulas

$$y_{xx} = \frac{y(x_{i-1}, t) - 2y(x_i, t) + y(x_{i+1})}{h^2} + o(h^2)$$
(92)

$$y_x = \frac{y(x_{i+1}, t) - y(x_{i-1})}{2h} + o(h^2)$$
(93)

to discretize the equation (86) at each inner mesh point x_i , i = 0, ..., N, we obtain a system of N first order ordinary equations of the form

$$y'(t) = Ay(t) + s(y, y(t)) + B(y(t))u(t),$$
(94)

where y(t) is the approximation of the vector solution $(y(x_1, t), \ldots, y(x_N, t))^t$; A and B are the following $N \times N$ matrices:

$$A = \begin{pmatrix} -(\frac{2a}{h^2} + c) & \frac{a}{h^2} + \frac{b}{2h} \\ \frac{a}{h^2} - \frac{b}{2h} & -(\frac{2a}{h^2} + c) & \frac{a}{h^2} + \frac{b}{2h} \\ & \ddots \\ & & \ddots \\ & & \frac{a}{h^2} - \frac{b}{2h} & -(\frac{2a}{h^2} + c) \end{pmatrix}$$
(95)

$$B(y(x)) = diag(\tilde{\sigma}(y(x_1, t)), \dots, \tilde{\sigma}(y(x_N, t))).$$
(96)

Furthermore, we have

$$u(t) = (u(x_1, t), \dots, u(x_N, t))^t$$
 (97)

$$s(t, y(t)) = \begin{pmatrix} d(x_1, t, y(x_1, t)) + (\frac{a}{h^2} - \frac{b}{2h})g_0(t) \\ d(x_2, t, y(x_2, t)) \\ \dots \\ d(x_{N-1}, t, y(x_{N-1}, t)) \\ d(x_N, t, y(x_N, t)) + (\frac{a^2}{h^2} + \frac{b}{2h})g_1(t)^t \end{pmatrix}.$$
(98)

The vector solution y(t) of the differential system (94) is subject to the initial vector condition

$$y(0) = (y_0(x_1), \dots, y_0(x_N)).$$
 (99)

For each h such that

$$h < \frac{2a}{|b|} \tag{100}$$

the tridiagonal matrix A is irreducibly diagonnaly dominant. Thus, the matrix A is nonsingular. Since the diagonal entries of A are negative, the eigenvalues λ_i of A belong to the negative part of the complex plane, i.e. $Re(\lambda_i) < 0, i = 1, 2, ..., N$ (see [20], p. 23). Then, if the matrix B has constant diagonal entries and the source term d is independent from y(x,t), so that $s(t, y(t)) \equiv s(t)$, then the continuous dynamic system (94) is asymptotically stable (see [18], p. 65). Suppose that the fixed-time process (94)–(99) is of M steps duration. Then, the interval [0,1] is divided into M subintervals, each of size k, so that Mk = 1; we assume that the controls are piecewise constant, $u(t) = u_j$ for $t \in (t_j, t_{j+1}], j = 0, 1, ..., M - 1$. Using the backward difference implicit method for solving the differential system (94), we obtain, at the time t = (j-1)k for any time level j = 0, 1, ..., M - 1, the following difference equations:

$$\frac{y_{j+1} - y_j}{k} = Ay_{j+1} + s_{j+1}(y_{j+1}) + B(y_j)u_j \qquad j = 0, 1, \dots, M-1 \quad (101)$$

or

$$(I - kA)y_{j+1} = -y_j + ks_{j+1}(y_{j+1}) + kB(y_j)u_j \qquad j = 0, 1, \dots, M - 1$$
(102)

where $B(y_j)$ is the $N \times N$ diagonal matrix

$$B(y_j) = diag(\tilde{\sigma}(x_{1j}), \dots, \tilde{\sigma}(x_{Nj})), \qquad j = 0, 1, \dots, M-1$$
(103)

with $y_0 = y(0)$.

Any scalar equation of the system (102) has the form

$$-k\left(\frac{a}{h^{2}}-\frac{b}{2h}\right)y_{i-1j+1}+\left(1+k\left(\frac{2a}{h^{2}}+c\right)\right)y_{ij+1}-k\left(\frac{a}{h^{2}}-\frac{b}{2h}\right)y_{i+1j+1}=$$

= $y_{ij}+ks_{ij}(y_{ij})+k\tilde{\sigma}(y_{ij})u_{ij}$
(104)

for $i = 1, \dots, N, j = 0, 1, \dots, M - 1$.

Since the real parts of the eigenvalues of A are negative $(Re(\lambda_i) < 0)$, the eigenvalues of the matrix (I - kA) have the real parts strictly positive and greater than 1 (i.e. $Re(\lambda_i) > 1$) for any k > 0, so the spectral radius of (I - kA) is greater than 1. Then the matrix (I - kA) is nonsingular and the spectral radius of the inverse $(I - kA)^{-1}$ is strictly less then 1. This means that, if the source term is independent of y so that

$$s_{j+1} = \begin{pmatrix} d(x_1, t_{j+1}) + (\frac{a}{h^2} - \frac{b}{2h})g_0(t_{j+1}) \\ d(x_2, t_{j+1}) \\ \dots \\ d(x_{N-1}, t_{j+1}) \\ d(x_N, t_{j+1})) + (\frac{a^2}{h^2} + \frac{b}{2h})g_1(t_{j+1}) \end{pmatrix}$$

and the matrix B has constant diagonal entries equal to $\tilde{\sigma}$, then the discrete dynamic system (102) is asymptotically stable for any k > 0 (see [18], p.71). If we denote by z the vector whose entries are the approximations y_{ij+1} and u_{ij} of the control and state at any point x_i , $i = 1, \ldots, N$ and any level time t_j , $j = 1, \ldots, M - 1$, we have

$$z = (y_1^t, y_2^t, \dots, y_M^t, u_0^t, \dots, u_{M-1}^t)^t = (y_{11}, \dots, y_{N1}, y_{12}, \dots, y_{N2}, \dots, y_{1M}, \dots, y_{NM}, u_{10}, \dots, u_{N0}, \dots, u_{1M-1}, \dots, u_{N,M-1})^t$$
(105)

where $z \in \mathbb{R}^{2MN}$. Furthermore,

$$s = (s_1(y_1), \ldots, s_M(y_M))$$

and the equation (102) can be written in the form

$$G(z) = 0$$

where $G(z) \in \mathbb{R}^{MN}$. The analogous discrete form for the state constraints (89) and for the control constraints (90) is respectively

$$y_{min}e \le [I_{MN} \quad 0_{MN}]z \le y_{max}e \tag{106}$$

$$u_{min}e \le [0_{MN} \quad I_{MN}]z \le u_{max}e \tag{107}$$

where $e = (1, \ldots, 1)^t \in \mathbb{R}^{MN}$.

To discretize the cost functional (85), we use the rectangular rule to integrate with respect to the space variable and we obtain

$$F(u(t)) = h \int_0^1 \sum_{i=0}^N (y^2(x_i, t) + \alpha u^2(x_i, t)) dt + h \sum_{i=0}^N y^2(x_i, 1).$$
(108)

Then, using again the rectangular rule to integrate with respect to the time variable and assuming $u(0,t) \equiv 0, t \in [0,1]$, we have

$$\tilde{F} = hk \sum_{i=0}^{M-1} \sum_{i=0}^{N} y_{ij}^2 + h \sum_{i=0}^{N} y_{iM}^2 + \alpha hk \sum_{i=0}^{M-1} \sum_{i=0}^{N} u_{ij}^2 + \gamma.$$
(109)

where $\gamma = hk \sum_{i=0}^{N} y_0(x_i) + hk \sum_{i=0}^{M-1} g_0^2(t_j) + hg_0^2(t_M)$. Then, we define the $2MN \times 2MN$ matrix H as follows:

$$H = \left(\begin{array}{cc} H_y & 0\\ 0 & H_u \end{array}\right) \tag{110}$$

where

$$H_{y} = \begin{pmatrix} 2hkI_{N} & & & \\ & 2hkI_{N} & & \\ & & \ddots & \\ & & & 2hkI_{N} \\ & & & & 2hI_{N} \end{pmatrix}$$
(111)

and

$$H_u = 2\alpha h k I_{MN}. \tag{112}$$

The minimization of the functional \tilde{F} is equivalent to minimize the quadratic form

$$\bar{F}(z) = \frac{1}{2}z^t H z. \tag{113}$$

So, for any N and M we have to solve the following NLP problem:

$$\min_{\substack{s.t.\\G(z)=0\\y_{min}e \leq (I_{MN}, 0_{MN}z \leq y_{max}e\\u_{min}e \leq (0_{MN}, I_{MN}z \leq u_{max}e.}} F(z)$$
(114)

The Lagrangian function of the problem (114) has the form

$$L(z,q,\mu,\lambda) = \bar{F}(z) - G(z)^t q - \left(z - \left(\begin{array}{c} y_{min}e\\ y_{max}e\end{array}\right)\right)^t \mu - \left(\left(\begin{array}{c} y_{min}e\\ y_{max}e\end{array}\right) - z\right)^t \lambda$$
(115)

where $q \in \mathbb{R}^{MN}$, $\mu, \lambda \in \mathbb{R}^{2MN}$ are the Lagrange multipliers corresponding to the equality constraints and to the lower and upper bounds respectively. The Jacobian matrix J of the equality constraints is an $MN \times 2MN$ sparse matrix of the form

$$J = \begin{bmatrix} R & D \end{bmatrix} \tag{116}$$

with

$$R = \begin{pmatrix} \Omega - E_1 & & \\ -I_N - C_1 & \Omega - E_2 & & \\ & \ddots & \ddots & \\ & & -I_N - C_{M-1} & \Omega - E_M \end{pmatrix}$$
(117)

$$\Omega = (I - kA) \tag{118}$$

$$E_j = k \ diag\left(\frac{\partial d(x_1, t_j, y_{1j})}{\partial y_{1j}}, \cdots, \frac{\partial d(x_N, t_j, y_{Nj})}{\partial y_{Nj}}\right) \quad j = 1, \dots M$$
(119)

$$C_j = k \ diag\left(\frac{\partial \tilde{\sigma}(y_{1j})}{\partial y_{1j}}u_{1j}, \cdots, \frac{\partial \tilde{\sigma}(y_{Nj})}{\partial y_{Nj}}u_{nj}\right) \quad j = 1, \dots M - 1$$
(120)

$$D = \begin{pmatrix} D_0 & & \\ & \ddots & \\ & & D_{M-1} \end{pmatrix} \quad D_j = -kB(y_j), \quad j = 0, ..., M - 1.$$
(121)

If the source term d and the function $\tilde{\sigma}$ are independent of y(x,t), then the Jacobian matrix J of (116) becomes

$$J = \begin{pmatrix} \Omega & -\tilde{\sigma}kI_N & \\ -I_N & \ddots & & \ddots \\ & -I_N & \Omega & & -\tilde{\sigma}kI_N \end{pmatrix}$$
(122)

and the equality constraints become

$$G(z) = Jz - \tilde{s} = 0, \tag{123}$$

where

$$\tilde{s} = ks + \begin{pmatrix} \Omega y_0 \\ 0_{(M-1)N} \end{pmatrix}.$$

The Hessian matrix \bar{H} of the Lagrangian function (115) is the following $2MN\times 2MN$ matrix

$$\bar{H} = H + \begin{pmatrix} L_1 + T_1 & & & \\ & \ddots & & & \\ & & L_{M-1} + T_{M-1} & & \\ & & & L_M & \\ \hline & & & s^t & & 0_{MN} \end{pmatrix}$$
(124)

where

$$L_{j} = k \, diag \left(q_{1j} \frac{\partial^{2} d(x_{1}, t_{j}, y_{1j})}{\partial y_{1j}^{2}}, ..., q_{Nj} \frac{\partial^{2} d(x_{N}, t_{j}, y_{Nj})}{\partial y_{Nj}^{2}} \right) \quad j = 1, ..., M$$

$$(125)$$

$$T_{i} = k \, diag \left(q_{1j+1} \frac{\partial^{2} \tilde{\sigma}(y_{1j})}{\partial y_{1j}^{2}} u_{1j}, ..., q_{Nj+1} \frac{\partial^{2} \tilde{\sigma}(y_{Nj})}{\partial y_{Nj}^{2}} u_{Nj} \right) \quad i = 1, ..., M$$

$$T_{j} = k \, diag \left(q_{1j+1} \frac{\partial \, \partial (g_{1j})}{\partial y_{1j}^{2}} u_{1j}, ..., q_{Nj+1} \frac{\partial \, \partial (g_{Nj})}{\partial y_{Nj}^{2}} u_{Nj} \right) \quad j = 1, ..., M - 1$$
(126)

$$S = \begin{pmatrix} 0_N & S_1 & & \\ & \ddots & \ddots & \\ & & 0_N & S_{M-1} \\ & & & & 0_N \end{pmatrix}$$
(127)

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where

$$S_j = k \ diag\left(q_{1j+1}\frac{\partial\tilde{\sigma}(y_{1j})}{\partial y_{1j}}, ..., q_{Nj+1}\frac{\partial\tilde{\sigma}(y_{Nj})}{\partial y_{Nj}}\right) \quad j = 1, ..., M - 1.$$
(128)

If the source term and the function $\tilde{\sigma}$ are independent of y(x, t), the Hessian matrix \bar{H} is equal to H.

Problem 3.1

We consider the following optimal control problem: minimize the functional (85) subject to

$$y_t = ay_{xx} + by_x - cy + d + \tilde{\sigma}u \quad (x,t) \in (0,1) \times (0,1]$$

$$y(x,0) = y_0(x) = x \cos(\frac{\pi}{2}x) \qquad x \in [0,1]$$

$$y(0,t) = 0 \qquad t \in [0,1]$$

$$y(1,t) = 0 \qquad t \in [0,1]$$

$$0 \le y(x,t) \le 2 \qquad (x,t) \in (0,1) \times (0,1]$$

where $d(x,t) = e^{-t} \left(\pi (a + b\frac{x}{2}) \sin(\frac{\pi}{2}x) - b \cos(\frac{\pi}{2}x) \right), \alpha = 0.5, \tilde{\sigma} = \frac{a\pi^2}{4} + c - 1, a = 1, b = 70, c = 12.$

In this case $\tilde{\sigma}$ is constant and d(x,t) is independent of y(x,y). Then, the condition (100) requires that N > 34.

The discretization of the problem leads to a strictly convex quadratic programming problem, where the matrix J is given by (122). The sparsity pattern of the Hessian matrix H and of the Jacobian matrix J, for M = N = 5, are reported in figure 19.

Problem 3.2

The data of this problem are the same of problem 3.1, unless for $\tilde{\sigma} = 1 - \frac{a\pi}{4} - c$. Also in this case, the discretized problem is a strictly convex QP problem.

Problem 3.3

We consider the following optimal control problem: minimize the functional (85) subject to

$$\begin{array}{rcll} y_t &=& ay_{xx} + by_x - cy + d + \tilde{\sigma}u & (x,t) \in (0,1) \times (0,1] \\ y(x,0) &=& y_0(x) = x \cos(\frac{\pi}{2}x) & x \in [0,1] \\ y(0,t) &=& 0 & t \in [0,1] \\ y(1,t) &=& 0 & t \in [0,1] \\ & & y(x,t) \leq 2 & (x,t) \in (0,1) \times (0,1] \end{array}$$



where

$$d(x,t) = e^{-t} \left(\cos(\frac{\pi}{2}x)(-b + x(-2 + \frac{aM^2}{4} + c)) \right) + \sin(\frac{\pi}{2}x) \left((a + \frac{bx}{2})\pi \right) + \delta e^y,$$

and $\alpha = 0.5$, $\tilde{\sigma} = 1$, a = 1, b = 70, c = 12, $\delta = 1$.

The discretization of the problem leads to an NLP problem where $H = \bar{H}$. The sparsity pattern of the Hessian matrix H and of the Jacobian matrix J are the same than those of Problem 3.1.

Problem 3.4

We consider the following optimal control problem: minimize the functional (85) subject to

$$\begin{array}{rcl} y_t &=& ay_{xx} + by_x - cy + d + \tilde{\sigma}u & (x,t) \in (0,1) \times (0,1] \\ y(x,0) &=& y_0(x) = x \cos(\frac{\pi}{2}x) & x \in [0,1] \\ y(0,t) &\leq& 2 & t \in [0,1] \\ u(1,t) &\leq& 2 & t \in [0,1] \end{array}$$

where

$$d(x,t) = e^{-t} \left(\cos(\pi x/2) \left(-b + x(a\pi^2/4 + c - 1 - \delta e^{-t}x\cos(\pi x/2)) \right) \right) + \pi(a + bx/2) \sin(\pi x/2),$$

and $\alpha = 0.5$, $\tilde{\sigma} = \delta y$, a = 1, b = 70, c = 12, $\delta = 1$

The discretization of the problem leads to an NLP problem whose Hessian and Jacobian matrices \bar{H} and J have the structure depicted in figure 19.

Problem 3.5

We consider the following optimal control problem: minimize the functional (85) subject to

$$\begin{array}{rcl} y_t &=& ay_{xx} + by_x - cy + d + \tilde{\sigma}u & (x,t) \in (0,1) \times (0,1] \\ y(x,0) &=& y_0(x) = x \cos(\frac{\pi}{2}x) & x \in [0,1] \\ y(0,t) &=& 0 & t \in [0,1] \\ y(1,t) &=& 0 & t \in [0,1] \\ y(t,x) &\leq& 2 & (x,t) \in (0,1) \times (0,1] \end{array}$$

where

$$d(x,t,y) = e^{-t} \left(\cos(\pi x/2) \left(-2x + cx - b + \delta e^{-t} x^2 \cos(\pi x/2) + a\pi^2/4 \right) \right) + x(a + bx/2) \sin(\pi x/2) - \delta y^2,$$

and $\alpha = 0.5$, $\tilde{\sigma} = 1$, a = 1, b = 70, c = 12, $\delta = 1$. The discretization of the problem leads to an NLP problem whose Hessian and Jacobian matrices \bar{H} and J have the structure depicted in Figure 19.

Problem 3.6

We consider the following optimal control problem: minimize the functional

$$\int_{0}^{1} \int_{0}^{1} \left(y(x,t) . \bar{y}(x,t) \right)^{2} dx dt + \int_{0}^{1} \left(y(x,1) - \bar{y}(x,1) \right)^{2} dx \tag{129}$$

subject to

$$\begin{array}{rcl} y_t &=& ay_{xx} + by_x - cy + d + \tilde{\sigma}u & (x,t) \in (0,1) \times (0,1] \\ y(x,0) &=& y_0(x) = x\cos(\frac{\pi}{2}x) + 4 & x \in [0,1] \\ y(0,t) &=& 4 & t \in [0,1] \\ y(1,t) &=& 4 & t \in [0,1] \\ y(t,x) &\geq& 3 & (x,t) \in (0,1) \times (0,1] \end{array}$$

where

$$d(x,t) = e^{-t} \left(\pi (a + bx/2) \sin(\pi x/2) - b \cos(\pi x/2) \right) + 4c$$

and $\tilde{\sigma} = 1 - a\pi^2/4$, a = 1, b = 70, c = 12, $\bar{y}(x,t) = xe^{-t}\cos(\pi x/2) + 4$. The discretization of the functional (129) has the form

$$\tilde{F}(z) = hk \sum_{j=1}^{M-1} \sum_{i=1}^{N} (y_{ij} - \bar{y}(x_i, t_j))^2 + h \sum_{i=1}^{N} (y_{iM} - \bar{y}(x_i, t_M))^2$$



The Hessian matrix H of the function $\tilde{F}(z)$ has the form

$$H = \left(\begin{array}{cc} H_y & 0\\ 0 & 0 \end{array}\right)$$

where H_y is given in (111). The discretization of this optimal control problem leads to a convex QP problem, where the Jacobian matrix J has the form (122) depicted in the figure 20 and $H = \overline{H}$.

Problem 3.7

We consider the following optimal control problem: minimize the cost functional

$$F(y,u) = \int_0^{t_f} \int_0^{x_f} D_1(x) \left(y(x,t) - y_S(x,t) \right)^2 dx dt + \tilde{\alpha} \int_0^{t_f} \int_0^{x_f} D_2(x) u^2(x,t) dx dt,$$
(130)

subject to

$$y_t = -Vy_x - K_3y - K_1L + K_3y_S + u, (x,t) \in (0, x_f] \times (0, t_f]$$
(131)

$$y(x,0) = y_0(x) \qquad x \in [0, x_f]$$
 (132)

$$y(0,t) = \rho_0(t) \qquad t \in [0, t_f]$$
 (133)

$$y(x,t) \leq y_{max}(x) \quad (x,t) \in [0, x_f] \times [0, t_f]$$
 (134)

This is a special case of a water quality problem, described in [12], where y(x,t) is the dissolved oxygen concentration in a river of length x_f , u(x,t) is the rate of an artificial aeration mechanism and t_f is the time duration of the control. The functions $D_1(x)$ and $D_2(x)$ are two weighting functions, and they are non negative and positive respectively, while $\tilde{\alpha}$ is a positive scalar parameter. For the meaning of the other parameter see [12]. The equation (131) is related to a special case of a stream, assuming no tidal action and the cross sectional area constant. Here, we consider

$$L(x,t) = \begin{cases} \frac{J_1}{V} e^{-(K_1/V)x} & x < Vt\\ 0 & x \ge Vt \end{cases}$$

and we set the data as follows: $x_f = 5$ miles, $t_f = 4$ days, $V(x) \equiv \bar{V} \equiv V = 1$ mile/day, $J_1 = 15$, $K_1 = 0.16$ day⁻¹, $K_3 = 0.66$ day⁻¹, $y_0(x) = 6$ mg/l, $y_S(x) = 6$ mg/l, $\rho_0 = 6$ mg/l, $y_{max}(x) \equiv y_{max} = 7$ mg/l, $D_1(x) = 1$, $D_2 = 1$, $\tilde{\alpha} \in [0.1, 10]$.

The discretization technique used employed for this distributed control problem is described in [11] and leads to a QP problem,

In the following, we describe the main aspects of this approach. Setting $h = x_f/N$ and $x_i = x_f + ih$, i = 0, 1, ..., N, the space derivative y_x in (131) is replaced by the difference formula

$$\frac{y(x_i,t) - y(x_{i-1},t)}{h}$$
(135)

By substituting (135) in (131) for each i = 1, ..., N, we obtain a system of N first order differential equation of the following form

$$\frac{dy(t)}{dt} = Ay(t) + s(t) + u(t),$$
(136)

where

$$\begin{array}{lll} y(t) &=& (y(x_1,t),\ldots,y(x_N,t))^t \\ u(t) &=& (y(u_1,t),\ldots,y(u_N,t))^t \\ s(t) &=& \left(\frac{V_1}{h}\rho_0(t) + K_3y_S(x_1,t) - K_1L(x_1,t), K_3y_S(x_2,t) - K_1L(x_2,t),\ldots \right. \\ & & \quad K_3y_S(x_N,t) - K_1L(x_N,t)\right)^t \end{array}$$

and the $N \times N$ matrix A has the form

$$A = \begin{pmatrix} -\left(\frac{V_1}{h} + K_3\right) & & \\ \frac{V_2}{h} & -\left(\frac{V_2}{h} + K_3\right) & & \\ & \ddots & \ddots & \\ & & \ddots & \ddots & \\ & & & \frac{V_N}{h} & -\left(\frac{V_N}{h} + K_3\right) \end{pmatrix}$$
(137)

with $V_i = V(x_i), i = 1, ..., N$.

The vector solution y(t) of the differential system (136) is subject to the initial condition

$$y(0) = y_0 = (y_0(x_1), \dots, y_0(x_N))^{t}.$$
(138)

Since the matrix A is a strictly diagonal dominant matrix, it is non singular, and its eigenvalues are $\lambda_i = -(V_i/h + K_3) < 0, i = 1, ..., N$. The continuous dynamic system (136) is asymptotically stable [18].

Suppose that the fixed-time process (136)–(138) is of M step duration. Then the interval $[0, t_f]$ is divided into M subintervals of width k, so that $kM = t_f$; we assume $u(t) = u_j$ for $t \in [t_j, t_{j+1}), j = 0, 1, ..., M - 1$.

Using the forward difference method for solving the system (136), we obtain the following difference equations

$$\frac{y_{j+1} - y_j}{k} = Ay_j + s(t_j) + u_j$$

for any time $t_{j+1} = (j+1)k$, j = 0, 1, ..., M - 1, that can be written also as

$$y_{j+1} = (I + kA)y_j + ks(t_j) + ku_j, \qquad j = 0, ..., M - 1,$$
(139)

with $y_0 = y(0)$. Here $y_j = y(t_j) = (y(x_1, t_j), ..., y(x_N, t_j))^T = (y_{1j}, ..., y_{Nj})^T$ and $u_j = u(t_j) = (u(x_1, t_j), ..., u(x_N, t_j))^T = (u_{1j}, ..., u_{Nj})^T$. The eigenvalue of the matrix $\Omega = I + kA$ are $1 - k(\frac{v_i}{h} + k_3)$, i = 1, ..., N. Then, for

$$k < \frac{2}{\left(\frac{\bar{\nu}}{\bar{h}} + k_3\right)} \tag{140}$$

with $\bar{v} = \max_{i=1,...,N}(v_i)$, the discrete dynamic system (139) is asymptotically stable [18]. If we set $z = (y_1^T, ..., y_M^T, u_0^T, ..., u_{M-1})^T \in \mathbb{R}^{2MN}$,

$$\tilde{s} = \begin{pmatrix} ks(t_0) + \Omega y_0 \\ ks(t_i) \\ \vdots \\ ks(t_{M-1}) \end{pmatrix}$$

and

$$J = \begin{pmatrix} I_N & & \\ -\Omega & & \\ & -\Omega & I_N \end{pmatrix} \begin{pmatrix} -kI_N & & \\ & & -kI_N \end{pmatrix}$$

then the equation (139) can be written in the form

$$Jz - \tilde{s} = 0 \tag{141}$$

and the discrete form of the state constraint (134) is

$$\begin{bmatrix} I_{MN} & 0 \end{bmatrix} z \le y_{max} e \tag{142}$$

where, in this case, y_{max} is a constant parameter.

The discretization of the functional (130) is obtained by using the trapezoidal rule to integrate with respect to the space variable and then the rectangular rule to integrate with respect to the time variable.

The final form of the discretized functional that we have to minimize is

$$\bar{F}(z) = \frac{1}{2}z^T H z - r^T z \tag{143}$$

where H is a $2NM \times 2NM$ matrix with the form

$$H = \begin{pmatrix} H_y \\ H_u \end{pmatrix}$$
(144)

where $H_y = diag(hkD_1, ...hkD_1, 0_N), H_u = \tilde{\alpha}k diag(D_2, D_2, ..., D_2), D_1 = diag(2D_1(x_1), ..., 2D_1(x_{N-1}), D_1(x_N)), D_2 = diag(D_2(x_1), 2D_2(x_2), ..., 2D_2(x_{N-1}), D_2(x_N))$ and

$$r = hk \begin{pmatrix} D_1 y_{s1} \\ D_1 y_{s2} \\ \vdots \\ D_1 y_{sM-1} \\ 0_N \\ \vdots \\ 0_N \end{pmatrix}$$
(145)

with $y_{sj} = (y_s(x_1, t_j), ..., y_s(x_N, t_j)), j = 1, ..., M-1$. Then, an approximate solution of the original problem can be obtained by solving the following convex QP problem

$$\min_{\substack{\text{s.t. } Jz = \tilde{s} \\ (I_{MN} \ 0)z \le y_{max}e}} \bar{F}(z)$$
(146)

Since the QP problem is feasible (see [11]), there exists a unique optimal solution of the control problem [7]. In figure 21 the patterns of the matrices H and J are reported for N = M = 5. Finally, we observe that for the value assigned to the data in this case, the condition (140) is always satisfied.



References

- M. Bergounioux, K. Ito and K. Kunish (1997). Primal-dual strategy for constrained optimal control problems, SIAM J. Control Optim. 35, 1524–1543.
- [2] M. Bergounioux and K. Kunish (1999). Augmented Lagrangian techniques for elliptic state constrained optimal control problems, SIAM J. Control Optim. 37, 1176–1194.
- [3] J. T. Betts (2001). Practical methods for optimal control using nonlinear programming, Advances in Design and Control, SIAM.
- [4] F. Bonnans and E. Casas (1989). Optimal control of semilinear multistate systems with state constraints, SIAM J. Control Optim., 27, 303–325.
- [5] F. Bonnans and E. Casas (1995). An extension of Pontryagin's principle for state-constrained optimal control of semilinear elliptic equations and variational inequalities, SIAM J. Control Optim., 33, 274–298.
- [6] A. Canãda, J.L. Gámez and J. A. Montero (1998). Study of an optimal control problem for diffusive nonlinear elliptic equations of logistic type, SIAM J. Control Optim., 36, 1171–1189.
- [7] M.D. Canon, C. D. Cullum and E. Polak (1970). Theory of Optimal Control and Mathematical Programming, Mc Graw-Hill, New York.
- [8] E. Casas (1993). Boundary control with pointwise state constraints, SIAM J. Control Optim., 31, 993–1006.
- [9] E. Casas, F. Trölzsch and A. Unger (1996). Second order sufficient optimality conditions for a nonlinear ellptic control problem, J. for Analysis and its Applications, 15, 687–707.
- [10] E. Casas, F. Trölzsch and A. Unger (2000). Second order sufficient optimality conditions for some state constrained control problems of semilinear elliptic equations, SIAM J. Control Optim., 38, 1369–1391.
- [11] C. Durazzi and E. Galligani (2001). Nonlinear programming methods for solving optimal control problems, in "Equilibrium Problems: Nonsmooth Optimization and Variational Inequality Models" (F. Giannessi, A. Maugeri, P. M. Pardalos eds.), Nonconvex Optimization and Its Applications 58, Kluwer Academic Publ., 71–99.

- [12] W. Hullet (1974). Optimal estuary aeration: an application of distributed parameter control theory, Applied Mathematics and Optimization, 1, 20-63.
- [13] F. Leibfritz and E. W. Sachs (1994). Numerical Solution of Parabolic State Constrained Control Problems using SQP and Interior-Point-Methods, Large Scale Optimization: Stare of the Art, W. W. Hager et al. eds., Kluwer Academic Publisher, 245–258.
- [14] A. Leung and S. Stojanovic (1993). Optimal control for Volterra-Lotka equations, J. Math. Anal. Appl., 173, 603–619.
- [15] H. D. Mittelmann and H. Maurer (1999). Optimization techiques for solving elliptic control problems with control and state constraints: Part 1. Boundary control, Computational Optimization and Applications, 16, 29–55.
- [16] H. D. Mittelmann and H. Maurer (2001). Optimization techiques for solving elliptic control problems with control and state constraints: Part 2. Distributed control, Computational Optimization and Applications, 18, 141–160.
- [17] H. D. Mittelmann and H. Maurer (2000). Solving elliptic control problems with Interior Point and SQP Methods: control and state constraints, Journal of Computational and Applied Mathematics, 120, 175–195.
- [18] J. M. Ortega, (1972). Numerical Analysis: a second course, Academic Press inc.
- [19] S. Stojanovic (1991). Optimal damping control and nonlinear elliptic problem, SIAM J. Control Optim., 29, 594–608.
- [20] R. S. Varga (1962). *Matrix Iterative Analysis*, Prentice Hall inc.