Minimal invasion: An optimal L^∞ state constraint problem

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August 19, 2010

In this work, the least pointwise upper and/or lower bounds on the state variable on a specified subdomain of a control system under piecewise constant control action are sought. This results in a non-smooth optimization problem in function spaces. Introducing a Moreau-Yosida regularization of the state constraints, the problem can be solved using a superlinearly convergent semi-smooth Newton method. Optimality conditions are derived, convergence of the Moreau-Yosida regularization is proved, and well-posedness and superlinear convergence of the Newton method is shown. Numerical examples illustrate the features of this problem and the proposed approach.

1 Introduction

We consider the following relaxed L^∞-type control problem:

$$(\mathcal{P})\qquad \begin{cases} \min\limits_{c\in\mathbb{R},u\in\mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2}|u|_2^2 \\ \text{s.t. } Ay = f + \sum\limits_{i=1}^{m} u_i\chi_{\omega_i} & \text{in } \Omega, \\ -\beta_2 c + \psi_2 \leq y|_{\omega_0} \leq \beta_1 c + \psi_1 & \text{in } \omega_0. \end{cases}$$

Here $\alpha > 0$, Ω is a bounded domain in $\mathbb{R}^n$, A is a linear second order elliptic partial differential operator of convection-diffusion type carrying appropriate boundary conditions (to be made more explicit below), $\omega_i \subset \Omega$, $i = 0, \dots, m$ are subdomains and as such open and connected sets in Ω with characteristic functions

$$\chi_{\omega_i}(x) = \begin{cases} 1 & x \in \omega_i, \\ 0 & x \notin \omega_i, \end{cases}$$

and $f \in L^q(\Omega)$ for some $q < \max(2, n)$. Further

$$\beta_1, \beta_2 \in \mathbb{R} \text{ with } \beta_1, \beta_2 \geq 0 \quad \text{and} \quad \psi_1 \in L^\infty(\omega_0),\ \psi_2 \in L^\infty(\omega_0),$$

and we assume that $\beta_1 + \beta_2 > 0$ as well as $\max \psi_2 \leq \min \psi_1$. Furthermore, we assume that $\psi_1(\overline{x}) = \psi_2(\overline{x})$ for some $\overline{x} \in \overline{\omega}_0$, which can always be guaranteed by re-parametrization according to

$$\overline{\psi}_1 = \psi_1 + \beta_1 \overline{c}, \qquad \overline{\psi}_2 = \psi_2 - \beta_2 \overline{c},$$

where $\overline{c} = \frac{d}{\beta_1+\beta_2} \leq 0$ with $d = \max(\psi_2 - \psi_1) \leq 0$. Indeed, let $\overline{x} = \arg\max(\psi_2 - \psi_1)$. Then note that $\overline{\psi}_1 - \overline{\psi}_2 \leq 0$ and $\overline{\psi}_1(\overline{x}) - \overline{\psi}_2(\overline{x}) = 0$. Hence after re-parametrization it necessarily holds that $c \geq 0$.

To simplify notation, we introduce the control operator $B : \mathbb{R}^m \to L^\infty(\Omega)$,

$$Bu = \sum_{i=1}^{m} u_i \chi_{\omega_i}.$$

This problem can be given the following interpretation: A pollutant f enters the groundwater and is (diffusively and/or convectively) transported throughout the domain Ω. To minimize the concentration y of a pollutant in a city ω_0, wells $\omega_1, \ldots, \omega_m$ are placed in Ω, through which a counter-agent u_i can be introduced. The problem is therefore to minimize the upper bound c in the formulation $y|_{\omega_0} \leq c$, or, if the concentration is supposed to be non-negative, $0 \leq y|_{\omega_0} \leq c$. In general the concentration only satisfies inhomogeneous boundary conditions $\tilde{y} = g$ on $\partial\Omega$. To return to the formulation introduced above we transform to homogeneous boundary conditions by means of $y = \tilde{y} - g_{ext}$, where g_{ext} is a smooth extension of g into Ω. The resulting constraints on y are of the form $-g_{ext} \leq y \leq -g_{ext} + c$, and are a special case of the constrains considered above. The approach we present can readily be applied to a problem with a unilateral constraint on y.

In case $\beta_1 = \beta_2 = 1$ and $\psi_1 = \psi_2 = 0$ the inequality constraints in ($\mathcal{P}$) result in the norm constraint problem

$$\|y\|_{L^\infty(\omega_0)} \leq c.$$

which can equivalently be expressed as the following quadratic problem with affine constraints:

$$(1.1) \qquad \begin{cases} \min\limits_{u \in \mathbb{R}^m} \dfrac{1}{2} \|y\|^2_{L^\infty(\omega_0)} + \dfrac{\alpha}{2} |u|_2^2 \\ \text{s.t. } Ay = f + Bu. \end{cases}$$

Clearly ($\mathcal{P}$) is related to state-constrained optimal control problems but it is different since it involves c as a free variable. To find the smallest c such that the constraints in ($\mathcal{P}$) admit a feasible solution and such that the objective is minimized is the objective of this work. Note that for (1.1) with $f \neq 0$ it is required that $c > 0$ to guarantee that the constraint $\|y\|_{L^\infty(\omega_0)} \leq c$ is feasible.

Problem ($\mathcal{P}$) with $\omega_i = \Omega$ was treated in [3, 7]. In [3] a discretize before optimize approach was pursued so that phenomena due to lack of L^2- regularity of the Lagrange multipliers are not apparent. The work in [7] rests on an interior point treatment of the state constraints. In addition to the different treatment that we follow in this work, in the numerical examples we also focus on effects and the interpretation which result from the choice of the control and observation domains as proper subsets of Ω.

This article is organized as follows. In a short section 2 we present the regularization that we employ, prove existence and uniqueness of a solution to ($\mathcal{P}$) and establish the asymptotic behavior of the solutions to the regularized problems. Section 3 is devoted to the optimality systems for the original and the regularized problems. The semi-smooth Newton method and its analysis are considered in section 4, and the final section 5 contains numerical results.

2 Existence and regularization

This section is devoted to specifying the regularization that we use, and to establish existence and uniqueness results. We first address well-posedness of the state equation. We consider the operator

$$Ay = -\sum_{j,k=1}^{n} \partial_j (a_{jk}(x)\partial_k y + d_j(x)y) + \sum_{j=1}^{n} b_j(x)\partial_j y + d(x)y,$$

where the coefficients satisfy $a_{jk} \in C^{0,\delta}(\overline{\Omega})$ for some $\delta \in (0,1)$ and $b_j, d \in L^\infty(\Omega)$, and the corresponding Dirichlet problem

$$\begin{cases} Ay = g, & \text{in } \Omega, \\ y = 0, & \text{on } \partial\Omega, \end{cases} \tag{2.1}$$

where the domain Ω is open, bounded and of class $C^{1,\delta}$ and $g \in H^{-1}(\Omega)$ is given. If 0 is not an eigenvalue of A, this problem has a unique solution in $H_0^1(\Omega)$. A sufficient assumption for this is the existence of constants $\lambda, \Lambda\, \nu > 0$ such that

$$\begin{cases} \lambda|\xi|_2^2 \leq a_{jk}\xi_j\xi_k \quad \text{for all } \xi \in \mathbb{R}^n, & \displaystyle\sum_{j,k=1}^{n} |a_{j,k}|^2 \leq \Lambda^2, \\ \lambda^{-2}\displaystyle\sum_{j=1}^{n} \left(|d_j|^2 + |b_j|^2\right) + \lambda^{-1}|d| \leq \nu^2, & d - \partial_j d_j \geq 0, \quad \text{for all } 1 \leq j \leq n, \end{cases}$$

where the last inequality should be understood in the generalized sense (cf., e.g., [2, Th. 8.3]). Concerning the regularity of this solution, we have the following theorem [8, Th. 3.16]:

Proposition 2.1. *For each $g \in W^{-1,q}(\Omega)$ with $2 < q < \infty$, the solution y of (2.1) satisfies $y \in W_0^{1,q}(\Omega)$. Moreover, there exists a constant $C > 0$ independent of g such that*

$$\|y\|_{W^{1,q}(\Omega)} \leq C \|g\|_{W^{-1,q}(\Omega)} .$$

holds.

In particular, since $f \in L^q(\Omega)$ with $q > n$, this implies the existence of a unique solution $y \in W_0^{1,q}(\Omega)$ of the state equation $Ay = f + Bu$ for any control vector $u \in \mathbb{R}^m$. This affine solution mapping will be denoted by

$$y : \mathbb{R}^m \to W_0^{1,q}(\Omega), \text{ with } y(u) = A^{-1}(f + Bu).$$

Recalling the continuous embedding $W^{1,q}(\Omega) \hookrightarrow C(\overline{\Omega})$ for any $q > n$ we have moreover that $y \in C(\overline{\Omega})$.

To apply a semi-smooth Newton method, we introduce the Moreau-Yosida regularization of ($\mathcal{P}$), i.e. for $\gamma > 0$ we consider:

$$(\mathcal{P}_c) \qquad \begin{cases} \min\limits_{c \in \mathbb{R}, u \in \mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2} |u|_2^2 + \dfrac{\gamma}{2} \|\max(0, y|_{\omega_0} - (\beta_1 c + \psi_1))\|_{L^2}^2 \\ \qquad\qquad\qquad + \dfrac{\gamma}{2} \|\min(0, y|_{\omega_0} + \beta_2 c - \psi_2)\|_{L^2}^2 , \\ \text{s.t. } Ay = f + Bu. \end{cases}$$

For the case $\beta_1 = \beta_2 = 1$ and $\psi_1 = \psi_2 = 0$ this can be expressed compactly as

$$\begin{cases} \min\limits_{c \in \mathbb{R}, u \in \mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2} |u|_2^2 + \dfrac{\gamma}{2} \|\max(0, |y|_{\omega_0}| - c)\|_{L^2}^2, \\ \text{s.t. } Ay = f + Bu. \end{cases}$$

Proposition 2.2. *Problem ($\mathcal{P}$) admits a unique solution (c^*, u^*). Moreover, for every $\gamma > 0$ there exists a unique solution (c_γ, u_γ) to ($\mathcal{P}_c$). The associated states will be denoted by $y^* = y(u^*)$ and $y_\gamma = y(u_\gamma)$ respectively.*

Proof. Problem ($\mathcal{P}$) can equivalently be expressed as

$$\min_{u \in \mathbb{R}^m} J(u) = \min_{u \in \mathbb{R}^m} \frac{1}{2} \left[\operatorname*{ess\,sup}_{x \in \omega_0} \max \left(\frac{y - \psi_1}{\beta_1}, \frac{-y + \psi_2}{\beta_2} \right) \right]^2 + \frac{\alpha}{2} |u|_2^2,$$

where $J : \mathbb{R}^m \to \mathbb{R}$ is continuous and radially unbounded. The mapping

$$u \mapsto \operatorname*{ess\,sup}_{x \in \omega_0} \max \left(\frac{y(u) - \psi_1}{\beta_1}, \frac{-y(u) + \psi_2}{\beta_2} \right)$$

is convex and hence $u \mapsto J(u)$ is strictly convex. As a consequence ($\mathcal{P}$) has a unique solution with

$$0 \leq c^* = \operatorname*{ess\,sup}_{x \in \omega_0} \max \left(\frac{y(u^*) - \psi_1}{\beta_1}, \frac{-y(u^*) + \psi_2}{\beta_2} \right) .$$

An analogous argument implies the existence of a unique solution to ($\mathcal{P}_c$). □

We also define

$$\begin{cases} \lambda_\gamma = \lambda_{\gamma,1} + \lambda_{\gamma,2}, \\ \lambda_{\gamma,1} = \gamma \max(0, y_\gamma|_{\omega_0} - (\beta_1 c + \psi_1)), \quad \lambda_{\gamma,2} = \gamma \min(0, y_\gamma|_{\omega_0} + \beta_2 c - \psi_2), \end{cases}$$

which will turn out to be the regularized Lagrange multiplier associated to the inequality constraint on $y|_{\omega_0}$. Note that $\lambda_{\gamma,1} \geq 0$, $\lambda_{\gamma,2} \leq 0$ and that strict inequalities cannot hold simultaneously.

Proposition 2.3. *We have*

$$(c_\gamma, u_\gamma, y_\gamma) \to (c^*, u^*, y^*) \text{ in } \mathbb{R} \times \mathbb{R}^m \times W^{1,q}(\Omega),$$

and

$$\frac{1}{\sqrt{\gamma}} \|\lambda_\gamma\|_{L^2(\omega_0)} \to 0, \text{ as } \gamma \to \infty. \tag{2.2}$$

Proof. Due to the optimality of (c_γ, u_γ) we have

$$\frac{(c_\gamma)^2}{2} + \frac{\alpha}{2} |u_\gamma|_2^2 + \frac{1}{2\gamma} \|\lambda_\gamma\|^2_{L^2(\omega_0)} \leq \frac{(c^*)^2}{2} + \frac{\alpha}{2} |u^*|_2^2 . \tag{2.3}$$

Consequently

$$\{c_\gamma\}_{\gamma>0}, \ \{u_\gamma\}_{\gamma>0}, \ \{\frac{1}{\gamma} \|\lambda_\gamma\|^2_{L^2(\omega_0)}\}_{\gamma>0}, \ \{\|y_\gamma\|_{W^{1,q}}\}_{\gamma>0}$$

are bounded.

Thus there exists a sequence $\{\gamma_k\}$ and $(\hat{c}, \hat{u}, \hat{y}) \in \mathbb{R} \times \mathbb{R}^m \times W_0^{1,q}$ such that $(c_{\gamma_k}, u_{\gamma_k}, y_{\gamma_k})$ converges to $(\hat{c}, \hat{u}, \hat{y})$. Taking the limit (2.3) and in $Ay_{\gamma_k} - f - Bu_{\gamma_k} = 0$ we find that $(\hat{c}, \hat{u}, \hat{y})$ coincides with the unique solution (c^*, u^*, y^*) of ($\mathcal{P}$). Due to uniqueness of (c^*, u^*, y^*) the whole family $(c_\gamma, u_\gamma, y_\gamma)$ converges in $\mathbb{R} \times \mathbb{R}^m \times W^{1,q}(\Omega)$ to (c^*, u^*, y^*). Taking the limit in (2.3) implies (2.2). □

3 Optimality system

In this section we derive the optimality systems for ($\mathcal{P}$) and ($\mathcal{P}_c$) and the relationship between them.

We introduce the Lagrangian for the regularized problem

$$\begin{aligned} L(u, c, y, p) = \frac{c^2}{2} + \frac{\alpha}{2} |u|_2^2 + \frac{\gamma}{2} \|\max(0, y|_{\omega_0} - (\beta_1 c + \psi_1))\|^2_{L^2} \\ + \frac{\gamma}{2} \|\min(0, y|_{\omega_0} + \beta_2 c - \psi_2)\|^2_{L^2} + \langle p, Ay - f - Bu \rangle_{W_0^{1,q'}, W^{-1,q}}, \end{aligned}$$

where

$$L : \mathbb{R}^m \times \mathbb{R} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega) \to \mathbb{R}, \qquad \frac{1}{q} + \frac{1}{q'} = 1.$$

Since the linearized equality constraint in ($\mathcal{P}$) given by

$$(\overline{u}, \overline{y}) \mapsto A\overline{y} - B\overline{u}$$

is surjective, the necessary and sufficient optimality system for ($\mathcal{P}_c$) is found to be

$$\text{(3.1)} \qquad \begin{cases} \alpha u_{\gamma,i} - \langle p_\gamma, \chi_{\omega_i} \rangle & = 0, \quad i = 1, \ldots, m \\ c_\gamma - \langle \lambda_{\gamma,1}, \beta_1 \rangle + \langle \lambda_{\gamma,2}, \beta_2 \rangle & = 0, \\ A^* p_\gamma + \tilde{\lambda}_\gamma & = 0, \\ A y_\gamma - f - B u_\gamma & = 0 \end{cases}$$

where $\tilde{\lambda}_\gamma$ denotes the extension by zero to $\Omega \setminus \omega_0$ of λ_γ.

Theorem 3.1 (Optimality system for ($\mathcal{P}$))**.** *There exist $\lambda_i \in L^\infty(\omega_0)^*$, $i = 1, 2$, and $p^* \in W_0^{1,q'}(\Omega)$ such that*

$$\text{(3.2)} \qquad \begin{cases} \alpha u_i^* - \langle p^*, \chi_{\omega_i} \rangle = 0, \; i = 1, \ldots, m \\ c^* - \langle \lambda_1, \beta_1 \rangle_{(L^\infty)^*, L^\infty} + \langle \lambda_2, \beta_2 \rangle_{(L^\infty)^*, L^\infty} = 0, \\ \langle p^*, A\varphi \rangle + \langle \lambda_1 + \lambda_2, \varphi|_{\omega_0} \rangle_{(L^\infty)^*, L^\infty} = 0, \text{ for all } \varphi \in W_0^{1,q}(\Omega) \\ A y^* - f - B u^* = 0, \\ \langle \lambda_1, y^*|_{\omega_0} - (\beta_1 c^* + \psi_1) \rangle_{(L^\infty)^*, L^\infty} = 0, \; \langle \lambda_2, y^*|_{\omega_0} + (\beta_2 c^* - \psi_2 \rangle_{(L^\infty)^*, L^\infty} = 0, \\ \langle \lambda_1, \varphi \rangle_{(L^\infty)^*, L^\infty} \geq 0, \; \langle \lambda_2, \varphi \rangle_{(L^\infty)^*, L^\infty} \leq 0, \text{ for all } \varphi \in L^\infty(\Omega). \end{cases}$$

Moreover $\{p_\gamma, \lambda_\gamma\}_{\gamma > 0}$ is bounded in $W_0^{1,q'}(\Omega) \times L^1(\omega_0)$ and for every subsequence such that p_{γ_k} converges weakly in $W_0^{1,q'}(\Omega)$ and λ_{γ_k} converges weakly in $(L^\infty(\omega_0))^*$ the subsequential limits satisfy (3.2).*

Proof. Let $G : \mathbb{R}^m \times \mathbb{R} \to L^\infty(\omega_0) \times L^\infty(\omega_0)$ be defined by

$$G(u, c) = \begin{pmatrix} y(u)|_{\omega_0} - \beta_1 c - \psi_1 \\ -y(u)|_{\omega_0} - \beta_2 c + \psi_2 \end{pmatrix},$$

and

$$K = \{k \in L^\infty(\omega_0) : k \leq 0\}.$$

Then ($\mathcal{P}$) can be expressed in abstract form as

$$\min_{u\in\mathbb{R}^m, c\in\mathbb{R}} J(u,c) = \frac{1}{2}c^2 + \frac{\alpha}{2}\|u\|^2 \qquad \text{subject to } G(u,c) \in K \times K. \tag{3.3}$$

The regular point condition for (3.3) (cf. [6, 5]) is given by

$$0 \in \left\{G'(u^*,c^*)(\mathbb{R}^m \times \mathbb{R}) + G(u^*,c^*) - (K\times K)\right\}. \tag{3.4}$$

To verify (3.4) we consider for arbitrary $(g_1,g_2) \in \mathrm{L}^\infty(\omega_0) \times \mathrm{L}^\infty(\omega_0)$

$$\begin{pmatrix} A^{-1}(Bu)|_{\omega_0} - \beta_1 c \\ -A^{-1}(Bu)|_{\omega_0} - \beta_2 c\end{pmatrix} + \begin{pmatrix} y^*|_{\omega_0} - \beta_1 c^* - \psi_1 \\ -y^*|_{\omega_0} - \beta_2 c^* + \psi_2\end{pmatrix} - \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}. \tag{3.5}$$

Set $u = 0$ and

$$c = \max\left(\beta_1^{-1}\operatorname{ess\,sup}(-g_1), \beta_2^{-1}\operatorname{ess\,sup}(-g_2), 0\right).$$

Then the first coordinate in (3.5) is satisfied with

$$k_1 = -g_1 + y^*|_{\omega_0} - \beta_1 c^* - \psi_1 - \beta_1 c \le 0.$$

Similarly for the second coordinate we have

$$k_2 = -g_2 - y^*|_{\omega_0} - \beta_2 c^* + \psi_2 - \beta_2 c \le 0.$$

Hence there exist $(\lambda_1,\lambda_2) \in \mathrm{L}^\infty(\omega_0)^* \times \mathrm{L}^\infty(\omega_0)^*$ such that the last two lines in (3.2) hold.

For later reference we specify that the above argument implies that

$$\left\{\begin{array}{l} \text{for all } \rho > 0 \text{ there exists } M \ge 0 \text{ such that for all } g = (g_1,g_2) \in B_\rho \\ \ \text{there exists } (u,c,k_1,k_2) \text{ satisfying} \\ G'(u^*,c^*)(u,c) + G(u^*,c^*) - \begin{pmatrix} k_1 \\ k_2\end{pmatrix} = \begin{pmatrix} g_1 \\ g_2\end{pmatrix} \text{ and} \\ |(u,c,k_1 - y^*|_{\omega_0} + \beta_1 c^* + \psi_1, k_2 + y^*|_{\omega_0} + \beta_2 c^* - \psi_2)|_{\mathbb{R}^m\times\mathbb{R}\times\mathrm{L}^\infty\times\mathrm{L}^\infty} \le M\rho, \end{array}\right. \tag{3.6}$$

where $B_\rho = \{(g_1,g_2) \in \mathrm{L}^\infty \times \mathrm{L}^\infty : \|g_i\|_{\mathrm{L}^\infty} \le \rho\}$. In fact, $u = 0$ is possible.

We also have

$$J'(u^*,c^*) + \langle(\lambda_1,-\lambda_2), G'(u^*,c^*)\rangle_{(\mathrm{L}^\infty\times\mathrm{L}^\infty)^*,\mathrm{L}^\infty\times\mathrm{L}^\infty} = 0.$$

Exploiting this equality we find

$$c^* - \langle\lambda_1,\beta_1\rangle_{(\mathrm{L}^\infty)^*,\mathrm{L}^\infty} + \langle\lambda_2,\beta_2\rangle_{(\mathrm{L}^\infty)^*,\mathrm{L}^\infty} = 0,$$

which is the second equation in (3.2), and

$$\alpha u_i + \langle\lambda_1 + \lambda_2, A^{-1}(\chi_{\omega_i})|_{\omega_0}\rangle = 0, \text{ for all } i = 1,\ldots,m = 0.$$

Introducing the adjoint state as the solution to

$$\langle p^*, A\varphi\rangle + \langle \chi_{\omega_0}, (\lambda_1+\lambda_2)\varphi\rangle = 0, \text{ for all } \varphi \in C_0^\infty(\Omega)$$

provides the first and third equation in (3.2). Since $\lambda_1, \lambda_2 \in L^\infty(\omega_0)^*$ we have that $p^* \in W_0^{1,q'}(\Omega)$. This concludes the proof of the optimality system (3.2).

Next we argue that $\{\lambda_{\gamma,1}\}_{\gamma>0}$ and $\{\lambda_{\gamma,2}\}_{\gamma>0}$ are bounded in $L^1(\omega_0)$. For this purpose we set

$$\vec\lambda_\gamma = (\lambda_{\gamma,1}, -\lambda_{\gamma,2})^T = (\gamma \max(0, y_\gamma|_{\omega_0} - (\beta_1 c + \psi_1), -\gamma \min(0, y|_{\omega_0} + \beta_2 c - \psi_2))^T.$$

For $\rho > 0$ fixed choose $g = (g_1, g_2) \in B_\rho$ arbitrarily. Appealing to (3.6) for $-g$, there exists $(\tilde u, \tilde c, k)$, with $k = (k_1, k_2) \in K \times K$, such that for $(u, c) = (\tilde u + u^*, \tilde c + c^*)$,

$$-g = \big(G'(u^*, c^*)((u,c) - (u^*, c^*))\big) - (k - G(u^*, c^*))$$

holds. Taking the inner product with $\vec\lambda_\gamma$ we have

$$\begin{aligned} -\langle g, \vec\lambda_\gamma\rangle &= \big\langle G'(u_\gamma, c_\gamma)((u,c) - (u^*,c^*)), \vec\lambda_\gamma\big\rangle - \big\langle k - G(u^*,c^*)), \vec\lambda_\gamma\big\rangle \\ &= \big\langle G'(u_\gamma, c_\gamma)((u,c) - (u_\gamma,c_\gamma)), \vec\lambda_\gamma\big\rangle + \big\langle G'(u_\gamma, c_\gamma)((u_\gamma,c_\gamma) - (u^*,c^*)), \vec\lambda_\gamma\big\rangle \\ &\quad - \big\langle k, \vec\lambda_\gamma\big\rangle + \big\langle G(u^*,c^*) - G(u_\gamma,c_\gamma), \vec\lambda_\gamma\big\rangle + \big\langle G(u_\gamma,c_\gamma), \vec\lambda_\gamma\big\rangle. \end{aligned}$$

Note that $\langle k, \vec\lambda_\gamma\rangle \le 0$, $\langle G(u_\gamma, c_\gamma), \vec\lambda_\gamma\rangle \le 0$ and $J'(u_\gamma, c_\gamma) + G'(u_\gamma, \lambda_\gamma)^*\vec\lambda_\gamma = 0$. Therefore

$$\begin{aligned} \langle g, \vec\lambda_\gamma\rangle &\le \big\langle J'(u_\gamma, c_\gamma), (u,c) - (u_\gamma, c_\gamma)\big\rangle \\ &\qquad - \big\langle G'(u_\gamma,c_\gamma)((u_\gamma,c_\gamma) - (u^*,c^*)), \vec\lambda_\gamma\big\rangle - \big\langle G(u^*,c^*) - G(u_\gamma,c_\gamma), \vec\lambda_\gamma\big\rangle. \end{aligned}$$

Hence by (2.3) and (3.6) there exists $\tilde M$ independent of γ and (u, c) such that

$$\sup_{g\in B_\rho} \langle g, \vec\lambda_\gamma\rangle \le \tilde M\,(1 + \|\vec\lambda_\gamma\|_{L^1\times L^1}\, \|(u^*,c^*) - (u_\gamma,c_\gamma)\|).$$

Using (2.3) once again there exists $\hat M$ independent of γ such that

$$\sup_{g\in B_\rho} \langle g, \vec\lambda_\gamma\rangle \le \tilde M\,(1 + \|\vec\lambda_\gamma\|_{L^1\times L^1}).$$

This implies boundedness of $\{\|\lambda_{\gamma,1}\|_{L^1}\}_{\gamma>0}$ and $\{\|\lambda_{\gamma,2}\|_{L^1}\}_{\gamma>0}$. It follows that the sequence $\{\|p_\gamma\|_{W_0^{1,q'}}\}_{\gamma>0}$ is bounded as well. From Proposition 2.3 we recall that $(c_\gamma, u_\gamma, y_\gamma) \to (c^*, u^*, y^*)$ in $\mathbb{R} \times \mathbb{R}^m \times W^{1,q}(\Omega)$, and in particular $y_\gamma \to y^*$ in $C(\overline\Omega)$. Since $W_0^{1,q'}(\Omega)$ embeds compactly into $L^r(\Omega) \subset L^1(\Omega)$ for $r = \frac{\frac{nq}{q-1}}{n - \frac{q}{q-1}} = \frac{nq}{nq-(n+q)}$, there exist subsequences of p_γ, $\lambda_{\gamma_1}, \lambda_{\gamma_2}$, denoted by the same symbols, and $p^*, \lambda_1, \lambda_2$ such that $p_\gamma \to p^*$ weakly in $W^{1,q'}(\Omega)$ and strongly in $L^1(\Omega)$, and $\lambda_{\gamma,1}, \lambda_{\gamma,2}$ converge to λ_1, λ_2 weakly* in $L^\infty(\omega_0)^*$.

From (2.2) we have $0 = \lim_{\gamma\to\infty} \frac{1}{\gamma}\|\lambda_\gamma\|^2_{L^2(\omega_0)}$ and hence

$$0 = \lim_{\gamma\to\infty} \frac{1}{\gamma}\|\lambda_{\gamma,1}\|^2_{L^2(\omega_0)}, \qquad 0 = \lim_{\gamma\to\infty} \frac{1}{\gamma}\|\lambda_{\gamma,2}\|^2_{L^2(\omega_0)}.$$

Consequently

$$\begin{aligned} 0 &= \lim_{\gamma\to\infty} \langle \lambda_{\gamma,1}, \max(0, y_\gamma|_{\omega_0} - (\beta_1 c_\gamma + \psi)) \rangle \\ &= \lim_{\gamma\to\infty} \langle \lambda_{\gamma,1}, y_\gamma|_{\omega_0} - (\beta_1 c_\gamma + \psi) \rangle = \langle \lambda_1, y^*|_{\omega_0} - (\beta_1 c^* + \psi_1) \rangle_{(L^\infty)^*, L^\infty}. \end{aligned}$$

In a similar way one shows that $0 = \langle \lambda_2, y^*|_{\omega_0} + (\beta_2 c^* - \psi_2) \rangle_{(L^\infty)^*, L^\infty}$. This gives the fifth line of the optimality system (3.2). The remaining properties of the optimality system (3.2) can easily be obtained by passing to the limit in (3.1). □

Remark 3.2. The regularity of the Lagrange multipliers $\lambda_1, \lambda_2 \in L^\infty(\omega_0)^*$ is associated to the fact that the obstacle functions ψ_1, ψ_2 are in $L^\infty(\omega_0)$. If ψ_1, ψ_2 are taken in $C(\overline{\omega}_0)$, the above proof can be adapted to show that λ_1, λ_2 are bounded Radon measures in $C(\overline{\omega}_0)^*$.

Since the problem ($\mathcal{P}$) is strictly convex, the system (3.2) provides a sufficient optimality condition. In particular, the $(\overline{u}, \overline{c}, \overline{y})$ satisfying (3.2) are unique.

In the final result of this section we address the question of rate of convergence of the regularized solutions to the solution of the original problem as $\gamma \to \infty$.

Proposition 3.3. *We have*

$$\frac{1}{2}|c_\gamma - c^*|^2 + \frac{\alpha}{2}|u_\gamma - u^*|_2^2 = \mathcal{O}\left(\frac{1}{\gamma^{\frac{1-\theta}{1+\theta}}}\right),$$

where $\theta = \frac{nq}{nq+2(q-n)}$.

Proof. Let $z^1_\gamma = y_\gamma|_{\omega_0} - (\beta_1 c_\gamma + \psi_1)$ and $z^2_\gamma = y_\gamma|_{\omega_0} + (\beta_2 c_\gamma - \psi_2)$. Due to optimality of $(c_\gamma, u_\gamma, y_\gamma)$ we find

$$\frac{(c_\gamma)^2}{2} + \frac{\alpha}{2}|u_\gamma|_2^2 + \frac{\gamma}{2}\|\max(0, z^1_\gamma)\|^2_{L^2} + \frac{\gamma}{2}\|\min(0, z^2_\gamma)\|^2_{L^2} \le \frac{(c^*)^2}{2} + \frac{\alpha}{2}|u^*|_2^2. \tag{3.7}$$

We shall use the relationships

$$\begin{aligned} &\frac{(c_\gamma)^2}{2} - \frac{(c^*)^2}{2} + \frac{\alpha}{2}|u_\gamma|_2^2 - \frac{\alpha}{2}|u^*|_2^2 \\ &\qquad = (c_\gamma - c^*)c^* + \frac{1}{2}|c_\gamma - c^*|^2 + \alpha\langle u_\gamma - u^*, u^*\rangle + \frac{\alpha}{2}|u_\gamma - u^*|_2^2, \end{aligned} \tag{3.8}$$

and

$$\langle A(y_\gamma - y^*), p^*\rangle = \langle u_\gamma - u^*, B^* p^*\rangle = \alpha\langle u_\gamma - u^*, u^*\rangle, \tag{3.9}$$

and, using (3.2),

(3.10)

$$\begin{aligned}\langle A(y_\gamma - y^*), p^*\rangle &= -\langle \lambda_1, y_\gamma|_{\omega_0} - y^*|_{\omega_0}\rangle - \langle \lambda_2, y_\gamma|_{\omega_0} - y^*|_{\omega_0}\rangle \\ &= -\langle \lambda_1, y_\gamma|_{\omega_0} - (c_\gamma\beta_1 + \psi_1)\rangle - \beta_1\langle \lambda_1, c_\gamma - c^*\rangle + \langle \lambda_1, y^*|_{\omega_0} - (c^*\beta_1 + \psi_1)\rangle \\ &\quad - \langle \lambda_2, y_\gamma|_{\omega_0} + (c_\gamma\beta_2 - \psi_2)\rangle + \beta_2\langle \lambda_2, c_\gamma - c^*\rangle + \langle \lambda_2, y^*|_{\omega_0} + (c^*\beta_2 - \psi_2)\rangle \\ &= -\langle \lambda_1, z_\gamma^1\rangle - \langle \lambda_2, z_\gamma^2\rangle - c^*(c_\gamma - c^*).\end{aligned}$$

Combining (3.7), (3.8), (3.9), and (3.10), we obtain

$$\begin{aligned}\frac{1}{2}|c_\gamma - c^*|^2 + \frac{\alpha}{2}|u_\gamma - u^*|^2 &\le -(c_\gamma - c^*)c^* - \alpha\langle u_\gamma - u^*, u^*\rangle \\ &\quad - \frac{\gamma}{2}\|\max(0, z_\gamma^1)\|_{L^2}^2 - \frac{\gamma}{2}\|\min(0, z_\gamma^2)\|_{L^2}^2 \\ &= \langle \lambda_1, z_\gamma^1\rangle + \langle \lambda_2, z_\gamma^2\rangle \\ &\quad - \frac{\gamma}{2}\|\max(0, z_\gamma^1)\|_{L^2}^2 - \frac{\gamma}{2}\|\min(0, z_\gamma^2)\|_{L^2}^2 \\ &\le \|\lambda_1\|_{(L^\infty)^*}\,\|\max(0, z_\gamma^1)\|_{L^\infty} - \frac{\gamma}{2}\|\max(0, z_\gamma^1)\|_{L^2}^2 \\ &\quad + \|\lambda_2\|_{(L^\infty)^*}\,\|\min(0, z_\gamma^2)\|_{L^\infty} - \frac{\gamma}{2}\|\min(0, z_\gamma^2)\|_{L^2}^2 \end{aligned} \tag{3.11}$$

In the following estimates K denotes a generic constant, which is independent of $\alpha > 0$ and $\gamma > 0$. We use the estimate

$$\|\hat{z}\|_{L^\infty} \le K\|\hat{z}\|_{W^{1,q}}^{\theta}\,\|\hat{z}\|_{L^2}^{1-\theta},$$

for $\hat{z} = \max(0, z_\gamma^1)$, where $\theta = \frac{nq}{nq+2(q-n)}$, see e.g. [1, p. 141]. This further implies that

$$\|\hat{z}\|_{L^\infty} \le K\left(\frac{\|\lambda_1\|_{(L^\infty)^*}}{\gamma}\right)^{\frac{1-\theta}{2}}\|\hat{z}\|_{W^{1,q}}^{\theta}\left(\frac{\gamma}{\|\lambda_1\|_{(L^\infty)^*}}\right)^{\frac{1-\theta}{2}}\|\hat{z}\|_{L^2}^{1-\theta},$$

and

$$\|\hat{z}\|_{L^\infty} \le K\left(\frac{\|\lambda_1\|_{(L^\infty)^*}}{\gamma}\right)^{\frac{1-\theta}{1+\theta}}\|\hat{z}\|_{W^{1,q}}^{\frac{2\theta}{1+\theta}} + \frac{\gamma}{2\,\|\lambda_1\|_{(L^\infty)^*}}\|\hat{z}\|_{L^2}^2,$$

where we use that $\frac{1-\theta}{2} + \frac{1+\theta}{2} = 1$. Arguing similarly for $\hat{z} = \min(0, z_\gamma^2)$ and combining these estimates with (3.11) implies that

$$\frac{1}{2}|c_\gamma - c^*|^2 + \frac{\alpha}{2}|u_\gamma - u^*|_2^2 \le K\frac{1}{\gamma^{\frac{1-\theta}{1+\theta}}}\left(\|\lambda_1\|_{(L^\infty)^*}^{\frac{2}{1+\theta}}\|z_\gamma^1\|_{W^{1,q}}^{\frac{2\theta}{1+\theta}} + \|\lambda_2\|_{(L^\infty)^*}^{\frac{2}{1+\theta}}\|z_\gamma^2\|_{W^{1,q}}^{\frac{2\theta}{1+\theta}}\right).$$

Since $\{y_\gamma\}_{\gamma\ge 1}$ is bounded in $W^{1,q}(\Omega)$ this implies the claim. □

In the case $n = 2$ we find that $\theta = \frac{q}{2q-4}$ and so we obtain the convergence rate $\mathcal{O}(\frac{1}{\gamma^{1/3-\epsilon}})$ for any $\epsilon > 0$, provided that q is sufficiently large. For $n = 2$, using solutions $y_\gamma \in H^2(\Omega)$, the above proof can also be adapted to obtain the rate $\mathcal{O}(\gamma^{-1/3})$.

4 Semi-smooth Newton Method

This section is devoted to the solution of the optimality system (3.1) by a semi-smooth Newton method. For this purpose we define

$$F : \mathbb{R}^m \times \mathbb{R} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega) \to \mathbb{R}^m \times \mathbb{R} \times W^{-1,q'}(\Omega) \times W^{-1,q}(\Omega)$$

by

(4.1)

$$F(u,c,y,p) = \begin{pmatrix} \alpha u - \langle p, \vec{\chi}_\omega \rangle \\ c - \gamma \langle \beta_1, \max(0, y|_{\omega_0} - (\beta_1 c + \psi_1)) \rangle + \gamma \langle \beta_2, \min(0, y|_{\omega_0} + \beta_2 c - \psi_2) \rangle \\ \gamma \widetilde{\max}(0, y|_{\omega_0} - (\beta_1 c + \psi_1)) + \gamma \widetilde{\min}(0, y|_{\omega_0} + \beta_2 c - \psi_2) + A^* p \\ Ay - Bu \end{pmatrix},$$

where we have set

$$\langle \vec{\chi}_\omega, \overline{p} \rangle = (\langle \chi_{\omega_1}, \overline{p} \rangle, \ldots, \langle \chi_{\omega_m}, \overline{p} \rangle)^T,$$

and $\widetilde{\max}$, $\widetilde{\min}$ denote extensions by zero from ω_0 to $\Omega \setminus \omega_0$. Recall from [5] that $z \mapsto \max(0,z)$ is Newton differentiable from $L^{p_1}(\Omega) \to L^{p_2}(\Omega)$ provided that $1 \leq p_1 < p_2 \leq \infty$ with Newton derivative given in the a.e. sense by

$$D \max(0,z) = \begin{cases} 1, & \text{if } z(x) \geq 0 \\ 0, & \text{if } z(x) < 0. \end{cases}$$

An analogous statement holds for the min operation. It follows that

$$G_1(y,c) = \widetilde{\max}(0, y|_{\omega_0} - (\beta_1 c + \psi_1))$$

is Newton differentiable for fixed c from $W_0^{1,q}(\Omega) \to W^{-1,q'}(\Omega)$ with Newton derivative with respect to y given by

$$D_y G_1(y,c)\, \overline{y} = \overline{\chi}\, \overline{y},$$

where $\overline{\chi}$ is given in the a.e. sense by

(4.2) $$\overline{\chi} = \overline{\chi}(y,c) = \begin{cases} 1, & \text{if } x \in \omega_0 \text{ and } y|_{\omega_0}(x) - (\beta_1 c + \psi_1(x)) > 0, \\ 0, & \text{otherwise.} \end{cases}$$

Analogously

$$G_2(y,c) = \widetilde{\min}(0, y|_{\omega_0} + \beta_2 c - \psi_2)$$

is Newton differentiable for fixed c from $W_0^{1,q}(\Omega) \to W^{-1,q'}(\Omega)$ with Newton derivative with respect to y given by

$$D_y G_2(y,c)\, \overline{y} = \underline{\chi}\, \overline{y},$$

where $\underline{\chi}$ is given in the a.e. sense by

$$\underline{\chi} = \underline{\chi}(y,c) = \begin{cases} 1, & \text{if } x \in \omega_0 \text{ and } y|_{\omega_0}(x) + \beta_2 c - \psi_2(x) < 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.3}$$

Let us also consider the mappings $H_1, H_2 : W_0^{1,q}(\Omega) \times \mathbb{R} \to \mathbb{R}$, defined by

$$H_1(y,c) = \langle \beta_1, \max(0, y|_{\omega_0} - (\beta_1 c + \psi_1)) \rangle_{L^2(\omega_0)} = \langle \beta_1, \widetilde{\max}(0, y|_{\omega_0} - (\beta_1 c + \psi_1)) \rangle_{L^2(\Omega)}$$

and

$$H_2(y,c) = \langle \beta_2, \widetilde{\min}(0, y|_{\omega_0} + (\beta_2 c - \psi_2)) \rangle_{L^2(\Omega)}.$$

Their Newton derivatives with respect to y are found to be

$$D_y H_1(y,c)\,\overline{y} = \beta_1 \langle \overline{\chi}, \overline{y} \rangle, \qquad D_y H_2(y,c)\,\overline{y} = \beta_2 \langle \underline{\chi}, \overline{y} \rangle.$$

Similarly, we obtain

$$D_c G_1(y,c)\overline{c} = \beta_1 \overline{\chi} \overline{c},$$

and

$$D_c H_1(y,c)\overline{c} = \beta_1^2 \langle \overline{\chi} \rangle \overline{c},$$

where $\langle z \rangle = \int_\Omega z\,dx$. One proceeds analogously for $D_c G_2$ and $D_c H_2$.

All together the Newton derivative of F at an arbitrary point $(u,c,y,p) \in \mathbb{R}^{m+1} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega)$ is given by

$$DF(u,c,y,p)(\overline{u},\overline{c},\overline{y},\overline{p}) = \begin{pmatrix} \alpha\overline{u} - \langle \overline{p}, \vec{\chi}_\omega \rangle \\ (1 + \gamma\beta_1^2 \langle \overline{\chi} \rangle + \gamma\beta_2^2 \langle \underline{\chi} \rangle)\overline{c} - \gamma\beta_1 \langle \overline{\chi}, \overline{y} \rangle + \gamma\beta_2 \langle \underline{\chi}, \overline{y} \rangle \\ -\gamma\beta_1 \overline{\chi}\overline{c} + \gamma\beta_2 \underline{\chi}\overline{c} + \gamma\overline{\chi}\overline{y} + \gamma\underline{\chi}\overline{y} + A^*\overline{p} \\ A\overline{y} - B\overline{u} \end{pmatrix}, \tag{4.4}$$

where we have assumed that $c > 0$ holds. A semi-smooth Newton step is given by

$$DF(u,c,y,p)(\overline{u},\overline{c},\overline{y},\overline{p}) = -F(u,c,y,p).$$

We next address its well-posedness.

Proposition 4.1. *For each $(u,c,y,p) \in \mathbb{R}^m \times \mathbb{R} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega)$, the mapping $DF(u,c,y,p)$ is invertible, and there exists a constant $C > 0$ independent of (u,c,y,p) such that*

$$\|DF(u,c,y,p)^{-1}\|_{\mathcal{L}(\mathbb{R}^{m+1} \times W^{-1,q'} \times W^{-1,q},\, \mathbb{R}^{m+1} \times W_0^{1,q} \times W_0^{1,q'})} \leq C.$$

Proof. For $w = (w_1, \ldots, w_4)^T \in \mathbb{R}^m \times \mathbb{R} \times W^{-1,q'}(\Omega) \times W^{-1,q}(\Omega)$ we consider the equation $DF(u,c,y,p)(\overline{u}, \overline{c}, \overline{y}, \overline{p}) = w$, i.e.,

$$\text{(4.5)} \qquad \begin{cases} \alpha\overline{u} - \langle \vec{\chi}_\omega, \overline{p} \rangle & = w_1 \\ (1 + \gamma\beta_1^2 \langle \overline{\chi} \rangle + \gamma\beta_2^2 \langle \underline{\chi} \rangle)\overline{c} - \gamma\beta_1 \langle \overline{\chi}, \overline{y} \rangle + \gamma\beta_2 \langle \underline{\chi}, \overline{y} \rangle & = w_2 \\ -\gamma\beta_1\overline{\chi}\overline{c} + \gamma\beta_2\underline{\chi}\overline{c} + \gamma\overline{\chi}\overline{y} + \gamma\underline{\chi}\overline{y} + A^*\overline{p} & = w_3 \\ -B\overline{u} + A\overline{y} & = w_4. \end{cases}$$

Therefore from the third and fourth equation in (4.5), we obtain

$$\overline{y} = A^{-1}(B\overline{u}) + A^{-1}w_4 = A^{-1}(B\overline{u}) + r_1,$$

$$\begin{aligned} \overline{p} &= A^{-*}\big(w_3 + \gamma\overline{c}(\beta_1\overline{\chi} - \beta_2\underline{\chi}) - \gamma\overline{y}(\overline{\chi} + \underline{\chi})\big) \\ &= A^{-*}\big(w_3 + \gamma\overline{c}(\beta_1\overline{\chi} - \beta_2\underline{\chi}) - \gamma A^{-1}(B\overline{u})(\overline{\chi} + \underline{\chi}) - \gamma(\overline{\chi} + \underline{\chi}\rangle A^{-1}w_4 \\ &= \gamma\overline{c}A^{-*}(\beta_1\overline{\chi} - \beta_2\underline{\chi}) - \gamma A^{-*}((\overline{\chi} + \underline{\chi})A^{-1}(Bu)) + r_2, \end{aligned}$$

where

$$r_1 = A^{-1}w_4 \in W_0^{1,q}(\Omega) \qquad r_2 = A^{-*}(w_3 - \gamma(\overline{\chi} + \underline{\chi})A^{-1}w_4) \in W_0^{1,q'}(\Omega).$$

Using these representations for $\overline{y}, \overline{p}$ in the first two equations of (4.5) we obtain for $\overline{u}, \overline{c}$ and $i = 1, \ldots, m$

$$\begin{cases} \alpha\overline{u}_i - \gamma\overline{c}\langle \chi_{\omega_i}, A^{-*}(\beta_1\overline{\chi} - \beta_2\underline{\chi}) \rangle + \gamma \sum_{j=1}^m \overline{u}_j \langle (A^{-1}\chi_{\omega_i})(\overline{\chi} + \underline{\chi}), A^{-1}\chi_{\omega_j} \rangle - \langle \chi_{\omega_i}, r_2 \rangle = w_{1,i}, \\ (1 + \gamma(\beta_1^2\langle \overline{\chi} \rangle + \beta_2^2 \langle \underline{\chi} \rangle))\overline{c} - \gamma \sum_{j=1}^m \overline{u}_j \langle \beta_1\overline{\chi} - \beta_2\underline{\chi}, A^{-1}\chi_{\omega_j} \rangle - \gamma\langle \beta_1\overline{\chi} - \beta_2\underline{\chi}, r_1 \rangle = w_2, \end{cases}$$

equivalently in matrix form

(4.6)

$$\begin{pmatrix} \alpha I + \gamma\langle \vec{\psi}, (\overline{\chi} + \underline{\chi})\vec{\psi} \rangle & -\gamma\langle \vec{\psi}, \beta_1\overline{\chi} - \beta_2\underline{\chi} \rangle \\ -\gamma\langle \beta_1\overline{\chi} - \beta_2\underline{\chi}, \vec{\psi} \rangle & 1 + \gamma(\beta_1^2\langle \overline{\chi} \rangle + \beta_2^2\langle \underline{\chi} \rangle) \end{pmatrix} \begin{pmatrix} \overline{u} \\ \overline{c} \end{pmatrix} = \begin{pmatrix} w_1 + \langle \vec{\chi}_\omega, r_2 \rangle \\ \gamma\langle \beta_1\overline{\chi} - \beta_2\underline{\chi}, r_1 \rangle + w_2 \end{pmatrix},$$

where I is the $m \times m$ identity matrix,

$$\psi_i = A^{-1}\chi_{\omega_i}, \quad \vec{\psi} = (\psi_1, \ldots, \psi_m)^T,$$

and

$$(\langle \vec{\psi}, (\overline{\chi} + \underline{\chi})\vec{\psi} \rangle)_{i,j} = \langle \vec{\psi}_i, (\overline{\chi} + \underline{\chi})\vec{\psi}_j \rangle.$$

The matrix on the left hand side of (4.6) can be expressed as

$$M = M_1 + \gamma M_2 + \gamma M_3,$$

where

$$M_1 = \begin{pmatrix} \alpha I & 0 \\ 0 & 1 \end{pmatrix}, \; M_2 = \begin{pmatrix} \langle \vec{\psi}, \overline{\chi}\vec{\psi} \rangle & -\beta_1 \langle \vec{\psi}, \overline{\chi} \rangle \\ -\beta_1 \langle \vec{\psi}, \overline{\chi} \rangle & \beta_1^2 \langle \overline{\chi} \rangle \end{pmatrix}, \; M_3 = \begin{pmatrix} \langle \vec{\psi}, \underline{\chi}\vec{\psi} \rangle & \langle \beta_2 \vec{\psi}, \underline{\chi} \rangle \\ \langle \beta_2 \vec{\psi}, \underline{\chi} \rangle & \beta_2^2 \langle \underline{\chi} \rangle \end{pmatrix}.$$

We next argue that the symmetric matrix M_2 is positive semi-definite. For $\langle \overline{\chi} \rangle = 0$, this is straight-forward. Henceforth assume that $\langle \overline{\chi} \rangle \neq 0$ and let $(\overline{u}, \overline{c}) \in \mathbb{R}^{m+1}$ be arbitrary.

Then we have, using that $2ab + b^2 \geq -a^2$,

$$\begin{aligned} (\overline{u}^T, \overline{c}) M_2 (\overline{u}^T, \overline{c})^T &= \overline{u}^T \langle \vec{\psi}, \overline{\chi}\vec{\psi} \rangle \, \overline{u} - 2\beta_1 \overline{c} \langle \vec{\psi}, \overline{\chi} \rangle^T \overline{u} + \beta_1^2 \langle \overline{\chi} \rangle \, \overline{c}^2 \\ &\geq \overline{u}^T \langle \vec{\psi}, \overline{\chi}\vec{\psi} \rangle \, \overline{u} - \frac{1}{\langle \overline{\chi} \rangle} \overline{u}^T \langle \vec{\psi}, \overline{\chi} \rangle \, \langle \vec{\psi}, \overline{\chi} \rangle^T \overline{u} = \overline{u}^T \mathcal{M}_2 \overline{u}, \end{aligned}$$

where

$$(\mathcal{M}_2)_{i,j} = \langle \vec{\psi}_i, \overline{\chi} \vec{\psi}_j \rangle \; - \frac{1}{\langle \overline{\chi} \rangle} \langle \vec{\psi}_i, \overline{\chi} \rangle \langle \vec{\psi}_j \, , \overline{\chi} \rangle.$$

The diagonal elements of $\mathcal{M}_2$ are given by

$$(\mathcal{M}_2)_{i,i} = \langle \psi_i, \overline{\chi} \psi_i \rangle - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_i, \overline{\chi} \rangle^2 = \| (\psi_i - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_i, \overline{\chi} \rangle) \overline{\chi} \|_{L^2}^2,$$

and for the off-diagonal elements we find

$$(\mathcal{M}_2)_{i,j} = \langle \psi_i, \overline{\chi} \psi_j \rangle - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_i, \overline{\chi} \rangle \, \langle \psi_j, \overline{\chi} \rangle = \big\langle \; \psi_i - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_i, \overline{\chi} \rangle, (\psi_j - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_j, \overline{\chi} \rangle) \overline{\chi} \; \big\rangle.$$

Therefore we have

$$(\mathcal{M}_2)_{i,j} = \big\langle \; \psi_i - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_i, \overline{\chi} \rangle, (\psi_j - \frac{1}{\langle \overline{\chi} \rangle} \langle \psi_j, \overline{\chi} \rangle) \overline{\chi} \; \big\rangle.$$

Consequently $\mathcal{M}_2$ is a Gramian matrix and thus positive semi-definite, and we find that the same holds true for M_2. Analogously one argues that M_3 is positive semi-definite. All together we obtain

$$\| M^{-1} \|_{\mathbb{R}^{(m+1)\times(m+1)}} \leq \max(\frac{1}{\sqrt{\alpha}}, 1).$$

This estimate is independent of $\overline{\chi}, \underline{\chi}, \omega_i, \omega_0$.

Using (4.6) there exist constants C_1 and C_2 such that

$$|(\overline{u}, \overline{c})|_{\mathbb{R}^{m+1}} \leq C_1 |w|_{\mathbb{R}^{m+1} \times W_0^{-1,q'} \times W_0^{-1,q}}$$

and

$$|(\overline{y}, \overline{p})|_{W_0^{1,q} \times W_0^{1,q'}} \leq C_2 |w|_{\mathbb{R}^{m+1} \times W_0^{-1,q'} \times W_0^{-1,q}}$$

hold. This implies the claim. □

Algorithm 1 Semi-smooth Newton method

1: Choose x^0, γ^0, $0 < \tau < 1$, $\varepsilon > 0$, k^*; set $j = 0$
2: **repeat**
3: Increment $j \leftarrow j + 1$
4: Set $x_0 = x^{j-1}$, $k = 0$
5: **repeat**
6: Increment $k \leftarrow k + 1$
7: Compute indicator function of active sets : $\overline{\chi}(y_{k-1}, c_{k-1})$, $\underline{\chi}(y_{k-1}, c_{k-1})$ from (4.2) and (4.3)
8: Solve for δx:
$$DF(x_{k-1})\delta x = -F(x_{x-1}),$$
where F and DF are given by (4.1) and (4.4), respectively
9: Update $x_k = x_{k-1} + \delta x$
10: **until** $\overline{\chi}(y_{k-1}, c_{k-1}) = \overline{\chi}(y_{k-2}, c_{k-2})$ and $\underline{\chi}(y_{k-1}, c_{k-1}) = \underline{\chi}(y_{k-2}, c_{k-2})$, or $k = k^*$
11: Set $x^j = x_k$
12: Set $\gamma^j = \tau\gamma^{j-1}$
13: **until** $\sup_{x\in\omega_0}(y - (\beta_1 c + \psi_1)) < \varepsilon$ and $\inf_{x\in\omega_0}(y + \beta_2 c - \psi_2) < \varepsilon$

Thus F is semi-smooth, and from standard results (e.g., [5, Th. 8.16]) we deduce the following convergence result for the semi-smooth Newton method. For convenience we set

$$x = (u, c, y, p) \in \mathbb{R}^m \times \mathbb{R} \times W_0^{1,q}(\Omega) \times W_0^{1,q'}(\Omega),$$

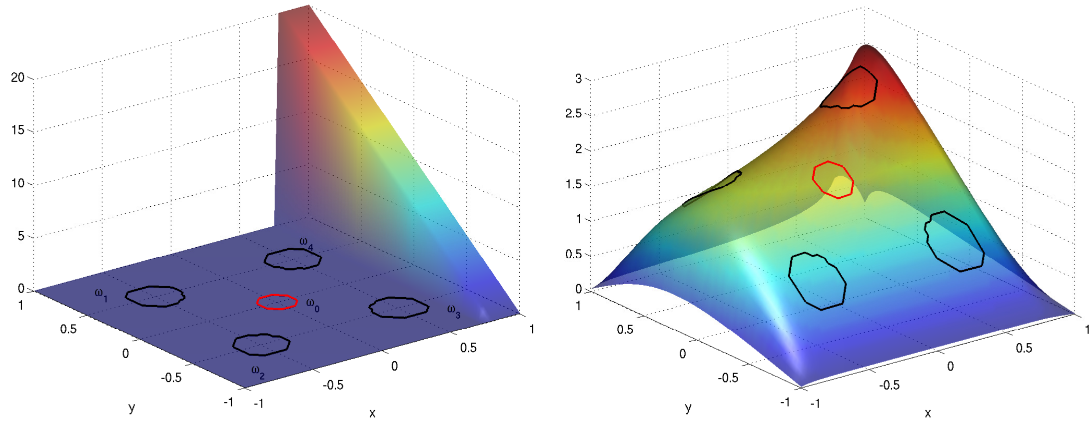
and similarly x_k, δx et cetera.

Theorem 4.2. *For each $\gamma > 0$ the iteration $DF(x_{k-1})(x_k - x_{k-1}) = -F(x_{k-1})$ converges superlinearly to $x_\gamma = (u_\gamma, c_\gamma, y_\gamma, p_\gamma)$ provided that x_0 is sufficiently close to x_γ.*

The full procedure for the solution of problem ($\mathcal{P}_c$) is given as Algorithm 1. Note that Algorithm 1 contains as inner loop the semi-smooth Newton method and as outer loop the increase of the penalty parameter γ. The convergence of these two processes was analyzed in Theorem 4.2 and Proposition 2.3 respectively. Here we choose a simple strategy for increasing γ. In related contexts [4] we proposed a path-following technique which could be adapted to the present situation. The termination criterion in step 10 is motivated by the following property of the semi-smooth Newton method.

Proposition 4.3. *If $\overline{\chi}(y_{k+1}, c_{k+1}) = \overline{\chi}(y_k, c_k)$ and $\underline{\chi}(y_{k+1}, c_{k+1}) = \underline{\chi}(y_k, c_k)$ holds, then x_{k+1} satisfies $F(x_{k+1}) = 0$.*

This can be verified by simple inspection, and is shown in [5, Rem. 7.1.1].



(a) Geometric setup. (b) Uncontrolled state y^0.

Figure 1: Model problem. The left plot shows the pollutant f, while the circles give the observation domain ω_0 (red) and the control domains $\omega_1, \ldots, \omega_4$ (black). The right plot shows the uncontrolled state $y^0 = A^{-1}f$.

5 Numerical results

Here we give the results of some numerical tests for a model problem in two dimensions. The geometric situation is given in Figure 1a: The circular observation domain ω_0 (the "town") is situated in the center of the unit square $[-1,1]^2$. On one side, a contaminant given by the function $f = 100(1+y)\chi_{\{x>.75\}}$ enters the domain. Around the town, $m = 4$ control domains ("wells") are spaced equally. We consider convective-diffusive transport, which is described by the operator $Ay = -\nu\Delta y + b \cdot \nabla y$ with $\nu = 0.1$ and $b = (-1,0)^T$ (i.e., transport parallel to the x-axis away from the source) with homogeneous Dirichlet conditions. The uncontrolled state y^0, which solves $Ay^0 = f$, is shown in Figure 1b.

The parameters were set to $x^0 = 0$, $\gamma^0 = 1$, $\tau = 0.1$, and $\varepsilon = 10^{-9}$. The penalty parameter was set to $\alpha = 10^{-6}$. The differential operators were discretized by finite differences with $N = 64$ grid points. We give results for $\psi_1 = \psi_2 = 0$. Since the convergence behavior is very similar in all test cases, we only show details for the motivating example of optimal L^∞-constraints, §5.3. A MATLAB code implementing the algorithm for these examples can be downloaded from http://www.uni-graz.at/~clason/codes/mininvasion.zip.

5.1 Unilateral constraint

We begin by considering the motivating example, which is the unilaterally constrained problem

$$\begin{cases} \min\limits_{c\in\mathbb{R},u\in\mathbb{R}^m} \dfrac{c^2}{2} + \dfrac{\alpha}{2}\,|u|_2^2 \\ \text{s.t. } Ay = f + Bu, \qquad y|_{\omega_0} \le c. \end{cases}$$

The numerical solution can be obtained using the above algorithm by simply dropping the min terms and setting all corresponding active sets to zero. Algorithm 1 terminated at $\gamma^* = 10^6$, using at most 8 (for $\gamma = 1$) Newton iterations. The computed optimal control is $u^* = (-0.0418744, -0.037166, -25.3717, -29.2032)^T$ (shown in Fig. 2c), which results in a minimal norm bound $c^* = 8.33217 \cdot 10^{-4}$. Correspondingly, the maximum value of y^* on ω_0 is $8.33217 \cdot 10^{-4}$, while its minimum value is -0.565084 (cf. Figs. 2a, 2b). It can be seen that only the controls acting on the control domains located between the source and the observation domain are active. For completeness, we also show the Lagrange multiplier p^* for the pde constraint in Fig. 2d.

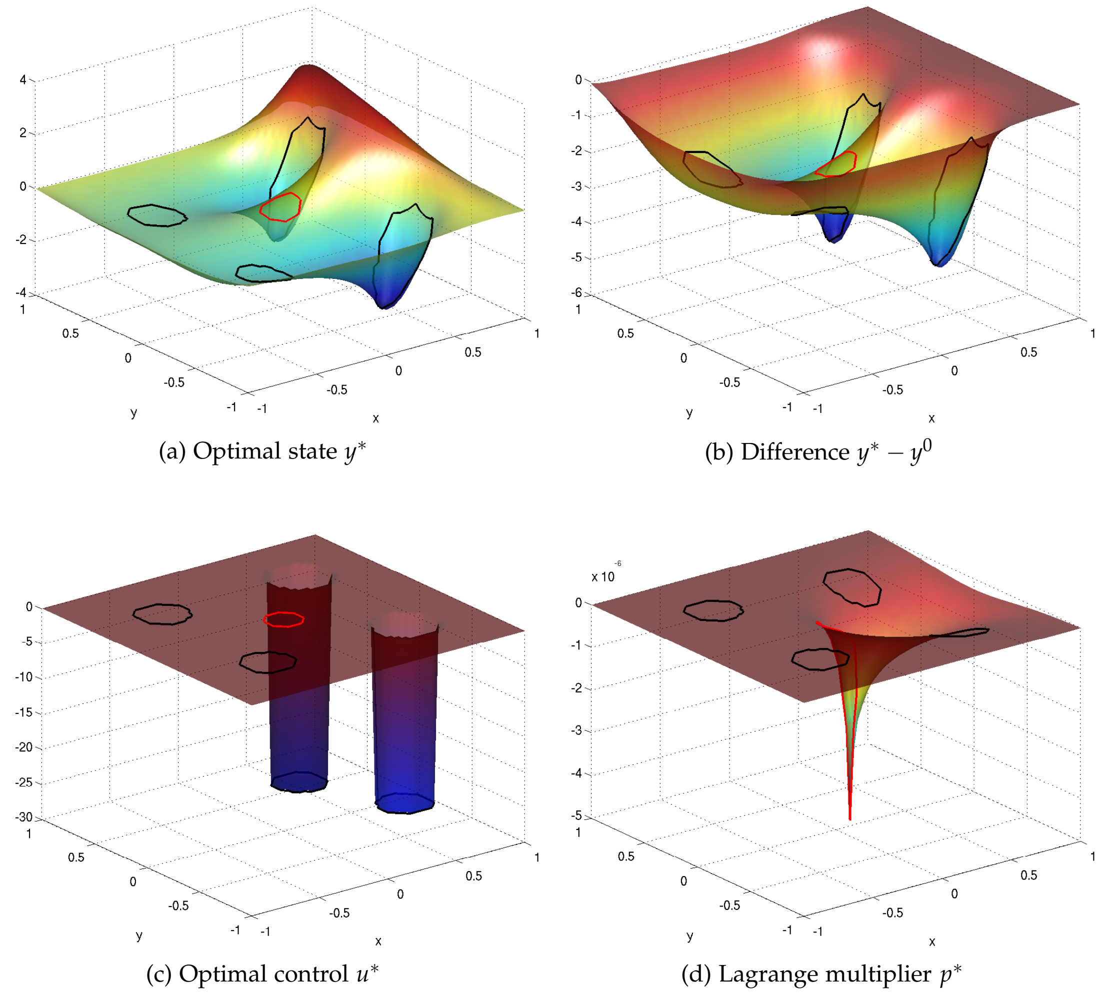
5.2 Non-negativity constraint

We next consider the case of minimizing an upper bound, while enforcing non-negativity of the state, i.e., we set $\beta_1 = 1$ and $\beta_2 = 0$. Again, Algorithm 1 terminated at $\gamma^* = 10^9$, after at most 7 Newton iterations. The computed optimal control is $u^* = (70.5931, 58.8345, -17.0403, -26.6347)^T$, which results in a minimal upper bound $c^* = 0.350723$ and identical maximal value of y^* on ω_0. The minimal value of y^* on ω_0 is $-1.67788 \cdot 10^{-10}$, within the prescribed tolerance of $\varepsilon = 10^{-9}$. Optimal state y^*, difference $y^* - y^0$, optimal control u^* and Lagrange multiplier p^* are shown in Figure 3.

We note that due to the non-negativity constraint, the controls near the contaminant inflow cannot act as strongly as in example 5.1, and that the optimal control is no longer uniformly negative. Thus the achievable upper bound is larger than in example 5.1.

5.3 L^∞ norm constraint

Finally, we consider the case $\beta_1 = \beta_2 = 1$, i.e., the L^∞ norm constraint problem (1.1). The iteration terminated at $\gamma^* = 10^9$, using at most 7 (for $c = 1$) Newton iterations. Table 1 shows the distance $d(\gamma) := \frac{1}{2}|c_\gamma - c_{\gamma^*}|^2 + \frac{\alpha}{2}|u_\gamma - u_{\gamma^*}|_2^2$, which indicates that the convergence rate proved in Proposition 3.3 is not optimal. For $\gamma = 1$, the norm of the residuals $|F(x_k)|_2$ in the semi-smooth Newton method is given in Table 2, verifying the locally superlinear convergence shown in Theorem 4.2. The computed optimal control is $u^* = (22.4538, 18.7443, -19.272, -28.7974)^T$ which results in a minimal norm bound $c^* = 0.202759$. The corresponding maximum and minimum value of y^* on ω_0 is 0.202759 (a difference of -1.70265 compared to the maximum of the uncontrolled state y^0) and -0.202759, respectively. Again, optimal state y^*, difference $y^* - y^0$, optimal control u^* and Lagrange multiplier p^* are shown in Figure 4.



(a) Optimal state y^* (b) Difference $y^* - y^0$

(c) Optimal control u^* (d) Lagrange multiplier p^*

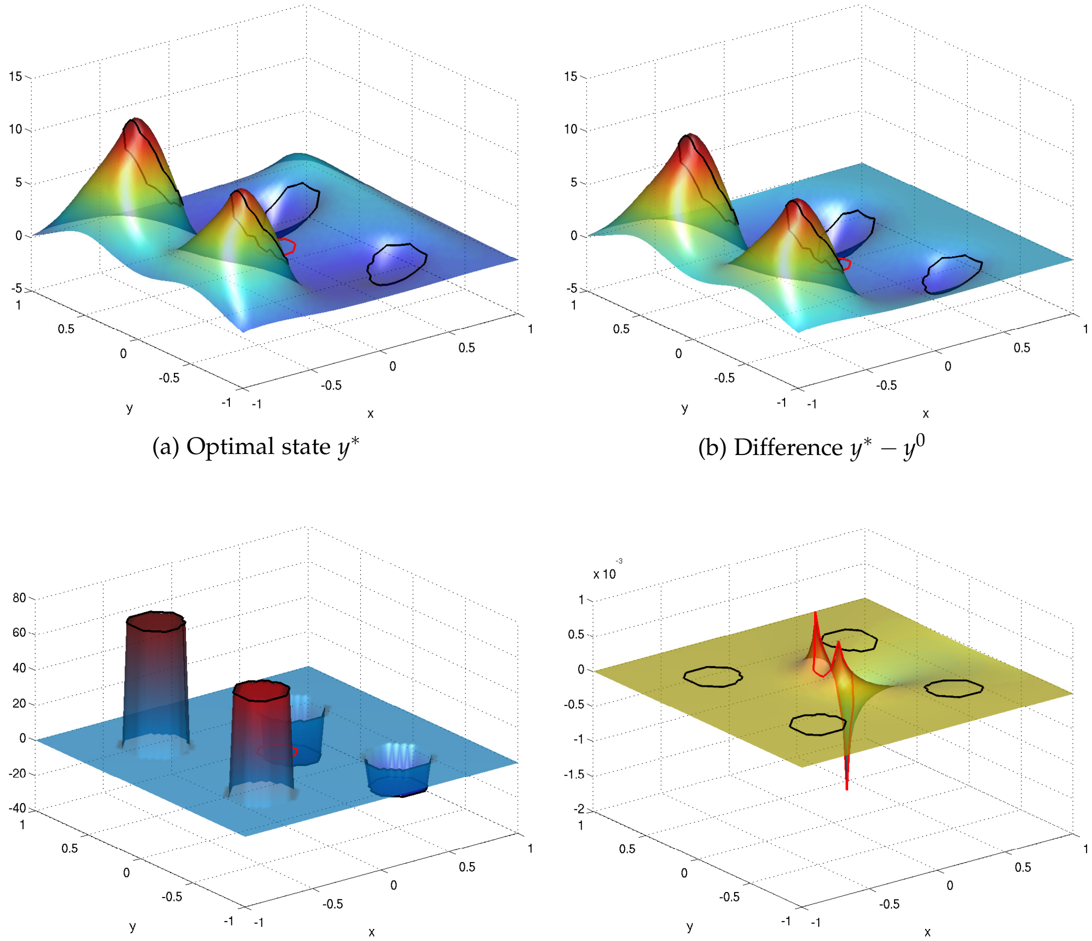
Figure 2: Results for unilateral constraint ($y|_{\omega_0} \leq c$).

Table 1: Convergence in γ. Shown are the distances $d(\gamma) := \frac{1}{2}|c_\gamma - c_{\gamma^*}|^2 + \frac{\alpha}{2}|u_\gamma - u_{\gamma^*}|_2^2$.

γ	1e0	1e1	1e2	1e3	1e4	1e5	1e6	1e7	1e8
$d(\gamma)$	5.11e-4	1.85e-5	3.34e-7	3.37e-9	3.37e-11	3.37e-13	3.37e-15	3.30e-17	2.73e-19

Acknowledgments

The research of the first and last named authors was supported in part by the Austrian Science Fund (FWF) under grant SFB F32 (SFB "Mathematical Optimization and Applications in Biomedical Sciences"). The research of the second named author was partially supported by the Army Research Office under DAAD19-02-1-0394.



(a) Optimal state y^*

(b) Difference $y^* - y^0$

(c) Optimal control u^*

(d) Lagrange multiplier p^*

Figure 3: Results for upper bound minimization with non-negativity constraint ($\beta_1 = 1$, $\beta_2 = 0$).

Table 2: Convergence of semi-smooth Newton method. Shown is the norm of the residual of (4.1) for the iterates x_k.

k	0	1	2	3	4	5	6
$\lvert F(x_k)\rvert_2$	2.62e+2	9.12e+1	1.34e+0	7.63e-1	3.26e-1	7.07e-2	2.85e-12

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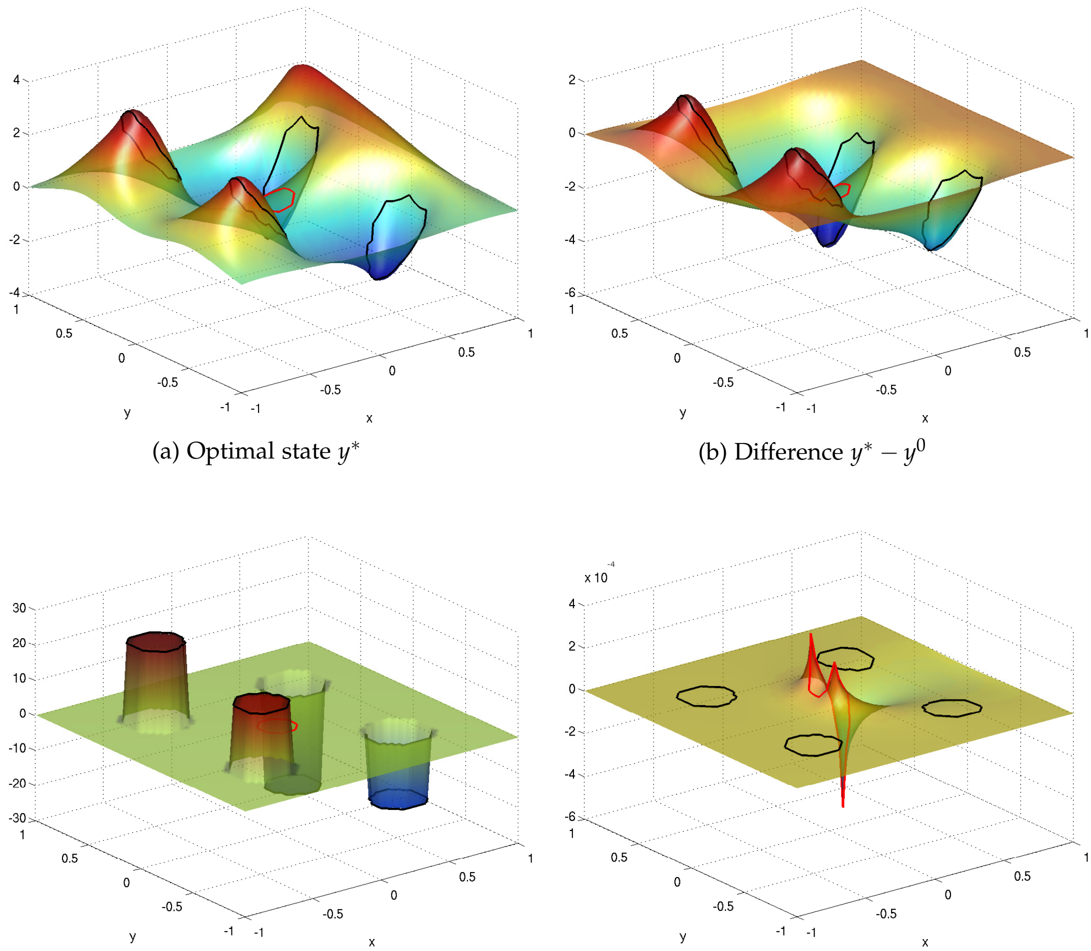

(a) Optimal state y^* (b) Difference $y^* - y^0$

(c) Optimal control u^* (d) Lagrange multiplier p^*

Figure 4: Results for L^∞ norm minimization ($\beta_1 = \beta_2 = 1$).

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