AN INEXACT SEMISMOOTH LEAST SQUARES METHOD FOR LARGE-SCALE COMPLEMENTARITY PROBLEMS

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Abstract: Recently, the reformulation of the complementarity problem as a nonlinear least squares problem was proposed by the authors, along with a corresponding nonsmooth Levenberg-Marquardt- or Gauss-Newton-type method. This method has some nice global and local convergence properties and turned out to be extremely robust when applied to several difficult test problems. However, it requires the exact solution of a linear least squares problem at each iteration and may therefore not be applicable to large-scale problems. Hence we suggest an inexact version of this method which allows inexact solutions of the linear least squares subproblems by using an appropriate iterative method. We show that the convergence properties of the exact method also hold for this inexact version, and we discuss several practical aspects related to a suitable implementation of this inexact method. Numerical results are presented for a number of large-scale problems taken from the MPCLIB collection or arising from finite difference discretizations of optimal control and obstacle problems.

Keywords: Complementarity problems; Nonlinear least squares reformulation; Semismooth functions; Levenberg-Marquardt method; LSQR method; Global convergence; Quadratic convergence

1 Introduction

The complementarity problem is to find a solution $x^* \in \mathbb{R}^n$ of the following system of equations and inequalities:

$$x_i \geq 0, \;\; F_i(x) \geq 0, \;\; x_i F_i(x) = 0 \quad \forall i = 1, \ldots, n, \tag{1}$$

where $F : \mathbb{R}^n \to \mathbb{R}^n$ denotes a given continuously differentiable mapping. This problem has a number of important applications, and the interested reader is referred to the survey paper [13] to get a first impression.

Most algorithms for the solution of the complementarity problem (1) were proposed during the last 15 years and are based on a suitable reformulation of this problem, either as a nonlinear system of equations or as a constrained or unconstrained optimization problem. Many of these methods are described in the excellent book [9, 10] by Facchinei and Pang.

One of the most prominent and efficient methods for solving the complementarity problem is the class of semismooth Newton methods, see the references [2, 5, 11, 12, 20, 30] for some examples. These methods can easily be extended to the slightly more general mixed complementarity problem, however, in order to keep our notation as simple as possible, we prefer to deal with the structurally simpler complementarity problem (1). We stress, however, that all results presented in this paper can be extended to mixed complementarity problems.

The reformulation of the complementarity problem used in this paper is based on the recent article [19]. The method described in [19] is a semismooth least squares Levenberg-Marquardt-type method and seems to be numerically much more stable than any other semismooth method proposed earlier. However, it solves at each iteration a linear least squares subproblem, and this can be done efficiently only if the dimension of the underlying complementarity problem is not too large. In particular, we have to expect storage problems when solving the linear least squares problems by any of the standard orthogonalization methods since these methods usually produce dense matrices.

The main motivation for this paper is therefore to modify the method from [19] in such a way that it can be applied to large-scale problems. This can be done by allowing inexact solutions of the linear least squares subproblem using an iterative solver that preserves the sparsity structure of the complementarity problem.

We describe this algorithm and the details of the reformulation of (1) as an overdetermined least squares problem in Section 2. The convergence of this method is analyzed in Section 3. Some details of the implementation including a discussion of suitable preconditioners are presented in Section 4. This section also contains numerical results for a number of different large-scale problems either taken from the MCPLIB library or obtained by discretization of optimal control and obstacle problems. We then conclude with some final remarks in Section 5.

Our notation is standard: $\mathbb{R}^n$ denotes the n-dimensional real vector space. The Euclidean vector norm or its associated matrix norm are denoted by $\|\cdot\|$, while $\|\cdot\|_\infty$

is used for the maximum norm in $\mathbb{R}^n$. For a continuously differentiable function $F : \mathbb{R}^n \to \mathbb{R}^m$, we write $F'(x)$ for the Jacobian of F at a point $x \in \mathbb{R}^n$, whereas $\nabla F(x)$ denotes the transposed Jacobian. In particular, if $m = 1$, then $\nabla F(x)$ is the gradient vector, which is considered to be a column vector. On the other hand, if $F : \mathbb{R}^n \to \mathbb{R}^m$ is locally Lipschitz only, then $\partial F(x)$ is the generalized Jacobian of F at x in the sense of Clarke [3]. It is well-known that the inclusion

$$\partial F(x)^T \subseteq \partial F_1(x) \times \ldots \times \partial F_m(x) \tag{2}$$

holds, where $\partial F_i(x)$ is the generalized gradient of F_i at x (again viewed as column vectors). The set on the right-hand side of (2) is sometimes called the C-subdifferential of F at x and denoted by $\partial_C F(x)$, see, e.g., [27]. Finally, we make frequent use of the Landau symbols $O(\cdot)$ and $o(\cdot)$ which are defined as follows: Given two sequences $\{\alpha_k\}$ and $\{\beta_k\}$ converging to zero, we write $\alpha_k = O(\beta_k)$ if $\limsup_{k\to\infty} \alpha_k/\beta_k < \infty$, whereas $\alpha_k = o(\beta_k)$ means that $\lim_{k\to\infty} \alpha_k/\beta_k = 0$.

2 Reformulation and Algorithm

The method to be considered in this paper is based on an approach from [19]. In this section, we only review the basic definitions and properties of that approach and refer the interested reader to [19] for a motivation.

The method from [19] exploits a reformulation of the complementarity problem (1) as an overdetermined nonlinear system of equations

$$\Phi(x) = 0 \tag{3}$$

with $\Phi : \mathbb{R}^n \to \mathbb{R}^{2n}$ being defined by

$$\Phi(x) := \begin{pmatrix} \vdots \\ \lambda\phi_{FB}(x_i, F_i(x)), \quad i = 1, \ldots, n \\ \vdots \\ (1-\lambda)\phi_+(x_i, F_i(x)), \quad i = 1, \ldots, n \\ \vdots \end{pmatrix}, \tag{4}$$

where $\lambda \in (0, 1)$ is a fixed but arbitrary parameter used as a weight between the first term and the second one, $\phi_+ : \mathbb{R}^2 \to \mathbb{R}$ is the function

$$\phi_+(a, b) := a_+ b_+ \ ,$$

where $z_+ := \max\{0, z\}$ for $z \in \mathbb{R}$, and $\phi_{FB} : \mathbb{R}^2 \to \mathbb{R}$ denotes the Fischer-Burmeister function (see [14])

$$\phi_{FB}(a, b) := \sqrt{a^2 + b^2} - a - b,$$

which belongs to the class of NCP-functions defined via the characterization

$$\phi(a,b) = 0 \Longleftrightarrow a \geq 0, b \geq 0, ab = 0$$

of their zeros.

These properties guarantee that x^* is a solution of the complementarity problem if and only if it solves the nonlinear least squares problem

$$\min \Psi(x) = \frac{1}{2}\|\Phi(x)\|^2 \tag{5}$$

with zero residual, where Φ denotes the mapping from (4). Here, it is interesting to note that (besides the nonsmoothness of Φ) the merit function Ψ is continuously differentiable everywhere (see [19]). Taking these observations into account, we are now able to state our inexact Levenberg-Marquardt-type method for the solution of the complementarity problem (1) via the nonlinear least squares reformulation (5).

Algorithm 2.1 (Inexact Semismooth Levenberg-Marquardt Method)

(S.0) Let $\beta \in (0,1)$, $\sigma \in (0, \frac{1}{2})$, $\rho > 0$, $p > 2$ and $\varepsilon \geq 0$. Choose any $x^0 \in \mathbb{R}^n$. Set $k := 0$.

(S.1) If $\|\nabla\Psi(x^k)\| \leq \varepsilon$: STOP.

(S.2) Choose $H_k \in \partial_C\Phi(x^k), \nu_k > 0$ and find an approximate solution $d^k \in \mathbb{R}^n$ of

$$\big(H_k^T H_k + \nu_k I\big)d = -\nabla\Psi(x^k), \tag{6}$$

where ν_k is the Levenberg-Marquardt parameter. If the condition

$$\nabla\Psi(x^k)^T d^k \leq -\rho\|d^k\|^p \tag{7}$$

is not satisfied, set $d^k = -\nabla\Psi(x^k)$.

(S.3) Compute $t_k = \max\{\beta^\ell \,|\, \ell = 0, 1, 2, \dots\}$ such that

$$\Psi(x^k + t_k d^k) \leq \Psi(x^k) + \sigma t_k \nabla\Psi(x^k)^T d^k. \tag{8}$$

(S.4) Set $x^{k+1} = x^k + t_k d^k$, $k \leftarrow k+1$, and go to (S.1).

Algorithm 2.1 is very similar to the one presented in [8] (see also [17]) which, however, is based on a different reformulation of the complementarity problem as a square system of equations. Nevertheless, this observation will simplify the convergence analysis of Algorithm 2.1 significantly, and we will come back to this point in the next section.

Before investigating the convergence properties of Algorithm 2.1, however, we need to say what we mean by solving the subproblem (6) inexactly in Step (S.2). To specify

this point, we will assume that the inexact solution d^k of (6) satisfies a relation of the form

$$(H_k^T H_k + \nu_k I)d^k = -\nabla\Psi(x^k) + r^k \tag{9}$$

for some residual vector r^k such that

$$\|r^k\| \leq \alpha_k \|\nabla\Psi(x^k)\| \tag{10}$$

for some a priori chosen number $\alpha_k \geq 0$. Note that the choice $\alpha_k = 0$ corresponds to an exact solution of the regularized linear least squares subproblem from (6).

3 Convergence Properties

In this section, we investigate the convergence properties of our algorithm. To this end, we assume that the termination parameter ε is equal to zero and that Algorithm 2.1 generates an infinite sequence. We further assume throughout this section that the subproblems (6) are solved inexactly in such a way that conditions (9) and (10) hold for some sequence $\{\alpha_k\}$.

We first state a global convergence result for Algorithm 2.1. Its proof is essentially the same as the one from [8, Theorem 12], and we therefore skip the details here.

Theorem 3.1 *Assume that the sequence $\{\nu_k\}$ is bounded and that the sequence of residual vectors $\{r^k\}$ satisfies condition (10) for some sequence of positive numbers $\{\alpha_k\}$ such that $\alpha_k \leq \bar{\alpha}$ for some $\bar{\alpha} \in [0, 1)$. Then every accumulation point of a sequence $\{x^k\}$ generated by Algorithm 2.1 is a stationary point of Ψ.*

Conditions for a stationary point of Ψ to be a solution of the complementarity problem (1) are given in [19] and therefore not repeated here.

In order to show local fast convergence, we need a regularity assumption. To this end, we define the index sets

$$\begin{aligned}\alpha &:= \{i \mid x_i^* > 0, F_i(x^*) = 0\},\\ \beta &:= \{i \mid x_i^* = 0, F_i(x^*) = 0\},\\ \gamma &:= \{i \mid x_i^* = 0, F_i(x^*) > 0\},\end{aligned}$$

and recall that a solution x^* of the complementarity problem is said to be *R-regular* if the submatrix $F'(x^*)_{\alpha\alpha}$ is nonsingular and the Schur complement

$$F'(x^*)_{\beta\beta} - F'(x^*)_{\beta\alpha}F'(x^*)_{\alpha\alpha}^{-1}F'(x^*)_{\alpha\beta}$$

is a P-matrix (see [29, 4]). For our subsequent analysis, we note that the R-regularity assumption implies that, if the sequence $\{x^k\}$ converges to an R-regular solution x^*, then the matrices $H_k^T H_k$ are uniformly positive definite, i.e., there is a constant $\gamma > 0$ such that

$$\|H_k d^k\|^2 = (d^k)^T H_k^T H_k d^k \geq \gamma \|d^k\|^2 \tag{11}$$

for all k sufficiently large, see [19].

We are now in the position to state a local convergence result.

Theorem 3.2 *Let $\{x^k\}$ be a sequence generated by Algorithm 2.1, let the sequence $\{\nu_k\}$ be bounded and assume that $\{\alpha_k\} \to 0$ with $\{\alpha_k\}$ being the sequence from (10). Assume that x^* is an accumulation point of $\{x^k\}$ such that x^* is an R-regular solution of the complementarity problem (1). Then the following statements hold:*

(a) The entire sequence $\{x^k\}$ converges to x^*.

(b) Eventually d^k is always given by the inexact solution of system (6).

(c) The full stepsize $t_k = 1$ is always accepted for k sufficiently large so that $x^{k+1} = x^k + d^k$ provided that $\nu_k \to 0$.

(d) The rate of convergence is Q-superlinear if $\nu_k \to 0$.

(e) The rate of convergence is Q-quadratic if $\nu_k = O(\|\Phi(x^k)\|)$, $\alpha_k = O(\|\Phi(x^k)\|)$ and, in addition, F' is locally Lipschitzian.

Proof. (a) Using the R-regularity assumption, we can argue exactly as in [19, Theorem 3.3 (a)] for proving that x^* is an isolated accumulation point of the sequence $\{x^k\}$.

Let $\{x^k\}_K$ denote any subsequence converging to x^*, and note that x^* is a stationary point of Ψ by Theorem 3.1. For all $k \in \mathbb{N}$ such that d^k is an inexact solution of (6), we have

$$\begin{aligned}
\|x^{k+1} - x^k\| &= t_k\|d^k\| \\
&\leq \|d^k\| \\
&\overset{(9)}{\leq} \|(H_k^T H_k + \nu_k I)^{-1}\| \, \| - \nabla\Psi(x) + r^k\| \\
&\leq \|(H_k^T H_k + \nu_k I)^{-1}\| \big(\|\nabla\Psi(x)\| + \|r^k\|\big) \\
&\overset{(10)}{\leq} (1 + \alpha_k)\|(H_k^T H_k + \nu_k I)^{-1}\| \, \|\nabla\Psi(x)\|.
\end{aligned}$$

On the other hand, for all $k \in \mathbb{N}$ with $d^k = -\nabla\Psi(x^k)$, we have

$$\|x^{k+1} - x^k\| = t_k\|d^k\| \leq \|d^k\| = \|\nabla\Psi(x^k)\|.$$

Together, it follows from $\{\nabla\Psi(x^k)\}_K \to 0$, the assumed boundedness of $\{\nu_k\}$ and [19, Lemma 2.5] that $\{\|x^{k+1} - x^k\|\}_K \to 0$. Hence statement (a) follows from [23, Lemma 4.10].

(b) First we prove that there is a constant $\kappa > 0$ such that

$$\nabla\Psi(x^k)^T d^k \leq -\kappa\|d^k\|^2 \tag{12}$$

for all $k \in \mathbb{N}$ sufficiently large, where d^k denotes an inexact solution of (6) in the sense that (9) and (10) are satisfied.

Since $\{\nu_k\}$ is bounded by assumption, $x^k \to x^*$ by (a) and the generalized Jacobian is upper semicontinuous, the sequence $\{H_k^T H_k + \nu_k I\}$ is bounded. Furthermore, it follows from $x^k \to x^*$, the assumed R-regularity and [19, Lemma 2.5] that the corresponding inverse matrices are also uniformly bounded. Hence there is a constant $c > 0$ such that

$$\|H_k^T H_k + \nu_k I\| \le c \quad \text{and} \quad \|(H_k^T H_k + \nu_k I)^{-1}\| \le c \quad \forall k \in \mathbb{N}. \tag{13}$$

Since

$$\|H_k^T H_k + \nu_k I\| = \lambda_{\max}(H_k^T H_k + \nu_k I) =: \lambda_{\max}^k$$

and

$$\|(H_k^T H_k + \nu_k I)^{-1}\| = \frac{1}{\lambda_{\min}(H_k^T H_k + \nu_k I)} =: \frac{1}{\lambda_{\min}^k},$$

we obtain from (13)

$$\frac{1}{c}\|d^k\|^2 \le \lambda_{\min}^k \|d^k\|^2 \le (d^k)^T (H_k^T H_k + \nu_k I) d^k \le \lambda_{\max}^k \|d^k\|^2 \le c\|d^k\|^2. \tag{14}$$

Furthermore, we have

$$\|\nabla\Psi(x^k) - r^k\| \overset{(9)}{=} \|(H_k^T H_k + \nu_k I) d^k\| \le \|H_k^T H_k + \nu_k I\| \, \|d^k\|$$

and therefore

$$\begin{aligned} \|d^k\| \ge \frac{\|\nabla\Psi(x^k) - r^k\|}{\|H_k^T H_k + \nu_k I\|} &\overset{(13)}{\ge} \frac{1}{c}\|\nabla\Psi(x^k) - r^k\| \\ &\ge \frac{1}{c}\big(\|\nabla\Psi(x^k)\| - \|r^k\|\big) \\ &\overset{(10)}{\ge} \frac{1}{c}\big(\|\nabla\Psi(x^k)\| - \alpha_k\|\nabla\Psi(x^k)\|\big) \\ &= \frac{1}{c}(1 - \alpha_k)\|\nabla\Psi(x^k)\|. \end{aligned} \tag{15}$$

The Cauchy-Schwarz inequality therefore implies

$$\begin{aligned} \nabla\Psi(x^k)^T d^k &\overset{(9)}{=} -(d^k)^T (H_k^T H_k + \nu_k I) d^k + (r^k)^T d^k \\ &\le -(d^k)^T (H_k^T H_k + \nu_k I) d^k + \|r^k\| \, \|d^k\| \\ &\overset{(10)}{\le} -(d^k)^T (H_k^T H_k + \nu_k I) d^k + \alpha_k \|\nabla\Psi(x^k)\| \|d^k\| \\ &\overset{(14)}{\le} -\frac{1}{c}\|d^k\|^2 + \alpha_k \|\nabla\Psi(x^k)\| \|d^k\| \\ &\overset{(15)}{\le} -\frac{1}{c}\|d^k\|^2 + c\frac{\alpha_k}{1 - \alpha_k}\|d^k\|^2. \end{aligned}$$

Hence inequality (12) follows immediately from the fact that $\alpha_k \to 0$.

Using (12), the Cauchy-Schwarz inequality implies

$$\kappa \|d^k\|^2 \leq \|\nabla \Psi(x^k)\| \, \|d^k\|$$

and therefore $\{\|d^k\|\} \to 0$. This together with $p > 2$ gives statement (b), i.e., the test (7) is satisfied for all k sufficiently large.

(c), (d) We first show that

$$\|x^k + d^k - x^*\| = o(\|x^k - x^*\|) \tag{16}$$

holds for all $k \in \mathbb{N}$ sufficiently large. To this end, we recall that, for any $k \in \mathbb{N}$, the matrix $H_k^T H_k + \nu_k I$ is nonsingular with $\|(H_k^T H_k + \nu_k I)^{-1}\| \leq c$ by (13). Furthermore, the sequence $\{H_k\}$ is bounded (since $\{x^k\}$ is convergent) and we can assume without loss of generality that we also have $\|H_k^T\| \leq c$. Since $\nabla \Psi(x^k) = H_k^T \Phi(x^k)$ in view of [19, Theorem 2.7], we obtain for all x^k sufficiently close to x^* that

$$\begin{aligned}
&\|x^k + d^k - x^*\| \\
&\overset{(9)}{=} \|x^k + (H_k^T H_k + \nu_k I)^{-1}(-\nabla \Psi(x^k) + r^k) - x^*\| \\
&\leq \|(H_k^T H_k + \nu_k I)^{-1}\| \, \|\nabla \Psi(x^k) - r^k - (H_k^T H_k + \nu_k I)(x^k - x^*)\| \\
&\leq c\|H_k^T \Phi(x^k) - H_k^T H_k (x^k - x^*) - \nu_k (x^k - x^*) - r^k\| \\
&\leq c\big(\|H_k^T (\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*))\| + \nu_k \|x^k - x^*\| + \|r^k\|\big) \\
&\overset{(10)}{\leq} c\big(\|H_k^T\| \|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| + \nu_k \|x^k - x^*\| + \alpha_k \|H_k^T \Phi(x^k)\|\big) \\
&\leq c\big(c\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| + \nu_k \|x^k - x^*\| + \alpha_k c \|\Phi(x^k) - \Phi(x^*)\|\big) \\
&= o(\|x^k - x^*\|) + o(\|x^k - x^*\|) + o(\|x^k - x^*\|) \\
&= o(\|x^k - x^*\|)
\end{aligned}$$

since $\nu_k \to 0, \alpha_k \to 0$, and Φ is locally Lipschitz and semismooth (see [19, Theorem 2.1]). Hence (16) holds.

In order to verify statement (c), we have to show that the full step $t_k = 1$ is eventually accepted by the line search rule in Algorithm 2.1. This fact may be derived from a general result in [7] using some additional properties of the merit function Ψ. However, we prefer to give a direct proof here which does not exploit any further properties of this merit function.

First note that (16) implies

$$\|x^k - x^*\| \leq \|x^k + d^k - x^*\| + \|d^k\| = o(\|x^k - x^*\|) + \|d^k\|.$$

Hence we have

$$\|x^k - x^*\| = O(\|d^k\|). \tag{17}$$

Together with (16), the local Lipschitz property of Φ and the fact that $\Phi(x^*) = 0$, we therefore obtain

$$\begin{aligned}\Psi(x^k + d^k) &= \frac{1}{2}\|\Phi(x^k + d^k)\|^2 \\ &= \frac{1}{2}\|\Phi(x^k + d^k) - \Phi(x^*)\|^2 \\ &= O(\|x^k + d^k - x^*\|^2) \\ &= o(\|x^k - x^*\|^2) \\ &= o(\|d^k\|^2).\end{aligned} \tag{18}$$

In a similar way, we also get from (10) and $\nabla\Psi(x^k) = H_k^T\Phi(x^k)$ that

$$\|r^k\| = o(\|\nabla\Psi(x^k)\|) = o(\|\Phi(x^k) - \Phi(x^*)\|) = o(\|x^k - x^*\|) = o(\|d^k\|). \tag{19}$$

Exploiting the semismoothness of Φ once again, we have

$$\big|\|\Phi(x^k)-\Phi(x^*)\|-\|H_k(x^k-x^*)\|\big| \le \|\Phi(x^k)-\Phi(x^*)-H_k(x^k-x^*)\| = o(\|x^k-x^*\|). \tag{20}$$

This means that there is a positive sequence $\tau_k \to 0$ such that

$$\big|\|\Phi(x^k) - \Phi(x^*)\| - \|H_k(x^k - x^*)\|\big| \le \tau_k\|x^k - x^*\|$$

for all k sufficiently large. Consequently, we have

$$\tau_k\|x^k - x^*\| + \|H_k(x^k - x^*)\| - \|\Phi(x^k) - \Phi(x^*)\| \ge 0$$

and

$$\tau_k\|x^k - x^*\| - \|H_k(x^k - x^*)\| + \|\Phi(x^k) - \Phi(x^*)\| \ge 0 \tag{21}$$

for all k large enough. Multiplying the last two inequalities, we obtain

$$\tau_k^2\|x^k - x^*\|^2 - \|H_k(x^k - x^*)\|^2 + 2\|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| \ge \|\Phi(x^k) - \Phi(x^*)\|^2.$$

We therefore have

$$\frac{1}{2}\|\Phi(x^k)-\Phi(x^*)\|^2 \le -\frac{1}{2}\|H_k(x^k-x^*)\|^2+\|H_k(x^k-x^*)\|\,\|\Phi(x^k)-\Phi(x^*)\|+o(\|x^k-x^*\|^2).$$

On the other hand, multiplying (21) with $\|\Phi(x^k) - \Phi(x^*)\|$ and rearranging terms, we get

$$\begin{aligned}&-\|\Phi(x^k) - \Phi(x^*)\|^2 \\ &\le \tau_k\|x^k - x^*\|\,\|\Phi(x^k) - \Phi(x^*)\| - \|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| \\ &\le -\|H_k(x^k - x^*)\|\,\|\Phi(x^k) - \Phi(x^*)\| + o(\|x^k - x^*\|^2)\end{aligned}$$

since Φ is locally Lipschitz. Adding the last two inequalities and using (17) gives

$$-\frac{1}{2}\|\Phi(x^k)-\Phi(x^*)\|^2 \leq -\frac{1}{2}\|H_k(x^k-x^*)\|^2 + o(\|d^k\|^2). \tag{22}$$

Since

$$\big|\|H_k(x^k+d^k-x^*)\| - \|H_k d^k\|\big| \leq \|H_k(x^k+d^k-x^*) - H_k d^k\| = \|H_k(x^k-x^*)\|$$

holds and the left-hand term is nonnegative, squaring both sides gives

$$\|H_k(x^k+d^k-x^*)\|^2 - 2\|H_k(x^k+d^k-x^*)\|\,\|H_k d^k\| + \|H_k d^k\|^2 \leq \|H_k(x^k-x^*)\|^2.$$

Multiplying this inequality by $-\frac{1}{2}$ and using (16), (17) as well as the boundedness of the sequence $\{H_k\}$, we obtain

$$\begin{aligned}
&-\frac{1}{2}\|H_k(x^k-x^*)\|^2 \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 - \frac{1}{2}\|H_k(x^k+d^k-x^*)\|^2 + \|H_k(x^k+d^k-x^*)\|\,\|H_k d^k\| \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 - \frac{1}{2}\|H_k(x^k+d^k-x^*)\|^2 + o(\|d^k\|^2) \\
&\leq -\frac{1}{2}\|H_k d^k\|^2 + o(\|d^k\|^2).
\end{aligned} \tag{23}$$

Summarizing our previous discussion, we now obtain for all x^k sufficiently close to x^* that

$$\begin{aligned}
&\Psi(x^k+d^k) - \Psi(x^k) - \sigma\nabla\Psi(x^k)^T d^k \\
&\overset{(9),(18)}{=} o(\|d^k\|^2) - \frac{1}{2}\|\Phi(x^k)\|^2 + \sigma(d^k)^T(H_k^T H_k + \nu_k I)d^k - \sigma(r^k)^T d^k \\
&\leq -\frac{1}{2}\|\Phi(x^k)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + \sigma\nu_k\|d^k\|^2 + o(\|d^k\|^2) + \sigma|(r^k)^T d^k| \\
&\overset{\nu_k\to 0}{\leq} -\frac{1}{2}\|\Phi(x^k)-\Phi(x^*)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + o(\|d^k\|^2) + \sigma\|r^k\|\|d^k\| \\
&\overset{(22),(19)}{\leq} -\frac{1}{2}\|H_k(x^k-x^*)\|^2 + \sigma(d^k)^T(H_k^T H_k)d^k + o(\|d^k\|^2) \\
&\overset{(23)}{\leq} -\frac{1}{2}\|H_k d^k\|^2 + \sigma\|H_k d^k\|^2 + o(\|d^k\|^2) \\
&= (\sigma-\frac{1}{2})\|H_k d^k\|^2 + o(\|d^k\|^2) \\
&\overset{(11)}{\leq} (\sigma-\frac{1}{2})\gamma\|d^k\|^2 + o(\|d^k\|^2) \\
&< 0,
\end{aligned}$$

where the last two inequalities follow from the fact that $\sigma \in (0, 1/2)$. This implies that the full step is eventually accepted, i.e., we have $x^{k+1} = x^k + d^k$ for all k sufficiently

large. Consequently, (16) shows that $\{x^k\}$ converges Q-superlinearly to x^*.

(e) The proof is essentially the same as for the local superlinear convergence. To this end, we only note that F' being locally Lipschitz implies that Φ is strongly semismooth by [19, Theorem 2.1], and that the relation

$$\|\Phi(x^k) - \Phi(x^*) - H_k(x^k - x^*)\| = O(\|x^k - x^*\|^2).$$

holds for strongly semismooth functions, see [28, 26, 25, 10]. □

Note that statement (e) of Theorem 3.2 remains true if the two sequences $\{\nu_k\}$ and $\{\alpha_k\}$ satisfy $\nu_k = O(\|\nabla\Psi(x^k)\|)$ and $\alpha_k = O(\|\nabla\Psi(x^k)\|)$.

4 Numerical Results

Since the previous sections showed that the good theoretical properties of the exact semismooth Newton method from [19] also hold for the inexact version from Algorithm 2.1, we now look at the practical behaviour of the algorithm. Here we are mainly interested in large-scale problems where the exact method from [19] may not necessarily be applied to because the solution of the linearized least squares problem at each iteration is either too time-consuming or simply not possible due to storage problems.

We first give some general comments regarding the implementation of Algorithm 2.1 in Subsection 4.1. We then give some more details and present our numerical results in Subsections 4.2 (for the large-scale problems from MCPLIB), 4.3 (for some problems from optimal control), and 4.4 (for a discretized obstacle problem).

4.1 General Considerations

We first note that Algorithm 2.1 can be extended in a relatively simple way to the more general class of mixed complementarity problems. Some details are given in [19]. Our implementation is therefore able to deal with mixed complementarity problems. Note, however, that we still write $\Phi(x) = 0$ for the corresponding reformulation as an overdetermined nonlinear system of equations, and we still write $\Psi(x) := \frac{1}{2}\|\Phi(x)\|^2$ for the associated merit function, i.e., we do not change our notation from the previous sections although Φ and Ψ are defined in a slightly different way.

We implemented Algorithm 2.1 in MATLAB. The implementation corresponds exactly to the statement of Algorithm 2.1 except that we use a nonmonotone line search. To be more precise, we use the standard (monotone) Armijo rule during the first five iterations and then switch to the nonmonotone line search where the maximum of the function values $\Psi(x^k)$ is taken over the last ten iterations, see [15] for further details.

Some preliminary numerical experiments indicated that small values of the Levenberg-Marquardt parameter ν_k give much better results than larger ones so that we decided

to take the limiting value $\nu_k = 0$ for all k, i.e., the Levenberg-Marquard step from (6) reduces to a Gauss-Newton step

$$\min_d \|H_k d + \Phi(x^k)\|. \tag{24}$$

The search direction d^k is always given by the inexact solution of system (24).

We terminate the iteration in step (S.1) of Algorithm 2.1 if one of the following conditions are satisfied:

$$\Psi(x^k) \leq 10^{-8} \quad \text{or} \quad \|\nabla\Psi(x^k)\|_\infty \leq 10^{-6} \quad \text{or} \quad k > 100.$$

The other parameters used in our implementation are $\lambda = 0.9, \beta = 0.9$ and $\sigma = 10^{-4}$.

For the inexact solution of the linearized least squares subproblems, we use the LSQR method from [24]. An implementation of LSQR is provided by MATLAB. LSQR is an iterative method for the solution of linear least squares problems and does not need any matrix factorizations. This allows us to apply LSQR to large-scale problems. The forcing sequence $\{\alpha_k\}$ from Algorithm 2.1, which determines the accuracy with which we actually solve the subproblems, is defined as

$$\alpha_k = \min\Big\{\frac{10^{-2}}{k+1}, \Psi(x^k), \|\nabla\Psi(x^k)\|_\infty\Big\}.$$

LSQR employs several termination criteria (see [24]). The two main criteria used in our implementation are

$$\frac{\|r_{LS}^k\|}{\|\Phi(x^k)\|} \leq \alpha_k \tag{25}$$

and

$$\|H_k^T r_{LS}^k\| \leq \max\big\{10^{-8}, \min\big\{\alpha_k, \theta\|H_k^T\Phi(x^k)\|\big\}\big\} \quad \text{with } \theta = 0.01, \tag{26}$$

where $r_{LS}^k := H_k d + \Phi(x^k)$ denotes the residual vector of (24) (note that this vector is different from the vector r^k occuring in (9)). Basically, the first criterion (25) checks whether the residuum is sufficiently small. In general, this condition will be satisfied only if the linearized least squares problem has a zero or small residuum in the solution d^k, and this will usually happen only if we are getting close to a solution x^* of our mixed complementarity problem.

The other condition (26) is applicable in more general situations and checks whether the error in the normal equation is small enough. Note that we use an absolute lower bound of 10^{-8} so that we do not force this error to become too small. The other two terms in (26) are easy to understand: We require the error in the normal equation to be at least as small as α_k, and, in addition, it has to satisfy the bound

$$\|H_k^T r_{LS}^k\| \leq \theta\|H_k^T\Phi(x^k)\|$$

for some constant $\theta \in (0, 1)$. This latter condition is important because otherwise it happens quite often that the zero vector (used as a starting point for the inner

LSQR iteration) is accepted by this criterion, meaning, however, that $x^k = x^{k+1}$ in the corresponding outer iteration, and this useless situation has to be avoided.

We also note that estimates of the quantities $\|r_{LS}^k\|$ and $\|H_k^T r_{LS}^k\|$ used within the inner termination criterion can be obtained at minimal cost from the LSQR method itself, see [24] for more details.

Finally, we turn to the question of a suitable preconditioner. Like all iterative methods for the solution of linear systems of equations, the practical performance of LSQR for the iterative solution of the linear least squares subproblem (24) may often be accelerated by the choice of a suitable preconditioner. Note, however, that we only have the possibility to choose a right preconditioner M since

$$\min_d \|Hd + \Phi(x)\| = \min_z \|HM^{-1}z + \Phi(x)\|, \quad \text{where } z = Md,$$

whereas a left preconditioner would change the subproblem. In order to find an appropriate preconditioner M, recall that any matrix $H \in \partial_C \Phi(x)$ has the representation

$$H = \begin{pmatrix} \lambda H_1 \\ (1-\lambda) H_2 \end{pmatrix}, \tag{27}$$

where

$$H_1 \subseteq D_a(x) + D_b(x)F'(x) \quad \text{and} \quad H_2 \subseteq \tilde{D}_a(x) + \tilde{D}_b(x)F'(x) \tag{28}$$

with certain diagonal matrices $D_a(x), D_b(x), \tilde{D}_a(x), \tilde{D}_b(x)$, see [19, Theorem 2.3] for more details. Taking into account this structure, a natural choice for M seems to be the first block matrix H_1 provided this matrix is nonsingular and the size and structure of H_1 allows the solution of linear systems of equations with this matrix. Note also that H_1 is the leading block since $\lambda = 0.9$ in our implementation, i.e., we put much more emphasis on this block than on the second part.

However, for some large-scale problems, it may not be possible to use H_1 or a suitable modification of this matrix as a preconditioner, and then we have to take a closer look at the particular structure of this matrix in order to find a suitable preconditioner. We will illustrate this point in more detail in some of the following subsections.

4.2 MCPLIB Test Problems

Our first test problems are the larger ones taken from the MCPLIB. Note that the test problem library used here is an updated version of the MCPLIB originally introduced in [6]. The starting point x^0 is the standard one provided by the MCPLIB collection.

Since the examples from the MCPLIB are difficult, but still of reasonable size, we basically take the suggestion from the previous subsection and use the slightly regularized H_1-block $M := H_1 + 10^{-4}I$ as a preconditioner. We note, however, that nonsingularity of this matrix M is not guaranteed, but the addition of the scaled identity seems to be quite helpful in order to avoid singularity problems at the solution of some test examples.

Our numerical results are summarized in Table 1. In this table, the first column gives the name of the problem; Dim is the number of the variables in the problem; o.it. denotes the number of outer iterations; column avg.i.it. presents the average number of inner LSQR iterations needed to solve the corresponding linear least squares problem (24) inexactly; $\Psi(x^0)$ gives the value of the merit function at the starting point; and $\Psi(x^f)$ and $\|\nabla\Psi(x^f)\|_\infty$ denote the values of $\Psi(x)$ and $\|\nabla\Psi(x)\|_\infty$ at the final iterate $x = x^f$.

Table 1: Numerical results for (large) MCPLIB test problems

Problem	Dim	o.it.	avg.i.it.	$\Psi(x^0)$	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|_\infty$
`bert_oc`	5000	5	1.8	5.13e+01	2.99e-12	1.07e-06
`bratu`	5625	8	1.6	1.41e+01	4.22e-10	4.21e-05
`bishop`	1645	—	—	1.00e+11	—	—
`lincont`	419	34	45.2	7.11e+03	1.19e-11	7.37e-06
`obstacle`	2500	7	1.0	2.36e-02	6.79e-10	4.88e-05
`opt_cont`	288	8	1.9	6.09e+01	5.86e-09	8.92e-05
`opt_cont31`	1024	10	1.5	6.76e+01	7.57e-10	3.36e-05
`opt_cont127`	4096	11	2.0	3.89e+01	1.12e-09	4.77e-05
`opt_cont255`	8192	10	2.9	2.64e+01	4.78e-09	1.37e-05
`opt_cont511`	16384	13	3.6	1.84e+01	2.54e-14	3.26e-07
`trafelas`	2904	39	4.2	5.28e+03	1.10e-11	3.86e-06

With the only exception of example `bishop`, we see from Table 1 that we can solve all other test examples. These other examples include some problems like `lincont` or `trafelas` which are usually regarded as being quite difficult. We also stress that the average number of inner iterations is extremely small for all problems except `lincont`. This indicates the effectiveness of our preconditioner.

4.3 Optimal Control Problems

In this section we look at the practical behaviour of the algorithm by considering a variety of large-scale complementarity problems resulting from suitable discretizations of optimal control problems. We consider both control problems with control constraints in Subsection 4.3.1 and control problems with control and state constraints in Subsection 4.3.2.

4.3.1 Control Problems with Control Constraints

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with boundary $\Gamma = \partial\Omega$, and let $y_d, u_d, \psi \in L^2(\Omega)$ be given functions such that y_d represents a desired state, u_d a desired control, and ψ describes the upper bounds on the control variable. Furthermore, let $\alpha \geq 0$ denote a

regularization parameter. Our aim is then to find a control u and a corresponding state y minimizing the functional

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

subject to the elliptic state equation

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

the Dirichlet boundary conditions

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

and the control constraints

$$u(x) \le \psi(x) \quad \text{a.e. in } \Omega.$$

To be more specific, consider the two-dimensional case $\Omega = (0,1) \times (0,1) \subseteq \mathbb{R}^2$, and let A denote the standard five-point finite difference approximation to the negative Laplacian with uniform stepsize $h := 1/(N+1)$ for some $N \in \mathbb{N}$, so that we have $n := N^2$ interior nodes. Then the discretized optimal control problem becomes

$$\min_{u,y} \frac{1}{2}\|y - y_d\|_2^2 + \frac{\alpha}{2}\|u - u_d\|_2^2 \quad \text{s.t.} \quad Ay = u, \;\; \psi - u \ge 0,$$

where, for simplicity of notation, the discretized functions u, y etc. are denoted by the same letters as their continuous counterparts.

Because the state variable is not constrained, we can remove the control variable using $u = Ay$ and obtain the equivalent problem

$$\min_{y} \frac{1}{2}\|y - y_d\|_2^2 + \frac{\alpha}{2}\|Ay - u_d\|_2^2 \quad \text{s.t.} \quad \psi - Ay \ge 0.$$

Setting $v := \psi - Ay$, we obtain

$$\min_{v} \frac{1}{2}\|A^{-1}(\psi - v) - y_d\|_2^2 + \frac{\alpha}{2}\|\psi - v - u_d\|_2^2 \quad \text{s.t.} \quad v \ge 0.$$

Defining $v_d := y_d - A^{-1}\psi$ and $\psi_d := u_d - \psi$, we finally obtain the convex problem

$$\min_{v} f(v) := \frac{1}{2}\|A^{-1}v + v_d\|_2^2 + \frac{\alpha}{2}\|v + \psi_d\|_2^2 \quad \text{s.t.} \quad v \ge 0.$$

Using the KKT theory, it follows that this convex quadratic optimization problem is equivalent to the linear complementarity problem

$$v \ge 0, \quad F(v) \ge 0, \quad v^T F(v) = 0$$

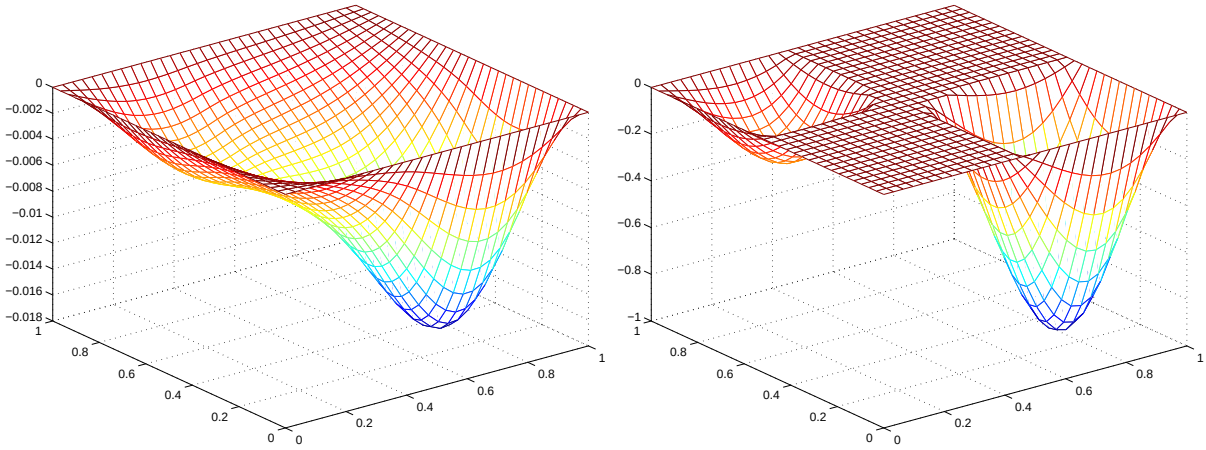

Figure 1: Optimal state (left) and optimal control (right) for Example 4.1

Table 2: Numerical results for Example 4.1

N	50	100	150	200	250	300
o. it.	10	10	9	13	16	15
avg. i. it.	6.3	20.7	38.0	25.1	31.0	37.5

with

$$F(v) := \nabla f(v) = (A^{-1}A^{-1} + \alpha I)v + A^{-1}v_d + \alpha\psi_d.$$

At this stage we can apply Algorithm 2.1 using the same parameter setting as in the previous subsection. In order to solve the corresponding linear least squares problem (24) inexactly, we apply the LSQR method with the same termination criteria as described above.

The matrix H_k arising in the subproblem (24) has the structure from (27), (28) with $F'(v) = A^{-1}A^{-1} + \alpha I$. Since we only need to compute matrix-vector products of the form $H_k v$ and $H_k^T u$ for certain vectors v and u, respectively, and since the matrix A corresponds to the standard five-point finite difference approximation of the negative Laplacian, these matrix-vector products can be computed quite efficiently by, e.g., a fast sine transform in only $O(N^2 \log_2 N)$ arithmetic operations which is not much more than $O(n)$ flops.

We apply our method to two examples taken from [1] (also used as test problems in, e.g., [31, 18]).

Example 4.1 (**Control Constraints**) The data are $\alpha = 0.01, \psi \equiv 0, u_d \equiv 0$ and $y_d(x_1, x_2) = \sin(2\pi x_1)\sin(2\pi x_2)\exp(2x_1)/6$. The optimal state and control are depicted in Figure 1.

We present our numerical results (number of outer iterations and average number of inner LSQR iterations) for this example in Table 2 using different discretizations $N \in \mathbb{N}$. Note that the dimension of the corresponding complementarity problem is $n = N^2$.

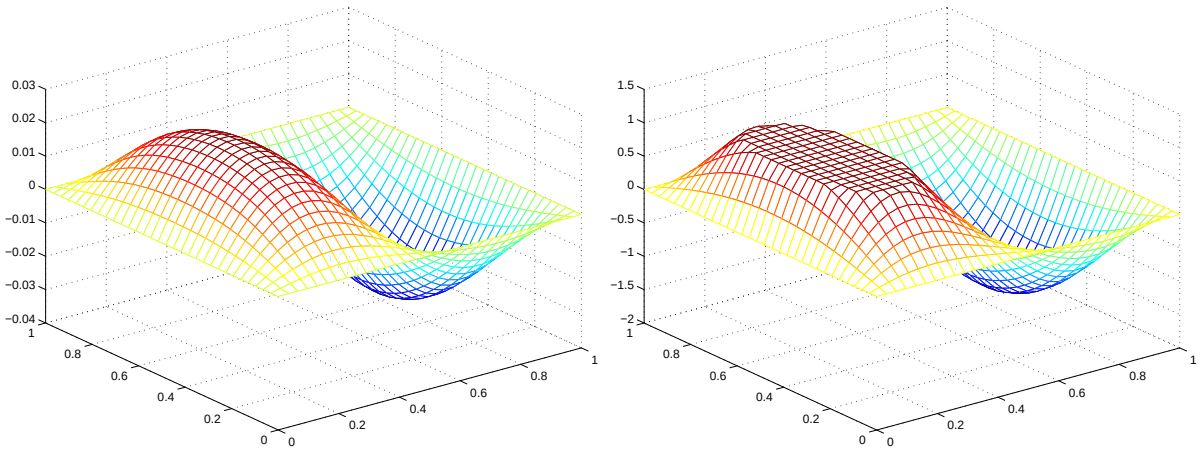

Figure 2: Optimal state (left) and optimal control (right) for Example 4.2

Table 3: Numerical results for Example 4.2

N	50	100	150	200	250	300
o. it.	12	16	10	10	11	11
avg.i. it.	6.2	12.6	21.2	37.5	45.6	45.2

Note also that the average number of inner iterations is relatively small for this example, so there was no need to use a fancy preconditioner for the LSQR method.

Example 4.2 (**Control Constraints**) The data are $\alpha = 0.01, \psi \equiv 1, u_d \equiv 0$ and

$$y_d(x_1, x_2) = \begin{cases} 200x_1x_2(x_1 - 0.5)^2(1 - x_2), & \text{if } 0 < x_1 \leq 0.5, \\ 200x_2(x_1 - 1)(x_1 - 0.5)^2(1 - x_2), & \text{if } 0.5 < x_1 \leq 1. \end{cases}$$

The optimal state and control are depicted in Figure 2.

Table 3 contains the number of inner and outer iterations needed by our method to solve Example 4.2. Again, we observe a relatively small number of average inner iterations, so there is no need to use a suitable preconditioner for this example.

Both examples clearly indicate that our inexact semismooth method can be applied very succesfully to optimal control problems with control constraints.

4.3.2 Control Problems with Control and State Constraints

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with boundary $\Gamma = \partial\Omega$. Given $y_d \in L^2(\Omega), u_d, u_1, u_2, \psi \in L^2(\Gamma), \alpha \geq 0$, and suitable functions $d : \Omega \times \mathbb{R} \to \mathbb{R}, b : \Gamma \times \mathbb{R} \to \mathbb{R}$, our aim is to find a control function $u \in L^2(\Gamma)$ and a corresponding state y minimizing the functional

$$J(y, u) = \frac{1}{2} \int_\Omega \big(y(x) - y_d(x)\big)^2 dx + \frac{\alpha}{2} \int_\Gamma \big(u(x) - u_d(x)\big)^2 dx, \tag{29}$$

subject to the state equation

$$-\Delta y(x) + d(x, y(x)) = 0, \quad \text{for } x \in \Omega, \tag{30}$$

the Dirichlet boundary conditions

$$y(x) = b(x, u(x)), \quad \text{for } x \in \Gamma, \tag{31}$$

and the control and state contraints

$$y(x) \leq \psi(x) \text{ a.e. in } \Omega, \quad u_1(x) \leq u(x) \leq u_2(x) \text{ a.e. in } \Gamma. \tag{32}$$

We discretize this problem is a similar way as described in the previous subsection, where Ω is again the unit square $(0,1) \times (0,1) \subset \mathbb{R}^2$. After discretization we then obtain a nonlinear programming problem of the form

$$\min f(z) \quad \text{s.t.} \quad g(z) \leq 0, \quad h(z) = 0. \tag{33}$$

The corresponding KKT conditions of (33) form a mixed complementarity problem which may be reformulated as an overdetermined nonlinear system of equations $\Phi(w) = 0$, with $\Phi : \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^m \to \mathbb{R}^n \times \mathbb{R}^p \times \mathbb{R}^{2m}$ being defined by

$$\Phi(w) := \Phi(z, \zeta, \xi) := \begin{pmatrix} \nabla f(z) + g'(z)^T \xi + h'(z)^T \zeta \\ h(z) \\ \lambda\, \varphi_{FB}(\xi, g(z)) \\ (1-\lambda)\varphi_+(\xi, g(z)) \end{pmatrix}, \tag{34}$$

for some $\lambda \in (0,1)$ (again, we use $\lambda = 0.9$ in our implementation),

$$\varphi_{FB}(\xi, g(z)) := \big(\phi_{FB}(\xi_1, g_1(z)), \ldots, \phi_{FB}(\xi_m, g_m(z)\big)^T \in \mathbb{R}^m$$

and

$$\varphi_+(\xi, g(z)) := \big(\phi_+(\xi_1, g_1(z)), \ldots, \phi_+(\xi_m, g_m(z)\big)^T \in \mathbb{R}^m.$$

We note that the last m components are again used in order to reduce the complementarity gap at the current point z.

We now follow [21] and try to achieve the form (33) by choosing a number $N \in \mathbb{N}$, a stepsize $h = 1/(N+1)$, considering the mesh points

$$x_{ij}, \quad 0 \leq i, j \leq N+1,$$

and defining the following sets of indices (i,j), residing either in the domain Ω or on the boundary Γ:

$$\begin{aligned} I(\Omega) &:= \{(i,j) \mid 1 \leq i, j \leq N+1\}, \\ I(\Gamma) &:= \{(i,j) \mid i = 1, \ldots, N,\ j = 0 \text{ or } j = N+1, \\ &\qquad\quad j = 1, \ldots, N,\ i = 0 \text{ or } i = N+1\ \}. \end{aligned}$$

Obviously, these index sets have the cardinality $|I(\Omega)| = N^2$ and $|I(\Gamma)| = 4N$, respectively.

The optimization variable z in (33) is taken as the vector

$$z := ((y_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma)}, (u_{ij})_{(i,j)\in I(\Gamma)}) \in \mathbb{R}^{N^2+8N}.$$

Since we have Dirichlet boundary conditions, the dimension of the optimization variable z can be reduced to a vector in the smaller space $\mathbb{R}^{N^2+4N}$ by determining the state variables $(y_{ij})_{(i,j)\in I(\Gamma)}$ out of the Dirichlet conditions (31).

The discretized form of the cost function (29) then becomes

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

The application of the five-point finite difference approximation of $-\Delta$ to the elliptic equation (30) yields the following equality constraints for all $(i, j) \in I(\Omega)$:

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

Note that the Dirichlet conditions (31) are used in the above equation to substitute the variables $(y_{ij})_{(i,j)\in I(\Gamma)}$, so we have $h : \mathbb{R}^{N^2+4N} \to \mathbb{R}^{N^2}$.

The control and state inequality constraints (32) yield the inequality constraints $g : \mathbb{R}^{N^2+4N} \to \mathbb{R}^{N^2+8N}$ defined by

$$\begin{array}{lll} g_{ij}(z) & := y_{ij} - \psi_{ij} \le 0 & \forall (i,j) \in I(\Omega), \\ g_{ij}(z) & := -u_{ij} + u_{1,ij} \le 0 & \forall (i,j) \in I(\Gamma), \\ g_{n+i,n+j}(z) & := u_{ij} - u_{2,ij} \le 0 & \forall (i,j) \in I(\Gamma). \end{array}$$

In summary, we obtain a problem of the form (33) and therefore get the corresponding equation reformulation $\Phi(w) = 0$ using certain Lagrange multipliers $\zeta = (\zeta_{ij})_{(i,j)\in I(\Omega)}$ and $\xi = (\xi_{ij})_{(i,j)\in I(\Omega)\cup I(\Gamma)\cup I(\Gamma)}$.

Example 4.3 (**Control and State Constraints**) This example is taken from [21] and has the following data

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

The cost function evaluated at the optimal control and state by the authors in [21] is $f(\bar{y}, \bar{u}) = 0.196525$ for a discretization factor $N = 99$. The optimal state and adjoint variable ζ are depicted in Figure 3. The control variable is depicted in Figure 4.

Example 4.4 (**Control and State Constraints**) This example is again taken from [21] and has the same data as Example 4.3 except that $\alpha = 0$. A singular control is obtained. The cost function evaluated at the optimal control and state by the autors in [21] is $f(\bar{y}, \bar{u}) = 0.096695$ for a discretization factor $N = 99$. The optimal state and adjoint variable ζ are depicted in Figure 5. The control variable is shown in Figure 6.

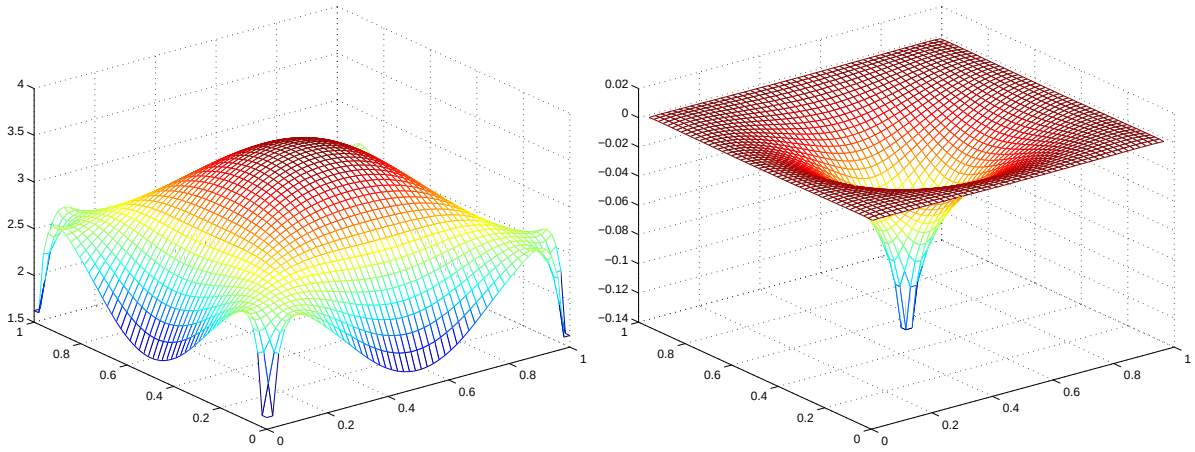

Figure 3: Optimal state (left) and adjoint variable (right) for Example 4.3

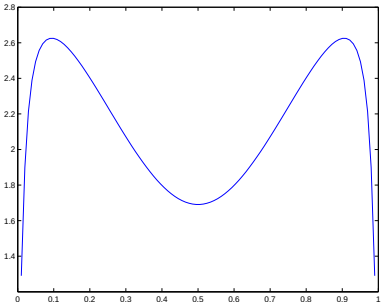

Figure 4: Optimal control for Example 4.3

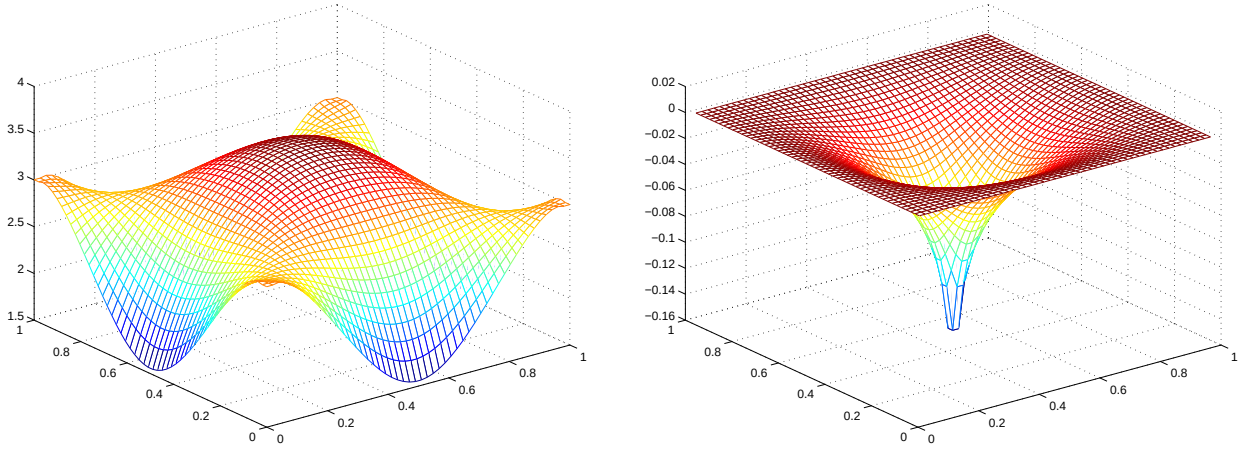

Figure 5: Optimal state (left) and adjoint variable (right) for Example 4.4

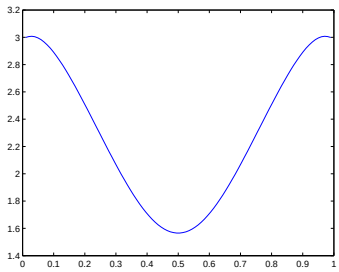

Figure 6: Optimal control for Example 4.4

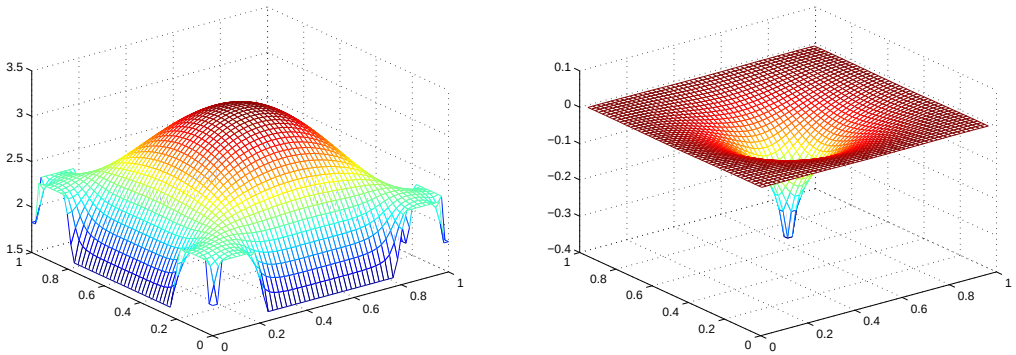

Figure 7: Optimal state (left) and adjoint variable (right) for Example 4.5

Example 4.5 (**Control and State Constraints**) This is the third example from [21] and has the same data as Example 4.3 except that the state and control constraints are more restrictive:

$$\begin{array}{ll} \text{on } \Omega & : -\Delta y(x) = 20,\ y(x) \le 3.2, \qquad y_d(x) = 3 + 5x_1(x_1-1)x_2(x_2-1), \\ \text{on } \Gamma & : y(x) = u(x),\ 1.6 \le u(x) \le 2.3 \quad u_d(x) \equiv 0,\ \alpha = 0.01. \end{array}$$

The optimal state and adjoint variable ζ are depicted in Figure 7. The control variable is shown in Figure 8. The cost function evaluated at the optimal control and state by the authors in [21] is $f(\bar{y}, \bar{u}) = 0.321010$ when using $N = 99$.

Example 4.6 (**Control and State Constraints**) This is the fourth example from [21] and has the same data as Example 4.5 except that $\alpha = 0$. We obtain a bang-bang optimal control. The optimal state and adjoint variable ζ are depicted in Figure 9. The control variable is shown in Figure 10. The cost function evaluated at the optimal control and state by the authors in [21] is $f(\bar{y}, \bar{u}) = 0.249178$ for $N = 99$.

Note that, after discretization of these examples, we obtain a nonlinear programming problem (33) with convex objective function f and linear equality and linear inequality

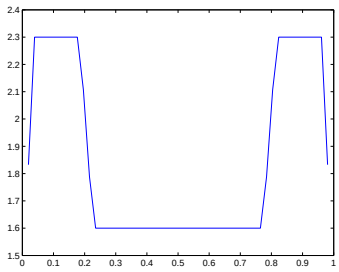

Figure 8: Optimal control for Example 4.5

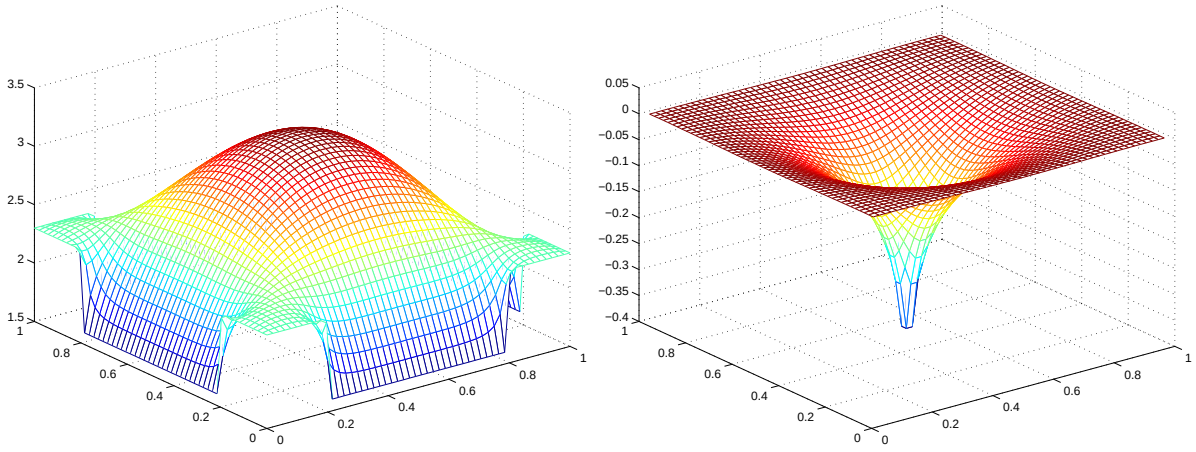

Figure 9: Optimal state (left) and adjoint variable (right) for Example 4.6

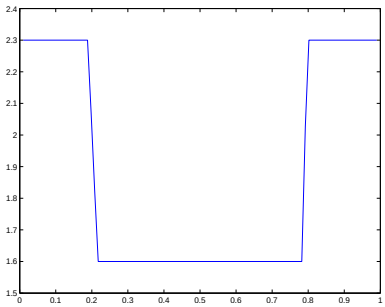

Figure 10: Optimal control for Example 4.6

constraints h and g. This implies the equivalence between (33) and the overdetermined system of equations $\Phi(x) = 0$ from (34).

We therefore applied Algorithm 2.1 using the same parameters as in the previous subsections. However, without a suitable preconditioner, LSQR was not able to solve the larger subproblems successfully. Therefore we had to find a suitable preconditioner M in order to improve the performance of the LSQR method. To this end, we note that the matrix H_k from the least squares subproblem (24) has the following structure for all test problems from Examples 4.3–4.6:

$$H_k = \left(\begin{array}{ccc|ccc} \frac{1}{(N+1)^2}I & 0 & A & I & 0 & 0 \\ 0 & \frac{\alpha}{N+1}I & B & 0 & -I & I \\ A & B^T & 0 & 0 & 0 & 0 \\ \hline \lambda D_1 & 0 & 0 & & & \\ 0 & -\lambda D_2 & 0 & & \lambda D_4 & \\ 0 & \lambda D_3 & 0 & & & \\ \hline (\lambda-1)\tilde{D}_1 & 0 & 0 & & & \\ 0 & (1-\lambda)\tilde{D}_2 & 0 & & (\lambda-1)\tilde{D}_4 & \\ 0 & (\lambda-1)\tilde{D}_3 & 0 & & & \end{array}\right),$$

where matrix $A \in \mathbb{R}^{N^2 \times N^2}$ is the five-point difference approximation to the negative Laplace operator, $B \in \mathbb{R}^{4N \times N^2}$ a sparse matrix with entries 0 or -1, and $D_i, \tilde{D}_i, i = 1, 2, 3$ are diagonal matrices of suitable dimension.

Taking into account this structure, we decided to take the matrix

$$M = \left(\begin{array}{ccc|c} 0 & 0 & A & \\ 0 & \frac{1}{N+1}I & B & 0 \\ A & B^T & 0 & \\ \hline & 0 & & I \end{array}\right)$$

as a preconditioner for the LSQR matrix since this matrix is both nonsingular and may be viewed as a suitable approximation to the leading block of H_k. Moreover, we can solve linear systems involving M once again very efficiently by a fast sine transform. The numerical results obtained with Algorithm 2.1 using this preconditioner are summerized in Table 4 using different discretizations $N \in \mathbb{N}$. The columns in Table 4 have the same meaning as those for Table 1 except that we now have one additional column which shows the optimal value $f(\bar{y}, \bar{u})$ of the cost function obtained by our method. Note that, for $N = 100$, this value is always very close to the corresponding results presented in [21].

Table 4: Numerical results for optimal control problems with mixed constraints

Example	N	Dim	o.it.	avg.i.it.	$\Psi(w^f)$	$\|\nabla\Psi(w^f)\|_\infty$	$f(\bar{y}, \bar{u})$
	50	8100	14	42.4	7.99e-09	6.19e-05	1.882782e-01

Table 4: Numerical results for optimal control problems with mixed constraints (continued)

Example	N	Dim	o.it.	avg.i.it.	$\Psi(w^f)$	$\|\nabla\Psi(w^f)\|_\infty$	$f(\bar{y},\bar{u})$
4.3	100	31200	13	55.1	3.79e-10	8.48e-06	1.965488e-01
	150	69300	23	96.5	3.53e-09	3.62e-05	1.993628e-01
4.4	50	8100	12	53.1	5.30e-10	2.63e-06	8.939136e-02
	100	31200	14	56.9	9.17e-07	9.79e-07	9.659419e-02
	150	69300	21	116.3	3.37e-07	7.93e-07	1.000500e-01
4.5	50	8100	77	1004.5	3.37e-09	5.09e-05	3.069800e-01
	100	31200	55	516.1	2.48e-06	6.35e-07	3.195118e-01
	150	69300	67	596.4	2.64e-06	7.88e-07	3.230811e-01
4.5	50	8100	84	1172.1	3.67e-09	5.02e-05	2.358106e-01
	100	31200	57	484.4	2.48e-06	4.45e-07	2.474559e-01
	150	69300	75	702.1	2.27e-06	5.43e-07	2.506512e-01

Table 4 shows that we are able to solve all optimal control problems with mixed constraints from Examples 4.3–4.6. The number of outer iterations is quite reasonable for all test runs. Also the number of inner iterations is at least acceptable taking into account the overall dimension of the problems.

4.4 Obstacle Problems

Let $\Omega \subset \mathbb{R}^2$ be a given domain with boundary $\Gamma = \partial\Omega$. The obstacle problem consists in finding the equilibrium position of an elastic membrane subject to en external force f and an obstacle ψ. Hence the infinite-dimensional problem is to minimize the total energy

$$E(u) := \frac{1}{2}\int_\Omega \|\nabla u\|^2 dx - \int_\Omega f u dx,$$

subject to the constraint

$$u \geq \psi \text{ a.e. in } \Omega.$$

The optimality conditions for this infinite-dimenional problem lead to a variational inequality which, under a weak regularity condition, is equivalent to the following complementarity problem

$$\begin{aligned} -\Delta u &\geq f \quad \text{on } \Omega, \\ u &\geq \psi \quad \text{on } \Omega, \\ (-\Delta u - f)(u-\psi) &= 0 \quad \text{on } \Omega, \\ u &\equiv 0 \quad \text{on } \Gamma. \end{aligned} \tag{35}$$

In order to discretize this problem, we take once again the standard rectangle $\Omega = (0,1)\times(0,1)$ and denote by A the five-point finite difference approximation to the

negative Laplace operator on a uniform grid with stepsize $h := 1/(n+1)$ for some $N \in \mathbb{N}$. Then, setting $v := u - \psi$, the discretized problem can be reformulated as a nonlinear complementarity problem

$$v \geq 0, F(v) \geq 0, v^T F(v) = 0 \tag{36}$$

with $F(v) := A(v + \psi) - f$. Using $f = f(v) := \lambda e^{-\psi - v}$ for some parameter $\lambda \geq 0$, we obtain the obstacle Bratu problem from [22].

We apply Algorithm 2.1 to this problem using the particular data $\psi \equiv -4, \lambda := 1$ and the same parameters as in the previous subsections. We use the matrix A as a preconditioner for the inner LSQR method. Note again that a linear system with this matrix can be solved very efficiently. The numerical results are summarized for different discretizations in Table 5.

Table 5: Numerical results for the obstacle Bratu problem

N	o.it	avg.i.it	$\Psi(x^f)$	$\|\nabla\Psi(x^f)\|_\infty$
100	7	9.9	2.67e-15	4.13e-05
200	7	11.6	3.28e-11	5.58e-02
300	8	13.9	3.55e-12	1.78e-04
400	8	14.1	6.59e-12	4.86e-04
500	8	14.2	1.05e-11	1.15e-03

Note that both the number of outer iterations and the average number of inner iterations is extremely small for this example. This is consistent with the observation made in [18] for a somewhat different method.

5 Conclusions

We have shown that the good theoretical properties of the exact semismooth Newton method applied to the least squares formulation with additional gap reduction for complementarity problems from [19] can be carried over to a inexact semismooth method. We also discussed several practical aspects of this inexact method when applied to several large-scale problems from MCPLIB, optimal control and obstacle problems. The main computational burden is then to solve a linearized least squares problem at each iteration. Here we used the LSQR method from [24] and discussed different preconditioners depending on the structure of the particular large-scale problem. Another alternative would be to use the modification of LSQR recently proposed in [16]. However, a successful application of that method also requires extra knowledge of the problem structure. We leave this as a future research topic.

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