

# A Power Penalty Method for a Bounded Nonlinear Complementarity Problem<sup>\*</sup>

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#### Abstract

We propose a novel power penalty approach to the bounded Nonlinear Complementarity Problem (NCP) in which a reformulated NCP is approximated by a nonlinear equation containing a power penalty term. We show that the solution to the nonlinear equation converges to that of the bounded NCP at an exponential rate when the function is continuous and  $\xi$ -monotone. A higher convergence rate is also obtained when the function becomes Lipschitz continuous and strongly monotone. Numerical results on discretized 'double obstacle' problems are presented to confirm the theoretical results.

**Keywords.** Bounded nonlinear complementarity problems, Nonlinear variational inequality problems, Power penalty methods, Convergence rates,  $\xi$ -monotone functions.

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### 1 Introduction

Complementarity Problems (CPs) appear naturally in many areas of science, engineering, management and finance. Typical examples of such problems are obstacle and frictional contact problems in mechanics, traffic equilibrium problem in transportation, Nash equilibrium problems in economics and option pricing problems in financial engineering (cf.,

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for example, [2, 7, 12]). Extensive studies have been done on the theoretical and computational aspects of CPs in both finite and infinite dimensional spaces. For details of these results, we refer the reader to the excellent monographs [2, 5, 7] and the references therein. Complementarity problems are in both finite and infinite dimensions. Infinite-dimensional problems usually contain partial differential operators. An infinite-dimensional CP is normally approximated by a finite dimensional one using an appropriate discretization technique (cf., for example, [5, 11]) so that numerical techniques for finite-dimensional problems can be used. Popular numerical methods for solving finite dimensional CPs, particularly for Linear Complementarity Problems (LCPs), include Newton methods, interior point methods and nonsmooth equation methods |2|. Methods for the numerical solution of Nonlinear Complementarity Problems (NCPs) have also been discussed in the open literature, though most of the existing numerical methods have been developed for unbounded NCPs, i.e., for problems defined on unbounded domains. Numerical methods for bounded complementarity problems are scarce in the open literature ([4]). On the other hand, many real world problems are often defined on bounded domains. One typical example is the 'double obstacle' type of problems arising in engineering, physics and financial engineering [3] in which the set of feasible solutions are bounded.

Penalty methods have been used very successfully for solving LCPs and NCPs in infinite dimensions such as the linear penalty methods in [5, 8, 9] and power penalty methods proposed in [12, 13]. They have also been widely used for solving continuous optimization problems (cf., for example, [10]). Recently, the power penalty methods have been also developed for LCPs and NCPs in finite dimensions [14, 6]. The main merit of the power penalty approach is its exponential convergence rates as established recently in [13, 12] for linear and nonlinear infinite dimensional problems and in [14, 6] for a finite dimensional linear and nonlinear problems. In this paper we present a power penalty approach to bounded NCPs, based on the idea in [14, 6]. To the best of our knowledge, there are no existing advances in the development of power penalty methods for bounded NCPs in finite dimensions in the open literature. Our present work aims to fill this gap by developing a power penalty method and establishing its convergence analysis. In this work, we first reformulate bounded NCPs as a standard NCP and then approximate the bounded NCPs by a nonlinear algebraic system of equations containing a power penalty term with a penalty constant  $\lambda > 1$  and a power parameter k > 0. We then show that, under certain conditions, the solution to the penalty equation converges to that of the bounded NCPs in the Euclidean norm at an exponential rate depending on  $\lambda$  and k as  $\lambda \to +\infty$ . We also carry out numerical experiments of the power penalty method on discretized non-trivial 'double obstacle' problems and our numerical results confirm our theoretical findings.

The rest of this paper is organized as follows. In the next section, we will state the bounded NCPs and reformulate it as a variational inequality. A penalty method in form of a system of nonlinear algebraic equations is then proposed to approximate the bounded NCPs. In Section 3, we establish a convergence theory for the penalty method. Numerical results are presented in Section 4.

### 2 The bounded nonlinear complementarity problem

Consider the following bounded nonlinear complementarity problem:

**Problem 2.1** Find  $x, y \in \mathbb{R}^n$  such that

$$f(x) + y \leq 0, \tag{2.1}$$

$$x \leq 0, \tag{2.2}$$

$$x^{\top}(f(x) + y) = 0, \qquad (2.3)$$

and

$$b - x \leq 0, \tag{2.4}$$

$$y \leq 0, \tag{2.5}$$

$$y^{\top}(b-x) = 0, (2.6)$$

where f(x) is an n-dimensional vector-valued function defined on  $\mathbb{R}^n$  and b < 0 is a given n-dimensional vector defining a lower bound on x.

It is easy to show that this problem arises from the KKT conditions for the minimization problem  $\min_{b \le x \le 0} \phi(x)$ , where  $\phi$  satisfies  $f(x) = \nabla \phi(x)$ . Problem 2.1 is equivalent to the bounded NCP discussed in [4]. Let

$$z = \begin{pmatrix} x \\ y \end{pmatrix}$$
 and  $w(z) = \begin{pmatrix} f(x) + y \\ b - x \end{pmatrix}$ . (2.7)

Then, Problem 2.1 can be written as the following unbounded NCP:

**Problem 2.2** Find  $z \in \mathbb{R}^{2n}$  such that

$$w(z) \leq 0, \tag{2.8}$$

$$z \leq 0, \tag{2.9}$$

$$z^{\top}w(z) = 0. (2.10)$$

Let  $\mathcal{K} = \{s \in \mathbb{R}^n : s \leq 0\}$  and denote  $\mathcal{K}^2 = \mathcal{K} \times \mathcal{K} \subset \mathbb{R}^{2n}$ . It is obvious that  $\mathcal{K}$  and  $\mathcal{K}^2$  are closed, convex and self-dual cones in respectively  $\mathbb{R}^n$  and  $\mathbb{R}^{2n}$ . Using this  $\mathcal{K}$ , we define the following variational inequality problem corresponding to Problem 2.2:

**Problem 2.3** Find  $z \in \mathcal{K}^2$  such that, for all  $u \in \mathcal{K}^2$ ,

$$(u-z)^{\top}w(z) \ge 0.$$
 (2.11)

Using a standard argument one can easily show that Problem 2.2 is equivalent to Problem 2.3 in the sense that z is a solution to Problem 2.3 if and only if it is a solution to Problem 2.2. For a detailed proof, we refer to, for example, [2, Vol.I, pp.4-5].

In what follows we use  $|| \cdot ||_p$  to denote the usual  $l_p$ -norm on  $\mathbb{R}^n$  or  $\mathbb{R}^{2n}$  for any  $p \ge 1$ . When p = 2, it becomes the Euclidean norm. We also let  $e_i$  denote the unit vector in  $\mathbb{R}^n$  defined by  $e_i = (0, ..., 0, \underbrace{1}_{i-\text{th}}, 0, ..., 0)^{\top}$  for any  $i \in \{1, 2, ..., n\}$ . Without causing confusion, we will frequently use 0 to denote the zero vector in any dimensions. Before further discussion, it is necessary to impose the following assumptions on the nonlinear function f in Problem 2.1 which will be used in the rest of this paper.

A1. f is Hölder continuous on  $\mathbb{R}^n$ , i.e., there exist constants  $\beta > 0$  and  $\gamma \in (0, 1]$  such that

$$||f(x_1) - f(x_2)||_2 \le \beta ||x_1 - x_2||_2^{\gamma}, \quad \forall x_1, x_2 \in \mathbb{R}^n.$$
(2.12)

A2. f is  $\xi$ -monotone, i.e., there exist constants  $\alpha > 0$  and  $\xi \in (1, 2]$  such that

$$(x_1 - x_2)^{\top} (f(x_1) - f(x_2)) \ge \alpha ||x_1 - x_2||_2^{\xi}, \quad \forall x_1, x_2 \in \mathbb{R}^n.$$

When f(x) = Mx, where M is a positive-definite matrix,  $\gamma = 1$  and  $\xi = 2$ , A1 and A2 were used in [14].

In the rest of this paper, we assume that Assumptions A1 and A2 are satisfied by f. Using these assumptions we are able to establish the continuity and the partial monotonicity of w(z) as given in the following theorem.

**Theorem 2.1** The function w defined in (2.7) is Hölder continuous on  $\mathbb{R}^{2n}$  and satisfies the following partial  $\xi$ -monotone property:

$$(z_1 - z_2)^{\top} (w(z_1) - w(z_2)) \ge \alpha ||x_1 - x_2||_2^{\xi}$$
(2.13)

for any  $z_1 = (x_1^{\top}, y_1^{\top})^{\top} \in \mathcal{K}^2$  and  $z_2 = (x_2^{\top}, y_2^{\top})^{\top} \in \mathcal{K}^2$ .

PROOF. From the definition of w it is easy seen that w is Hölder continuous on  $\mathbb{R}^{2n}$  because of Assumption A1. Thus, we omit this discussion and only prove (2.13).

Let  $z_1$  and  $z_2$  be two arbitrary elements in  $\mathcal{K}^2$  and partition them into  $z_1 = (x_1^{\top}, y_1^{\top})^{\top}$ and  $z_2 = (x_2^{\top}, y_2^{\top})^{\top}$  where  $x_1, x_2, y_1, y_2 \in \mathbb{R}^n$ . Then, from (2.7) we have

$$(z_1 - z_2)^{\top} (w(z_1) - w(z_2)) = \begin{pmatrix} x_1 - x_2 \\ y_1 - y_2 \end{pmatrix}^{\top} \begin{pmatrix} f(x_1) - f(x_2) + y_1 - y_2 \\ x_1 - x_2 \end{pmatrix}$$
  
=  $(x_1 - x_2)^{\top} (f(x_1) - f(x_2)) + (x_1 - x_2)^{\top} (y_1 - y_2)$   
+ $(y_1 - y_2)^{\top} (x_2 - x_1)$   
=  $(x_1 - x_2)^{\top} (f(x_1) - f(x_2))$   
 $\geq \alpha ||x_1 - x_2||_2^{\xi}$ 

by Assumption A2. Thus, we have proved (2.13).

Combining this theorem with the fact that  $\mathcal{K}^2$  is a self-dual cone we see from Theorem 2.3.5 of [2] that Problem 2.3, or equivalently Problem 2.2 has a solution. From Theorem 2.1 we see that the mapping w in Problem 2.2 is not  $\xi$ -monotone, and thus the uniqueness of the solution to Problem 2.2 is not guaranteed by existing known results. Nevertheless, for this particular problem, it is possible to show that the solution is also unique, as given in the following theorem.

#### **Theorem 2.2** There exists a unique solution to Problem 2.3.

PROOF. The existence of a solution to Problem 2.3 is simply a consequence of Theorem 2.3.5 of [2] as we commented above. Thus we omit this discussion and concentrate on the uniqueness of the solution.

Suppose  $z_1 := (x_1^{\top}, y_1^{\top})^{\top}$  and  $z_2 := (x_2^{\top}, y_2^{\top})^{\top}$  are solutions to Problem 2.3 with  $x_1, x_2, y_1, y_2 \in \mathcal{K}$ . Then  $z_1$  and  $z_2$  satisfy

$$(u-z_1)^{\top}w(z_1) \geq 0,$$
 (2.14)

$$(v - z_2)^{\top} w(z_2) \ge 0$$
 (2.15)

for any  $u, v \in \mathbb{R}^{2n}$ . Replacing u and v in (2.14) and (2.15) with  $z_2$  and  $z_1$  respectively, adding the resulting inequalities up and rearranging the terms, we have

$$(z_1 - z_2)^{\top} [w(z_1) - w(z_2)] \le 0.$$

Combining this inequality and (2.13) gives  $x_1 = x_2 =: x$ .

Now we show that  $y_1 = y_2$ . From the above we have that  $z_1 = (x^{\top}, y_1^{\top})^{\top}$  and  $z_2 = (x^{\top}, y_2^{\top})^{\top}$ . For any  $i \in \{1, 2, ..., n\}$ , if  $b^i \neq x^i$ , it is easy to see that both  $u := (x^{\top}, y_1^{\top} + e_i^{\top}(y_2^i - y_1^i)^{\top})^{\top}$  and  $v := (x^{\top}, y_2^{\top} + e_i^{\top}(y_1^i - y_2^i))^{\top}$  are in  $\mathcal{K}^2$ , where  $y_1^i$  and  $y_2^i$  denote respectively

the *i*th components of  $y_1$  and  $y_2$ . Thus, substituting these u and v into (2.14) and (2.15) respectively yields

$$\begin{array}{rcl} (y_2^i - y_1^i)(b^i - x^i) & \geq & 0, \\ (y_1^i - y_2^i)(b^i - x^i) & \geq & 0. \end{array}$$

The above two inequalities imply

$$(y_2^i - y_1^i)(b^i - x^i) = 0 (2.16)$$

for any  $i \in \{1, 2, ..., n\}$ . Thus  $y_2^i - y_1^i = 0$ .

In the case that  $b^i - x^i = 0$  for some  $i \in \{1, 2, ..., n\}$ , replacing u in (2.14) with respectively  $(x^{\top} \pm e_i^{\top} b^i, y_1^{\top})^{\top}$  (or simply use the complementarity condition (2.10)), we have

$$\begin{array}{rcl} -b^{i}(f^{i}(x)+y_{1}^{i}) & \geq & 0, \\ \\ b^{i}(f^{i}(x)+y_{1}^{i}) & \geq & 0. \end{array}$$

This implies  $y_1^i = f^i(x)$ . Similarly, replacing v in (2.15) by  $(x^\top \pm e_i^\top b^i, y_2^\top)^\top$  respectively, we have

$$\begin{aligned} -b^{i}(f^{i}(x) + y_{2}^{i}) &\geq 0, \\ b^{i}(f^{i}(x) + y_{2}^{i}) &\geq 0, \end{aligned}$$

implying  $y_2^i = f^i(x)$ . Therefore, we have  $y_1^i = y_2^i$  when  $b^i - x^i = 0$  for any  $i \in \{1, 2, ..., n\}$ . Combining this with (2.16) we get  $y_1 = y_2$ . Thus, we have proved the theorem.  $\Box$ 

## 3 The penalty formulation and its convergence analysis

Let k > 0 be a fixed parameter. Following [6], we propose the following penalty problem to approximate Problem 2.2:

**Problem 3.1** Find  $z_{\lambda} = (x_{\lambda}^{\top}, y_{\lambda}^{\top})^{\top} \in \mathbb{R}^{2n}$  with  $x_{\lambda}, y_{\lambda} \in \mathbb{R}^{n}$  such that

$$w(z_{\lambda}) + \lambda[z_{\lambda}]_{+}^{1/k} = \begin{pmatrix} f(x_{\lambda}) + y_{\lambda} \\ b - x_{\lambda} \end{pmatrix} + \lambda \begin{pmatrix} [x_{\lambda}]_{+}^{1/k} \\ [y_{\lambda}]_{+}^{1/k} \end{pmatrix} = 0,$$
(3.1)

where  $\lambda > 1$  is the penalty parameter,  $[u]_{+} = \max\{u, 0\}$  (componentwise) for any  $u \in \mathbb{R}^m$ and  $v^{\sigma} = (v_1^{\sigma}, ..., v_m^{\sigma})^{\top}$  for any  $v = (v_1, ..., v_m)^{\top} \in \mathbb{R}^m$  and constant  $\sigma > 0$ . Clearly, (3.1) is a penalty equation which approximates Problem 2.2. Equation (3.1) contains a penalty term  $\lambda[z_{\lambda}]^{1/k}_{+}$  which penalizes the positive part of  $z_{\lambda}$  when (2.8) is violated. It it easy to see from (3.1) that (2.8) is always satisfied by  $z_{\lambda}$  because  $\lambda[z_{\lambda}]^{1/k}_{+} \geq 0$ . For this penalty equation, we have the following theorem:

**Theorem 3.1** Problem 3.1 has a unique solution.

PROOF. In Lemma 2.1 we have shown that w is monotone. Since  $[v]_+$  is also monotone in v for any function v,  $\lambda[z_{\lambda}]_+^{1/k}$  is also monotone in  $z_{\lambda}$ . Therefore, from Theorem 2.3.5 of [2] we see that there exists a solution to Problem 3.1.

We now show that the solution to Problem 3.1 is unique. To achieve, we let, omitting the subscript  $\lambda$  for notation simplicity,  $z_j = (x_j^{\top}, y_j^{\top})^{\top}$ , j = 1, 2 be two solutions to Problem 3.1. Left-multiplying both sides of (3.1) by  $(z_1 - z_2)^{\top}$  and using (2.13) and the monotonicity of  $\lambda[z_{\lambda}]_{+}^{1/k}$  we have

$$\alpha ||x_1 - x_2||_2^{\gamma} \le (z_1 - z_2)^{\top} \left( w(z_1) - w(z_2) + \lambda ([z_1]_+^{1/k} - [z_2]_+^{1/k}) \right) = 0$$

Therefore,  $x_1 = x_2$ . Using this result, it is easy seen from the block of the first *n* equations in (3.1) that  $y_1 = y_2$ . Thus, the theorem is proved.

In [6] the authors show the convergence of this method for an unbounded NCPs. It would be thought that the proof in [6] applies to our present case straightforwardly. But this is not the case. As we will see later in this section, the convergence proof for Problem 3.1 is substantially different from that of the penalty method for unbounded NCPs. This is mainly because, unlike the case in [6], the function w is no longer  $\xi$ -monotone.

We start our convergence analysis with the following lemma.

**Lemma 3.1** Let  $z_{\lambda}$  be a solution to (3.1) for any  $\lambda > 1$ . Then, there exists a positive constant M, independent of  $z_{\lambda}$ ,  $\lambda$  and k, such that

$$||z_{\lambda}||_2 \le M. \tag{3.2}$$

PROOF. For any  $\lambda > 0$ , let  $z_{\lambda} = (x_{\lambda}^{\top}, y_{\lambda}^{\top})^{\top}$  be a solution to (3.1). Left-multiplying both sides of (3.1) by  $z_{\lambda}^{\top}$  gives

$$z_{\lambda}^{\top}w(z_{\lambda}) + \lambda z_{\lambda}^{\top}[z_{\lambda}]_{+}^{1/k} = 0.$$
(3.3)

Since  $z_{\lambda} = [z_{\lambda}]_{+} - [z_{\lambda}]_{-}$ , where  $[u]_{-} = \max\{-u, 0\}$ , we have

$$z_{\lambda}^{\top}[z_{\lambda}]_{+}^{1/k} = ([z_{\lambda}]_{+} - [z_{\lambda}]_{-})^{\top} [z_{\lambda}]_{+}^{1/k} = [z_{\lambda}]_{+}^{\top}[z_{\lambda}]_{+}^{1/k} \ge 0.$$

Thus, we have from (3.3)

$$z_{\lambda}^{\top}w(z_{\lambda}) \leq 0,$$

or

$$(z_{\lambda} - 0)^{\top} (w(z_{\lambda}) - w(0)) \leq -z_{\lambda}^{\top} w(0).$$

Using (2.13), we have from the above inequality

$$\alpha ||x_{\lambda}||_{2}^{\xi} \leq -z_{\lambda}^{\top} w(0) = -x_{\lambda}^{\top} f(0) - y_{\lambda}^{\top} b.$$
(3.4)

From the block of the first n equations in (3.1) we have

$$y_{\lambda} = -f(x_{\lambda}) - \lambda [x_{\lambda}]_{+}^{1/k}.$$

Substituting this into the right-hand side of (3.4) gives

$$\alpha ||x_{\lambda}||_{2}^{\xi} \leq -x_{\lambda}^{\top} f(0) + b^{\top} f(x_{\lambda}) + \lambda b^{\top} [x_{\lambda}]_{+}^{1/k}.$$

Since b < 0 and  $[x_{\lambda}]_{+} \ge 0$ , we have  $b^{\top}[x_{\lambda}]_{+}^{1/k} \le 0$ , and thus the above inequality becomes

$$\begin{aligned} \alpha ||x_{\lambda}||_{2}^{\xi} &\leq -x_{\lambda}^{\top} f(0) + b^{\top} f(x_{\lambda}) \\ &\leq ||f(0)||_{2} ||x_{\lambda}||_{2} + ||b||_{2} (\beta ||x_{\lambda}||_{2}^{\gamma} + ||f(0)||_{2}) \\ &\leq C_{1} \left( \max \left\{ ||x_{\lambda}||_{2}, ||x_{\lambda}||_{2}^{\gamma} \right\} + 1 \right), \end{aligned}$$
(3.5)

where  $C_1 = \max\{||f(0)||_2 + \beta ||b||_2, ||b||_2 ||f(0)||_2\}$ . In the above we used Cauchy-Schwarz inequality and (2.12). We assume  $||x_{\lambda}||_2 > 1$ , as otherwise  $||x_{\lambda}||_2$  is bounded above by unity. From (3.5) we have

$$\alpha ||x_{\lambda}||_{2}^{\xi} \leq C_{1} \left( ||x_{\lambda}||_{2} + 1 \right),$$

or

$$||x_{\lambda}||_{2}^{\xi-1} \le \frac{C_{1}}{\alpha} (1+||x_{\lambda}||_{2}^{-1}) \le \frac{2C_{1}}{\alpha}$$
(3.6)

since  $||x_{\lambda}||_2 > 1$  and  $\gamma \in (0, 1]$ . Therefore,  $||x_{\lambda}||_2$  is bounded for any  $\lambda > 0$ .

We now show  $y_{\lambda}$  is bounded. Left-multiplying both sides of  $f(x_{\lambda}) + y_{\lambda} + \lambda [x_{\lambda}]_{+}^{1/k} = 0$ by  $[y_{\lambda}]_{+}^{\top}$  gives

$$[y_{\lambda}]_{+}^{\top}f(x_{\lambda}) + [y_{\lambda}]_{+}^{\top}y_{\lambda} + \lambda[y_{\lambda}]_{+}^{\top}[x_{\lambda}]_{+}^{1/k} = 0.$$

$$(3.7)$$

But  $\lambda[y_{\lambda}]_{+}^{\top}[x_{\lambda}]_{+}^{1/k} \geq 0$  and

$$[y_{\lambda}]_{+}^{\top}y_{\lambda} = [y_{\lambda}]_{+}^{\top}([y_{\lambda}]_{+} - [y_{\lambda}]_{-}) = ||[y_{\lambda}]_{+}||_{2}^{2}.$$

Therefore, we have from (3.7)

$$||[y_{\lambda}]_{+}||_{2}^{2} \leq -[y_{\lambda}]_{+}^{\top}f(x_{\lambda}) \leq ||[y_{\lambda}]_{+}||_{2}||f(x_{\lambda})||_{2},$$

or there is a constant  $C_2 > 0$  such that

$$||[y_{\lambda}]_{+}||_{2} \le ||f(x_{\lambda})||_{2} \le C_{2}$$
(3.8)

since  $x_{\lambda}$  is bounded for any  $\lambda > 0$  and f is continuous. This shows that  $[y_{\lambda}]_+$  is bounded uniformly in  $\lambda$ .

Suppose  $[y_{\lambda}]_{-}$  is unbounded. Then there exists an index  $i \in \{1, 2, ..., n\}$  such that  $y_{\lambda}^{i} \to -\infty$  as  $\lambda \to \infty$ . The *i*th equation in (3.1) is

$$f^{i}(x_{\lambda}) + y^{i}_{\lambda} + \lambda [x^{i}_{\lambda}]^{1/k}_{+} = 0$$

Since  $f^i(x_{\lambda})$  is bounded uniformly in  $\lambda$ ,  $\lambda [x_{\lambda}^i]^{1/k}_+ \to \infty$  since  $y_{\lambda}^i \to -\infty$  when  $\lambda \to \infty$ . Therefore,  $x_{\lambda}^i > 0$  when  $\lambda$  is sufficiently large. Now the (n+i)th equation in (3.1) is

$$b^i - x^i_\lambda + \lambda [y^i_\lambda]^{1/k}_+ = 0.$$

When  $\lambda$  is sufficiently large,  $y_{\lambda}^{i} < 0$ , and thus from the above equation we have  $x_{\lambda}^{i} = b^{i} < 0$ , contradicting the fact that  $x_{\lambda}^{i} > 0$ . Therefore,  $[y_{\lambda}]_{-}$  is also bounded uniformly in  $\lambda$ . Combining this with (3.6) and (3.8), we have (3.2).

**Remark 3.1** Lemma 3.1 shows that for any positive  $\lambda > 1$ , the solution of (3.1) always lies in a bounded closed set  $\mathcal{D} = \{u \in \mathbb{R}^{2n} : ||u||_2 \leq M\}$ . This guarantees that there exists a positive constant L, independent of  $z_{\lambda}$ ,  $\lambda$  and k, such that

$$||w(z_{\lambda})||_2 \le L,\tag{3.9}$$

due to Assumption A1. This result will be used in the proof of the following lemma which establishes an upper bound for  $||[z_{\lambda}]_{+}||_{2}$ .

**Lemma 3.2** Let  $z_{\lambda}$  be the solution to (3.1). Then, there exists a positive constant C, independent of  $z_{\lambda}$ ,  $\lambda$  and k, such that

$$||[z_{\lambda}]_{+}||_{2} \leq \frac{C}{\lambda^{k}}.$$
(3.10)

PROOF. Decompose  $z_{\lambda}$  into  $z_{\lambda} = (x_{\lambda}^{\top}, y_{\lambda}^{\top})^{\top}$  with  $x_{\lambda}, y_{\lambda} \in \mathbb{R}^{n}$ . Left-multiplying both sides of  $(b - x_{\lambda}) + \lambda [y_{\lambda}]_{+}^{1/k} = 0$  by  $[y_{\lambda}]_{+}^{\top}$  gives

$$[y_{\lambda}]_{+}^{\top}(b-x_{\lambda}) + \lambda[y_{\lambda}]_{+}^{\top}[y_{\lambda}]_{+}^{1/k} = 0.$$

This is of the form

$$[y_{\lambda}]_{+}^{\top}(b - x_{\lambda}) + \lambda \sum_{i=1}^{n} [y_{\lambda}^{i}]_{+}^{1+1/k} = 0.$$

Let p = 1 + 1/k and q = 1 + k. Clearly, p and q satisfy 1/p + 1/q = 1. Using Hölder's inequality, we have from the above equation

$$\lambda ||[y_{\lambda}]_{+}||_{p}^{p} = [y_{\lambda}]_{+}^{\top}(x_{\lambda} - b) \leq ||[y_{\lambda}]_{+}||_{p}(||x_{\lambda}||_{q} + ||b||_{q}).$$

Therefore,

$$||[y_{\lambda}]_{+}||_{p}^{p-1} \leq \frac{1}{\lambda}(||x_{\lambda}||_{q} + ||b||_{q}) \leq \frac{C_{1}}{\lambda},$$

where  $C_1$  denotes a positive constant, independent of  $z_{\lambda}$  and  $\lambda$ . In the above we used the fact that all norms on  $\mathbb{R}^n$  are equivalent and Lemma 3.1. Taking (p-1)-root on both sides of the above estimate and noticing p-1=1/k, we finally have

$$|[y_{\lambda}]_{+}||_{p} \leq \frac{C_{1}^{k}}{\lambda^{k}}.$$

Using the fact that all norms on  $\mathbb{R}^n$  are equivalent again we see that the above inequality implies

$$||[y_{\lambda}]_{+}||_{2} \le \frac{C_{2}}{\lambda^{k}},$$
(3.11)

where  $C_2$  is also a positive constant, independent of  $z_{\lambda}$  and  $\lambda$ , that consists of  $C_1^k$  and the positive constant involved in the equivalence representation of  $||[y_{\lambda}]_+||_p$  and  $||[y_{\lambda}]_+||_2$ . This gives an upper bound for part of  $[z_{\lambda}]_+$ .

Now, left-multiplying (3.1) by  $([x_{\lambda}]^{\top}_{+}, 0^{\top})$  gives

$$[x_{\lambda}]_{+}^{\top}(f(x_{\lambda}) + y_{\lambda}) + \lambda ||[x_{\lambda}]_{+}||_{p}^{p} = 0.$$

Thus, using Hölder's inequality and the boundedness of  $||x_{\lambda}||$ , we have from the above equality

$$|[x_{\lambda}]_{+}||_{p}^{p} = -\frac{1}{\lambda}[x_{\lambda}]_{+}^{\top}(f(x_{\lambda}) + y_{\lambda})$$

$$\leq \frac{1}{\lambda}||[x_{\lambda}]_{+}||_{p}||f(x_{\lambda}) + y_{\lambda}||_{q}$$

$$\leq \frac{1}{\lambda}||[x_{\lambda}]_{+}||_{p}||w(z_{\lambda})||_{q}.$$

Using (3.9) and the fact that all norms on  $\mathbb{R}^n$  are equivalent we obtain from the above estimates

$$||[x_{\lambda}]_+||_p^{p-1} \le \frac{C_3}{\lambda},$$

where  $C_3$  is a combination of L in (3.9) and the positive constant involved in the equivalence representation of  $||w(z_{\lambda})||_q$  and  $||w(z_{\lambda})||_2$ . Taking (p-1)-root on both sides and noticing again that all norms on  $\mathbb{R}^n$  are equivalent, we get

$$|[x_{\lambda}]_+||_2 \le \frac{C_4}{\lambda^k},$$

where  $C_4$  is a positive constant, independent of  $z_{\lambda}$  and  $\lambda$ . Finally, using this estimate and (3.11) we have

$$||[z_{\lambda}]_{+}||_{2} = \sqrt{||[x_{\lambda}]_{+}||_{2}^{2} + ||[y_{\lambda}]_{+}||_{2}^{2}} \le \frac{C}{\lambda^{k}}$$

This completes the proof.

**Lemma 3.3** Let  $z = (x^{\top}, y^{\top})^{\top}$  be a solution to Problem 2.2. Then y and f(x) + y are orthogonal.

PROOF. When the *i*th component of y is non-zero, i.e.,  $y^i \neq 0$  for an  $i \in \{1, 2, ..., n\}$ , from the complementarity condition (2.6) (or (2.10)) we have

$$x^i = b^i < 0.$$

Thus, the complementarity condition (2.3) gives  $f^i(x) + y^i = 0$ . Therefore, we have

$$y^{\top}(f(x) + y) = 0.$$
 (3.12)

Using Lemmas 3.2 and 3.3, we are ready to present and prove our main convergence results as given in the following theorem.

**Theorem 3.2** Let  $z := (x^{\top}, y^{\top})^{\top}$  and  $z_{\lambda} := (x_{\lambda}^{\top}, y_{\lambda}^{\top})^{\top}$  be the solutions to Problems 2.2 and 3.1, respectively, where  $x^{\top}, y^{\top} \in \mathcal{K}$  and  $x_{\lambda}^{\top}, y_{\lambda}^{\top} \in \mathbb{R}^{n}$ . There exists a constant K > 0, independent of  $z_{\lambda}$ ,  $\lambda$  and k, such that

$$||x - x_{\lambda}||_{2} \leq K \max\left\{\frac{1}{\lambda^{k/(\xi - \gamma)}}, \frac{1}{\lambda^{k/\gamma}}\right\}, \qquad (3.13)$$

$$||y - y_{\lambda}||_{2} \leq K \max\left\{\frac{1}{\lambda^{k}}, \frac{1}{\lambda^{\xi k/[2(\xi - \gamma)]}}, \frac{1}{\lambda^{\gamma k/(\xi - \gamma)}}\right\},$$
(3.14)

for sufficiently large  $\lambda$ , where  $\gamma$  and  $\xi$  are constants used in Assumptions A1 and A2 respectively.

PROOF. In this proof we use  $C_i$  for any subscript *i* to denote a positive constant, independent of  $z_{\lambda}$  and  $\lambda$ . We first show (3.13) in a similar way as that in [6], as given below.

We decompose  $z - z_{\lambda}$  into

$$z - z_{\lambda} = z + [z_{\lambda}]_{-} - [z_{\lambda}]_{+} =: r_{\lambda} - [z_{\lambda}]_{+}, \qquad (3.15)$$

where  $r_{\lambda} = z + [z_{\lambda}]_{-}$ . Noticing

$$z - r_{\lambda} = -[z_{\lambda}]_{-} \le 0,$$

we have  $z - r_{\lambda} \in \mathcal{K}^2$ . Note that z is a solution to Problem 2.2 and thus satisfies (2.11). Therefore, replacing u in (2.11) with  $z - r_{\lambda}$  gives

$$-r_{\lambda}^{\top}w(z) \ge 0. \tag{3.16}$$

Since  $z_{\lambda}$  satisfies (3.1), left-multiplying both sides of (3.1) by  $r_{\lambda}^{\top}$ , we have

$$r_{\lambda}^{\top}w(z_{\lambda}) + \lambda r_{\lambda}^{\top}[z_{\lambda}]_{+}^{1/k} = 0.$$
(3.17)

Adding up both sides of (3.16) and (3.17) gives

$$r_{\lambda}^{\top} \left( w(z_{\lambda}) - w(z) \right) + \lambda r_{\lambda}^{\top} [z_{\lambda}]_{+}^{1/k} \ge 0.$$
(3.18)

Note that

$$r_{\lambda}^{\top}[z_{\lambda}]_{+}^{1/k} = (z + [z_{\lambda}]_{-})^{\top}[z_{\lambda}]_{+}^{1/k} = z^{\top}[z_{\lambda}]_{+}^{1/k} \le 0,$$

because  $[z_{\lambda}]_{-}^{\top}[z_{\lambda}]_{+}^{1/k} = 0, \ z \leq 0 \ \text{and} \ [z_{\lambda}]_{+} \geq 0$ . Thus, (3.18) reduces to

$$r_{\lambda}^{\top}(w(z) - w(z_{\lambda})) \le 0.$$

Using (3.15), we have from the above inequality

$$(z - z_{\lambda} + [z_{\lambda}]_{+})^{\top} (w(z) - w(z_{\lambda})) \le 0,$$

or equivalently

$$(z - z_{\lambda})^{\top} (w(z) - w(z_{\lambda})) \leq -[z_{\lambda}]^{\top}_{+} (w(z) - w(z_{\lambda})).$$

Using (2.13) and Cauchy-Schwarz inequality we have from the above inequality

$$\begin{aligned} \alpha ||x - x_{\lambda}||_{2}^{\xi} &\leq (z - z_{\lambda})^{\top} (w(z) - w(z_{\lambda})) \\ &\leq -[z_{\lambda}]_{+}^{\top} (w(z) - w(z_{\lambda})) \\ &\leq ||[z_{\lambda}]_{+}||_{2} ||w(z) - w(z_{\lambda})||_{2}. \end{aligned}$$
(3.19)

From (3.9) and (3.10) we have from the above

$$||x - x_{\lambda}||_{2} \le \frac{C_{1}}{\lambda^{k/\xi}} < 1$$
 (3.20)

when  $\lambda$  is sufficiently large.

Now, using (2.12), (3.10) and (2.7) we have from (3.19)

$$\begin{aligned} ||x - x_{\lambda}||_{2}^{\xi} &\leq 2||[z_{\lambda}]_{+}||_{2} \left(||f(x) - f(x_{\lambda})||_{2} + ||y - y_{\lambda}||_{2} + |x - x_{\lambda}||_{2}\right) \\ &\leq C_{2}||[z_{\lambda}]_{+}||_{2} \left(||x - x_{\lambda}||_{2}^{\gamma} + ||y - y_{\lambda}||_{2} + ||x - x_{\lambda}||_{2}\right) \\ &\leq \frac{C_{3}}{\lambda^{k}} \left(||x - x_{\lambda}||_{2}^{\gamma} + ||y - y_{\lambda}||_{2}\right) \end{aligned}$$
(3.21)

when  $\lambda$  is sufficiently large, where  $C_2 = \max\{\beta, 1\}$  and  $C_3 = 2C_2C_1$ . In the above we used  $||x - x_{\lambda}||_2 < ||x - x_{\lambda}||_2^{\gamma}$  because of (3.20) and  $\gamma \leq 1$ .

We now consider the estimation of  $||y - y_{\lambda}||_2$ . Let  $s_{\lambda} = y + [y_{\lambda}]_{-}$ . Then,

$$y - y_{\lambda} = y - ([y_{\lambda}]_{+} - [y_{\lambda}]_{-}) = s_{\lambda} - [y_{\lambda}]_{+}.$$
(3.22)

Left-multiplying (3.1) by  $(s_{\lambda}^{\top}, 0^{\top})$  yields

$$s_{\lambda}^{\top}(f(x_{\lambda}) + y_{\lambda}) + \lambda s_{\lambda}^{\top}[x_{\lambda}]_{+}^{1/k} = 0.$$
(3.23)

From the definition of  $s_{\lambda}$  we see that  $y - s_{\lambda} = -[y_{\lambda}]_{-} \leq 0$  and so  $y - s_{\lambda} \in \mathcal{K}$ . Thus, letting  $u = z + ((y - s_{\lambda})^{\top}, 0^{\top})^{\top}$  in (2.11), we get

$$(y - s_{\lambda})^{\top} (f(x) + y) \ge 0,$$

or equivalently,

$$-s_{\lambda}^{\top}(f(x)+y) + y^{\top}(f(x)+y) \ge 0.$$
(3.24)

Adding up both sides of (3.23) and (3.24) gives

$$s_{\lambda}^{\top}[(f(x_{\lambda}) - f(x)) + (y_{\lambda} - y)] + \lambda s_{\lambda}^{\top}[x_{\lambda}]_{+}^{1/k} + y^{\top}(f(x) + y) \ge 0.$$
(3.25)

From Lemma 3.3, y and f(x) + y are orthogonal. For the term  $s_{\lambda}^{\top}[x_{\lambda}]_{+}^{1/k}$  in (3.25), we have from the definition of  $s_{\lambda}$ 

$$s_{\lambda}^{\top} [x_{\lambda}]_{+}^{1/k} = y^{\top} [x_{\lambda}]_{+}^{1/k} + [y_{\lambda}]_{-}^{\top} [x_{\lambda}]_{+}^{1/k}.$$
(3.26)

If  $y_{\lambda}^i < 0$  (or  $[y_{\lambda}^i]_- > 0$ ) for some  $i \in \{1, 2, ..., n\}$ , we have  $[y_{\lambda}^i]_+ = 0$ , and the (n + i)th (scalar) equation of (3.1) becomes

$$b^i - x^i_\lambda = 0 \quad \text{or} \quad x^i_\lambda = b^i < 0.$$

This implies that  $[x_{\lambda}^{i}]_{+} = 0$ . We thus have

$$[y_{\lambda}]_{-}^{\top}[x_{\lambda}]_{+} = 0.$$

Using this complementarity relationship, we have from (3.26)

$$s_{\lambda}^{\top} [x_{\lambda}]_{+}^{1/k} = y^{\top} [x_{\lambda}]_{+}^{1/k} \le 0, \qquad (3.27)$$

since  $y \leq 0$  and  $[x_{\lambda}]^{1/k}_{+} \geq 0$ . Using (3.12) and (3.27) we obtain from (3.25)

$$s_{\lambda}^{\top}[f(x_{\lambda}) - f(x)] + s_{\lambda}^{\top}(y_{\lambda} - y) \ge 0.$$

But  $s_{\lambda} = y - y_{\lambda} + [y_{\lambda}]_{+}$  by (3.22). Thus, the above inequality becomes

$$(y - y_{\lambda} + [y_{\lambda}]_{+})^{\top} [f(x_{\lambda}) - f(x)] + [y_{\lambda}]_{+}^{\top} (y_{\lambda} - y) - (y_{\lambda} - y)^{\top} (y_{\lambda} - y) \ge 0.$$

Using Cauchy-Schwarz inequality, (2.12) and (3.10) we have from the above inequality

$$\begin{aligned} ||y_{\lambda} - y||_{2}^{2} &\leq (y - y_{\lambda} + [y_{\lambda}]_{+})^{\top} [f(x_{\lambda}) - f(x)] + [y_{\lambda}]_{+}^{\top} (y_{\lambda} - y) \\ &\leq (||y_{\lambda} - y||_{2} + ||[y_{\lambda}]_{+}||_{2})||f(x_{\lambda}) - f(x)||_{2} \\ &+ ||[y_{\lambda}]_{+}||_{2}||y_{\lambda} - y||_{2} \\ &\leq C_{4} \left( \left( ||x - x_{\lambda}||_{2}^{\gamma} + \frac{1}{\lambda^{k}} \right) ||y_{\lambda} - y||_{2} + \frac{||x - x_{\lambda}||_{2}^{\gamma}}{\lambda^{k}} \right), \end{aligned}$$

since  $\gamma \in (0, 1]$ , where  $C_4 = \max\{\beta, C, C\beta\}$ . Let  $u = ||x - x_\lambda||_2$  and  $v = ||y - y_\lambda||_2$ . Then, the above inequality becomes

$$v^2 \le C_4 \left( u^{\gamma} + \frac{1}{\lambda^k} \right) v + \frac{C_4 u^{\gamma}}{\lambda^k}.$$

This can be rewritten as

$$\left(v - \frac{C_4}{2}\left(u^{\gamma} + \frac{1}{\lambda^k}\right)\right)^2 \le \frac{C_4 u^{\gamma}}{\lambda^k} + \frac{C_4^2}{4}\left(u^{\gamma} + \frac{1}{\lambda^k}\right)^2.$$

Taking square-root on both sides of the above and rearranging the resulting inequality, we have

$$v \leq \left(\frac{C_4 u^{\gamma}}{\lambda^k} + \frac{C_4^2}{4} \left(u^{\gamma} + \frac{1}{\lambda^k}\right)^2\right)^{1/2} + \frac{C_4}{2} \left(u^{\gamma} + \frac{1}{\lambda^k}\right)$$
$$\leq \frac{C_4^{1/2} u^{\gamma/2}}{\lambda^{k/2}} + C_4 \left(u^{\gamma} + \frac{1}{\lambda^k}\right)$$
$$\leq C_5 \left(\frac{1}{\lambda^k} + \frac{u^{\gamma/2}}{\lambda^{k/2}} + u^{\gamma}\right), \qquad (3.28)$$

where  $C_5 = \max\{C_4^{1/2}, C_4\}$ . Replacing  $v = ||y - y_\lambda||_2$  on the right-hand side of (3.21) with the above bound and combining like terms, we get

$$u^{\xi} \le \frac{C_6}{\lambda^k} \left( \frac{1}{\lambda^k} + \frac{u^{\gamma/2}}{\lambda^{k/2}} + u^{\gamma} \right), \tag{3.29}$$

where  $C_6 = 1 + C_5$ . If  $u^{\gamma} \le u^{\gamma/2} / \lambda^{k/2}$ , we have

$$u \le \frac{1}{\lambda^{k/\gamma}}.\tag{3.30}$$

When  $u^{\gamma} > u^{\gamma/2}/\lambda^{k/2}$ , from (3.29) we have

$$u^{\xi} \le \frac{C_6 u^{\gamma}}{\lambda^k} + \frac{C_6}{\lambda^{2k}}.$$

Rearranging the above gives

$$u^{\gamma}\left(u^{\xi-\gamma} - \frac{C_6}{\lambda^k}\right) \le \frac{C_6}{\lambda^{2k}}.$$
(3.31)

Therefore, if  $u^{\xi-\gamma} - \frac{C_6}{\lambda^k} \leq 0$ , we have

$$u \le \frac{C_6}{\lambda^{k/(\xi-\gamma)}}.\tag{3.32}$$

When  $u^{\xi-\gamma} - \frac{C_6}{\lambda^k} > 0$ , from (3.31) it is easy seen

$$\min\left\{u^{2\gamma}, \left(u^{\xi-\gamma} - \frac{C_6}{\lambda^k}\right)^2\right\} \le u^{\gamma}\left(u^{\xi-\gamma} - \frac{C_6}{\lambda^k}\right) \le \frac{C_6}{\lambda^{2k}}.$$

This yields either (3.30) or (3.32). Therefore, combining the two cases we have (3.13) for some positive constant K, independent of  $z_{\lambda}$  and  $\lambda$ .

Finally, replacing u on the right-hand side of (3.28) with the upper bound in (3.13) we have (3.14). This completes the proof.

Theorem 3.2 establishes upper bounds for the approximation error between  $x_{\lambda}$  and xand that between  $y_{\lambda}$  and y. These upper bounds depend on the parameters in Assumptions A1 and A2 and Problem 3.1. In general,  $x_{\lambda}$  and  $y_{\lambda}$  converge respectively to x and y at the different rates as given in (3.13) and (3.14). However, when f(x) becomes strongly monotone and Lipschitz continuous, i.e.,  $\gamma = 1$  and  $\xi = 2$  in Assumptions A1 and A2 respectively, both  $x_{\lambda}$  and  $y_{\lambda}$  converge to their counterparts at the same rate  $\mathcal{O}(\lambda^{-k})$ . This is given in the following corollary.

**Corollary 3.1** Let z and  $z_{\lambda}$  be respectively the solutions to Problems 2.3 and 3.1. If f is Lipschitz continuous and strongly monotone, then, when  $\lambda$  is sufficiently large, we have

$$||z - z_{\lambda}||_2 \le \frac{K_1}{\lambda^k},\tag{3.33}$$

for some positive constant  $K_1$ , independent of  $z_{\lambda}$ ,  $\lambda$  and k.

PROOF. When f is Lipschitz continuous and strongly monotone, we have  $\gamma = 1$  and  $\xi = 2$  in Assumptions A1 and A2. Thus, (3.33) follows from (3.13)–(3.14) and the triangular inequality.

### 4 Numerical Results

We now present some numerical results to support our theoretical findings. Two infinitedimensional double obstacle problems have been solved using our penalty method. Note that the penalty equation (3.1) is nonlinear even when k = 1. To solve (3.1), we use the usual damped Newton's method with a damping parameter  $\theta$ . Also, the penalty term is non-smooth and in computation both  $[x_{\lambda}]^{1/k}_{+}$  and  $[y_{\lambda}]^{1/k}_{+}$  are smoothed out by the smoothing technique used in [6]). For all the test cases below, we use  $x_{\lambda}^{i} = -0.1 = y_{\lambda}^{i}$  as the initial guess for the Newton's method for all feasible *i*. The damping parameter is chosen to be  $\theta = 0.2$  for all of the computation. All the computations have been performed in double precision on a MacBook Pro with Intel Core i5 under Matlab R2012a programming environment.

**Test 1.** The first test problem is chosen to be the following problem: find u and v such that

$$\begin{aligned} -u''(s) + u^3(s) - g(s) + v(s) &\leq 0, \\ u(s) &\leq 0, \\ u(s)(-u''(s) + u^3(s) - g(s) + v(s)) &= 0, \\ p(s) - u(s) &\leq 0, \\ v(s) &\leq 0, \\ v(s)(p(s) - u(s)) &= 0 \end{aligned}$$

in  $s \in (0,1)$  satisfying the boundary conditions u(0) = u(1) = 0, where g and p are two given functions. It is easy to check that the above bounded NCP arises from the application of the KKT conditions and the calculus of variations to the following 'double obstacle' problem

$$\min_{p \le u \le 0} J(u) = \int_0^1 \left( \frac{1}{2} (u')^2 + \frac{1}{4} u^4 - ug \right) ds$$

satisfying that u is twice continuously differentiable and u(0) = u(1) = 0. We choose  $g(s) = -4\pi^2 \sin(2\pi s) + \sin^3(2\pi s)$  and  $p(s) = \sin(2\pi s) - 1.5$ . It is easy to verify that the unconstrained problem corresponding to the above one has the exact solution  $u = -\sin(2\pi s)$ .

To discretize the above bounded complementarity problem, we divide the solution interval [0,1] uniformly into n sub-intervals with n + 1 mesh points  $s_i = hi$  for i = 0, 1, ..., N, where h = 1/N. Applying the standard central finite difference scheme on the mesh to the above problem yields the finite-dimensional bounded NCP of the form (2.1)-(2.6) with

$$f(x) = Ax + x^3 - c,$$

where  $x = (x_1, ..., x_{N-1})^{\top}$  and  $y = (y_1, ..., y_{N-1})^{\top}$  are unknown nodal approximations to uand v respectively at the mesh points,  $b = (p(s_1), ..., p(s_{N-1}))^{\top}$ ,  $c = (g(s_1), ..., g(s_{N-1}))^{\top}$ and A is the following symmetric, positive-definite  $(N-1) \times (N-1)$  tri-diagonal matrix:

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}.$$

$\lambda = \frac{5^{2-k} \times 2^i}{h^2}$		i = 0	i = 1	i = 2	i = 3	i = 4	i = 5
k = 1	Errors	1.32e-1	7.95e-2	3.95e-2	1.97e-2	9.81e-3	4.90e-3
	Ratios	_	1.67	2.01	2.01	2.00	2.00
k = 2	Errors	2.30e-3	5.75e-4	1.44e-4	3.59e-5	8.97e-6	2.24e-6
	Ratios	_	4.01	4.00	4.00	4.00	4.00
k = 3	Errors	8.43e-4	1.05e-4	1.31e-5	1.64e-6	2.05e-7	2.57e-8
	Ratios	_	8.02	8.00	8.00	8.00	8.00
k = 4	Errors	8.01e-3	4.83e-4	3.01e-5	1.88e-6	1.18e-7	7.35e-9
	Ratios	_	16.6	16.0	16.0	16.0	16.0

Table 4.1: Computed rates of convergence in  $\lambda$  for Test 1.

We now choose N = 100 (h = 0.01) and consider the solution of the penalty equation (3.1) corresponding to the above finite-dimensional bounded NCP.

To test the rates of convergence, we use the solution with k = 2 and  $\lambda = 10^{10}/h^2$ as the 'exact' or reference solution, say  $z^*$ . Let us first investigate the computed rates of convergence of the method in  $\lambda$  for a fixed value of k. To achieve this, we solve the problem using one sequence of values of  $\lambda$  for each given value of k. This sequence is chosen to be  $\lambda_i = 5^{2-k} \times 2^i/h^2$  for i = 0, 1, ..., 5. The computed errors  $||z^* - z_{\lambda_i}||_2$  are listed in Table 4.1 for k = 1, 2, 3 and 4 and the chosen values of  $\lambda$ . We also list the ratios  $||z^* - z_{\lambda_{i-1}}||_2/||z^* - z_{\lambda_i}||_2(i = 1, ..., 5)$  of two consecutive errors in the table for each k. From (3.33) it is easy to see that the theoretical ratio for two consecutive values of  $\lambda$  is equal to  $\lambda_{i+1}^k/\lambda_i^k = 2^k$ . From Table 4.1, we see that our computed ratios are very close to these theoretical ones, i.e.,  $2^k$ , for all k = 1, 2, 3 and 4.

Finally, we plot the computed solution u along with the lower bound  $p(s) = \sin(2\pi s) - 1.5$  in Figure 4.1(a) and the computed v in Figure 4.1(b). From Figure 4.1 we see that u is bounded above and below by respectively 0 and p(s). From Figure 4.1 (b) we see that when the lower bound becomes active, v is negative. Otherwise, it is zero.

Test 2. Consider the following 2D obstacle problem:

$$\min_{p_1 \le u \le p_2} J(u) := \int_{\Omega} \left( \frac{1}{2} \nabla u(s,t) \cdot \nabla u(s,t) + \left( \frac{1}{4} u^4(s,t) - g(s,t) \right) u \right) ds dt, \tag{4.1}$$

satisfying u = 0 on the boundary of  $\Omega$ , where  $\Omega = (0, 1) \times (0, 1)$ ,  $g_1(s, t)$  and  $g_2(s, t)$  are given functions defining the lower and upper bounds on the solution u, and g(s, t) is also a known function. This test problem is given in [1] with the forcing term  $(\frac{1}{4}u^4 - g)$ .

As for Test 1, to solve this problem, it is necessary to discretize it first. Let  $\Omega$  be divided uniformly into  $N^2$  subdomains with mesh nodes  $(s_i, t_j) = (ih, jh)$  for i, j =0, 1, ..., N, where h = 1/N. We re-order the  $dof := (N - 1)^2$  mesh nodes inside  $\Omega$  as  $q_1 = (s_1, t_1), q_2 = (s_2, t_1), ..., q_N = (s_1, t_2), ..., q_{dof} = (s_{N-1}, t_{N-1})$ . As mentioned in

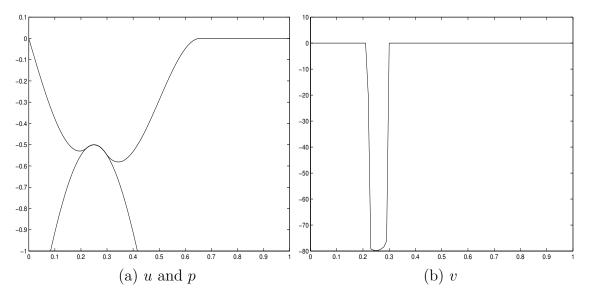


Figure 4.1: Computed solutions u and v along with the lower bound p of Test 1.

[1], application of a suitable finite difference scheme to (4.1) yields the following finite dimensional problem:

$$\min_{b_1 \le x \le b_2} \left( \frac{1}{2} x^\top A x + \frac{1}{4} ||x^2||_2^2 - d^\top x \right), \tag{4.2}$$

where x is an approximation of  $(u(q_1), ..., u(q_{dof}))^{\top}$ ,  $b_k = (p_k(q_1), ..., p_k(q_{dof}))^{\top}$  for k = 1, 2,  $d = (g(q_1), ..., g(q_{dof}))^{\top}$  and  $A = (a_{i,j})$  is the dof  $\times$  dof pentadiagonal matrix with the entries

$$a_{i,i} = 4$$
,  $a_{i,j-(N-1)} = a_{i,j-1} = a_{i,j+1} = a_{i,j+(N-1)} = -1$ ,

for all feasible (i, j) and  $a_{i,j} = 0$  otherwise.

Note that (4.2) is not in the desired form which has the KKT conditions as in Problem 2.1, as  $b_2 \neq 0$ . Let  $\bar{x} = x - b_2$  and  $b = b_1 - b_2$ , it is trivial to verify that (4.2) can be transformed into the following problem:

$$\min_{b \le \bar{x} \le 0} \left( \frac{1}{2} (\bar{x} + b_2)^\top A(\bar{x} + b_2) + \frac{1}{4} ||(\bar{x} + b_2)^2||_2^2 - d^\top (\bar{x} + b_2) \right).$$

The KKT conditions corresponding the above minimization problem is of the same form as in Problem 2.1 with  $f(\bar{x}) = A(\bar{x} + b_2) + (\bar{x} + b_2)^3 - d$ .

Now, we choose

$$p_1 = -s - t,$$
  

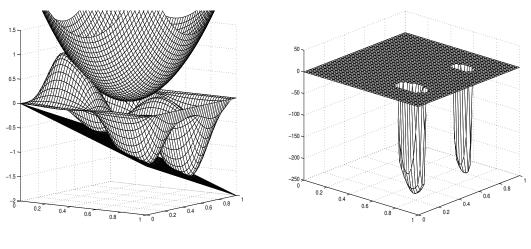
$$p_2 = 6[(s - 0.5)^2 + (t - 0.5)^2],$$
  

$$g = 4\pi \sin(2\pi s)(1 - 5\cos(4\pi t)) + \sin(2\pi s)^3(1 - \cos(4\pi t))^3.$$

It is easy to verify that the unconstrained solution to (4.1) is  $u_{\text{unc}} = \sin(2\pi s)[1-\cos(4\pi t)]$ . We also chose N = 50, and use the numerical solution from k = 2 and  $\lambda = 10^{10}/h^2$  as the

$\lambda = \frac{5^{3-k} \times 2^i}{h^2}$		i = 0	i = 1	i = 2	i = 3	i = 4	i = 5
k = 1	Errors	1.85e0	9.26e-1	4.72e-1	2.34e-1	1.17e-1	5.83e-2
	Ratios	_	2.00	1.96	2.01	2.01	2.00
k = 2	Errors	1.06e-1	2.63e-2	6.56e-3	1.64e-3	4.19e-4	1.03e-4
	Ratios	_	4.02	4.00	4.00	4.00	4.00
k = 3	Errors	1.78e-1	2.20e-2	2.74e-3	3.43e-4	4.28e-5	5.36e-6
	Ratios	_	8.09	8.01	8.00	8.00	8.00
k = 4	Errors	7.29e0	5.12e-1	3.13e-2	1.96e-3	1.23e-4	7.66e-6
	Ratios	_	14.2	16.2	16.0	16.0	16.0

Table 4.2: Computed rates of convergence in  $\lambda$  for Test 2.



(a)  $u, p_1$  and  $p_2$ 

(b) multiplier

Figure 4.2: Computed solution u and the multiplier, along with the lower and upper bounds  $p_1$  and  $p_2$  of Test 2.

reference solution for calculating rates of convergence. Table 4.2 contains the computed rates of convergence in the same way as used in Test 1. From the table we see that the computed rates match the theoretical one as for Test 1. The numerical solution to (4.1), the lower and upper bounds  $p_1$  and  $p_2$ , along with the multiplier y in Problem 2.1, are plotted in Figure 4.2. From Figure 4.2(b) we see that the multiplier is zero when the lower bound constraint  $p_1$  is inactive and negative when it is active. Note that the multiplier corresponding the upper bound  $p_2$  was eliminated during the formulation of Problem 2.1.

To conclude this section, we present some numerical results to demonstrate the influence of the size of the problem and k on the number of Newton's iterations and computational costs. In Table 4.3, we list the CPU time in seconds and numbers of Newton's iterations for difference mesh sizes and values of k. As can be seen from the figure, there is a small to moderate increase in the number of iterations as the dimension of Prob-

	No. of Newton's iter.				CPU times in sec.			
Mesh / $k =$	1	2	3	4	1	2	3	4
$10 \times 10$	124	115	96	96	0.29	0.24	0.21	0.23
$20 \times 20$	137	115	103	102	0.87	0.64	0.56	0.62
$40 \times 40$	151	126	112	110	2.61	2.34	2.25	2.25
$80 \times 80$	167	138	122	117	26.10	22.65	21.00	19.50
$160 \times 160$	187	156	140	127	120.86	99.65	92.58	82.67

Table 4.3: Numners of Newton's iterations and CPU time in seconds for Test 2.

lem 2.1 is quadrupled, indicating that the numerical solution of the penalty equation is insensitive to the number of unknowns. It is also interesting to see that the number of Newton's iterations decreases as k increases. However, the numbers of Newton's iterations for different values of k may not be absolutely comparable, as the results in Table 4.3 were obtained using the same damping parameter  $\theta = 0.2$ . Our numerical experiments show that  $\theta$  can be chosen to be larger than 0.2 for k < 4. For example, when k = 1, the standard Newton's method (i.e.,  $\theta = 1$ ) converges and thus it needs a smaller number of iterations than the corresponding ones listed in Table 4.3 to solve the problem.

We comment that it is non-trivial to find a non-trivial example in which the mapping only satisfies Hölder, not Lipschitz, continuity condition (2.12). We leave the numerical verification of the convergence rates for this general case to our future research.

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