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VALIDATED SOLUTIONS OF MIXED COMPLEMENTARITY PROBLEMS

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Abstract: We propose at first a method of computing validated solutions of mixed complementarity problem, here a validated solution is meant an approximate solution with guaranteed error bound. By utilizing the component identification property of the validated solution, we then give a method which sharpens the validated solution by solving systems of equations with reduced dimensions. The efficiency of the method is illustrated by numerical results.

Key words: *complementarity problem, error bound, validated solution*

Mathematics Subject Classification: *90C33, 65G30, 65K10*

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1 Introduction

Let $F : R^n \to R^n$, let $l = (l_i) \in \{R \cup \{-\infty\}\}^n$ and $u = (u_i) \in \{R \cup \{\infty\}\}^n$ be given with $l < u$. The mixed complementarity problem, denoted by MCP(l, u, F), is to find $x^* \in R^n$ with $l \leq x^* \leq u$ such that

$$(y - x^*)^T F(x^*) \geq 0 \qquad \text{for all } l \leq y \leq u \quad \text{and} \quad y \in R^n. \tag{1.1}$$

Particularly, when $l_i = 0$ and $u_i = \infty$, $i = 1, \ldots, n$, MCP(l, u, F) reduces to the standard nonlinear complementarity problem, which is to find an x^* such that

$$x^* \geq 0, \qquad F(x^*) \geq 0, \qquad (x^*)^T F(x^*) = 0. \tag{1.2}$$

MCPs have many real world applications, see [8]. For solving the problem, various methods have been developed, see Facchinei and Pang [7] for a comprehensive treatment. However, few of the existing methods can provide *validated solution*, which is meant an approximate solution with guaranteed error bounds accompanied. For solving the MCPs in a real-world setting, several types of error arise, like the approximation error caused in the practical implementation of an iterative method, the data error and the round-off error caused in the numerical computation performed on the floating point number system. An error bound is called guaranteed if it covers all these errors. Without reliable error information a numerical solution may be only of doubtful utility. In some application settings it does not even imply that the problem has a true solution.

In this paper, we propose a method for computing an interval vector that encloses a true solution of the MCP. If our method is performed on some interval-arithmetic based platform for tracking the round-off error and for controlling the data error, then the method delivers a validated solution, and this is very helpful for giving a safe solution of the applied problem. Moreover, by the output interval vector, one can identify some components of the true solution. Based on this, an approximate solution of the MCP can be computed by solving some equations with reduced dimensions.

Throughout this paper we restrict our study on the complementarity problem with the function F fulfilling the following conditions.

Assumption 1.1. Let $[z]$ be a given interval vector and let $\hat{x} = (\hat{x}_i) \in [z]$ be fixed. Assume:

- there exist constants γ_{ij}, $i, j = 1, \ldots, n$, $j \neq i$, such that for all $x = (x_i) \in [z]$, $x_j \neq \hat{x}_j$

$$\left| \frac{F_i(\hat{x}_1, \cdots, \hat{x}_{j-1}, x_j, x_{j+1}, \cdots, x_n) - F_i(\hat{x}_1, \cdots, \hat{x}_{j-1}, \hat{x}_j, x_{j+1}, \cdots, x_n)}{x_j - \hat{x}_j} \right| \leq \gamma_{ij};$$

- there exist nonnegative γ_{ii} and positive γ'_{ii} with $\gamma_{ii} \leq \gamma'_{ii}$, $i = 1, \ldots, n$, such that for all $x = (x_i) \in [z]$ with $x_i \neq \hat{x}_i$

$$\frac{F_i(\hat{x}_1, \cdots, \hat{x}_{i-1}, x_i, x_{i+1}, \cdots, x_n) - F_i(\hat{x}_1, \cdots, \hat{x}_{i-1}, \hat{x}_i, x_{i+1}, \cdots, x_n)}{x_i - \hat{x}_i} \in [\gamma_{ii}, \gamma'_{ii}].$$

These conditions are often satisfied in the realistic settings, like in the discretization of the free boundary problems. Actually, some special cases of the conditions were studied, for instance: the almost linear case [16] and the tridiagonal nonlinear case [2]. For the general case, a validated solution and an iterative method for sharpening it were given in [3], for which however, the convergence is quite slow. Here we utilize the dimension reduction technique used in [16] to give an algorithm, which can compute a sharp validated solution of the problem quite fast.

The remaining parts of the paper are organized as follows. In Section 2, we present some preliminaries on interval analysis and matrix analysis. In Section 3, we give a method for computing an error bound with a certain component identification property, the property is then used to give an algorithm for solving the MCP. In Section 4 we study the application of our method, and the numerical results are reported to support its practical performance.

2 Preliminaries and Notations

We present some preliminaries on interval analysis since our method is based on interval computation. Let $\underline{A} = (\underline{a}_{ij}), \overline{A} = (\overline{a}_{ij}) \in R^{n\times n}$ with $\underline{a}_{ij} \leq \overline{a}_{ij}$, $i = 1, \ldots, n$, $j = 1, \ldots, n$. We denote by $[A] = [\underline{A}, \overline{A}]$ an $n \times n$ interval matrix, which is a set

$$[A] := \{A = (a_{ij}) \in R^{n\times n} : \ \underline{a}_{ij} \leq a_{ij} \leq \overline{a}_{ij}\}.$$

The (i, j)-th element of $[A]$ is denoted by $[a_{ij}]$. We call an $n \times 1$ real interval matrix $[x] = [\underline{x}, \overline{x}]$ an interval vector, its i-th component is denoted by $[x_i]$. For the interval vector $[x]$ we denote

$$m([x]) := \frac{1}{2}(\underline{x} + \overline{x}) \quad \text{and} \quad r([x]) := \frac{1}{2}(\overline{x} - \underline{x}).$$

For an interval vector $[x] = [\underline{x}, \overline{x}]$, we define the interval operator

$$\text{median}\{l, u, [x]\} := [\text{median}\{l, u, \underline{x}\}, \text{median}\{l, u, \overline{x}\}],$$

where $\text{median}\{\cdot, \cdot, \cdot\}$ is the median operation taken componentwise. We take an example for clarification.

Example 2.1. Letting $l = (-1, 0)^T$, $u = (2, 1)^T$, $\underline{x} = (-9, -1)^T$ and $\overline{x} = (-2, 2)^T$, then we compute

$$\text{median}\{l, u, \underline{x}\} = (\text{median}\{-1, 2, -9\}, \text{median}\{0, 1, -1\})^T = (-1, 0)^T,$$

and

$$\text{median}\{l, u, \overline{x}\} = (\text{median}\{-1, 2, -2\}, \text{median}\{0, 1, 2\})^T = (-1, 1)^T,$$

and consequently

$$\text{median}\{l, u, [x]\} = [\text{median}\{l, u, \underline{x}\}, \text{median}\{l, u, \overline{x}\}] = \begin{pmatrix} [-1, -1] \\ [0, 1] \end{pmatrix}.$$

For an interval matrix $[A]$ we define the absolute value $|[A]| \in R^{n\times n}$ by

$$|[A]| := (\max\{|\underline{a_{ij}}|, |\overline{a_{ij}}|\}).$$

Let $F : R^n \to R^n$. Choose a fixed $\hat{x}$ from $[x]$. An interval slope, denoted by $\delta F(\hat{x}, [x])$, is an $n \times n$ interval matrix such that for all $x \in [x]$

$$F(x) - F(\hat{x}) \in \delta F(\hat{x}, [x])([x] - \hat{x}).$$

For more details on interval analysis and computation we refer to [12], for example.

A few words on matrix analysis. Let $A \in R^{n\times n}$, denote by Λ and $-B$ the diagonal and off-diagonal part of A, respectively. A is called a Z-matrix if its off-diagonal entries are nonnegative, A is called an M-matrix if it is a Z-matrix and has a nonnegative inverse, A is called an H-matrix if the so-called comparison matrix

$$\langle A\rangle := |\Lambda| - |B|$$

is an M-matrix.

3 Enclosure of Solution

Provided an approximate solution $\hat{x} \in R^n$ of $\text{MCP}(l, u, F)$ and an error guess $d \in R^n_+$, we have an interval vector $[x] = [\hat{x} - d, \hat{x} + d]$. If we can validate that the MCP has a true solution in $[x]$, then d is just a guaranteed componentwise error bound. The following theorem offers an existence validation.

Theorem 3.1. *Let $[x]$ be a given interval vector, and $\hat{x} \in [x]$ be fixed. Let F be Lipschitz continuous over $[x]$ and have an interval slope $\delta F(\hat{x}, [x])$ over $[x]$. Let $\Lambda = \text{diag}(\lambda_i) \in R^{n\times n}$ be a given diagonal matrix such that $\lambda_i > 0$, $i = 1, \ldots, n$. Define*

$$\Gamma(\hat{x}, [x], \Lambda) := \text{median}\{l, u, \hat{x} - \Lambda F(\hat{x}) + (I - \Lambda\delta F(\hat{x}, [x]))([x] - \hat{x})\}, \tag{3.1}$$

where I denotes the identity matrix. If $\Gamma(\hat{x}, [x], \Lambda) \subseteq [x]$, then the problem $\text{MCP}(l, u, F)$ has a solution $x^* \in [x]$. Moreover, if $[x]$ contains a solution x^*, then $x^* \in \Gamma(\hat{x}, [x], \Lambda)$.

The proof of the theorem can be found in [17]. Theorem 3.1 gives an existence validation of a solution of $\text{MCP}(l, u, F)$ in a given interval vector. Here we moreover use Theorem 3.1 to construct an interval $[x]$ containing a solution of $\text{MCP}(l, u, F)$, namely, we compute an interval vector $[x]$ such that the inclusion $\Gamma(\hat{x}, [x], \Lambda) \subseteq [x]$ holds, and as a consequence of Theorem 3.1, $\text{MCP}(l, u, F)$ must have a solution in $[x]$, and the radius of $[x]$ is just an error bound for the approximate solution given by the midpoint of the interval.

Theorem 3.2. *Let Assumption 1.1 be fulfilled for* $[z]$, $\hat{x} \in [z]$, $\tilde{M} = (\tilde{m}_{ij})$ *be defined by*

$$\tilde{m}_{ij} = \begin{cases} -\gamma_{ij} & \text{if} \quad j \neq i, \\ \gamma_{ii} & \text{if} \quad j = i. \end{cases} \tag{3.2}$$

If there exists $d \geq 0$ *such that* $\tilde{M}d \geq |F(\hat{x})|$, *and* $[x] := [\hat{x}-d, \hat{x}+d] \subseteq [z]$, *and* $[x] \cap [l, u] \neq \emptyset$, *then* $\mathrm{MCP}(l, u, F)$ *has a solution in* $[x]$.

Proof. Choose $\Lambda := \mathrm{diag}((\gamma'_{ii})^{-1})$, which is well defined under Assumption 1.1. Write

$$\begin{aligned} & F_i(x_1, \cdots, x_{i-1}, x_i, x_{i+1}, \cdots, x_n) - F_i(\hat{x}_1, \cdots, \hat{x}_{i-1}, \hat{x}_i, \hat{x}_{i+1}, \cdots, \hat{x}_n) \\ = \sum_{j=1}^{n} & \left[F_i(\hat{x}_1, \cdots, \hat{x}_{j-1}, x_j, x_{j+1}, \cdots, x_n) - F_i(\hat{x}_1, \cdots, \hat{x}_{j-1}, \hat{x}_j, x_{j+1}, \cdots, x_n)\right]. \end{aligned}$$

Assumption 1.1 gives moreover an interval slope $\delta F(\hat{x}, [z])$ of $F(x)$ over $[z]$:

$$[\delta F_i(\hat{x}, [z])]_j = \begin{cases} [-\gamma_{ij}, \gamma_{ij}] & \text{if} \quad j \neq i, \\ [\gamma_{ii}, \gamma'_{ii}] & \text{if} \quad j = i, \end{cases} \tag{3.3}$$

which gives an interval slope $\delta F(\hat{x}, [x]) := \delta F(\hat{x}, [z])$ of $F(x)$ over $[x]$. We verify the inclusion $\Gamma(\hat{x}, [x], \Lambda) = [\underline{\Gamma(\hat{x}, [x], \Lambda)}, \overline{\Gamma(\hat{x}, [x], \Lambda)}] \subseteq [x]$. It is easy to see

$$\begin{aligned} \overline{\Gamma(\hat{x}, [x], \Lambda)} &= \mathrm{median}\{l, u, \hat{x} - \Lambda F(\hat{x}) + |I - \Lambda \delta F(\hat{x}, [x])| d\}, \\ \underline{\Gamma(\hat{x}, [x], \Lambda)} &= \mathrm{median}\{l, u, \hat{x} - \Lambda F(\hat{x}) - |I - \Lambda \delta F(\hat{x}, [x])| d\}, \end{aligned}$$

where $\underline{\delta F(\hat{x}, [x])}$ and $\overline{\delta F(\hat{x}, [x])}$ denote the lower and the upper bound of the interval matrix $\delta F(\hat{x}, [x])$, respectively, and where

$$|I - \Lambda \delta F(\hat{x}, [x])| = \max\{|I - \Lambda A| : A \in \delta F(\hat{x}, [x])\}$$

with

$$|I - \Lambda \delta F(\hat{x}, [x])|_{ij} = \begin{cases} (\gamma'_{ii})^{-1}(\gamma_{ij}) & \text{if} \quad j \neq i, \\ 1 - (\gamma'_{ii})^{-1}(\gamma_{ii}) & \text{if} \quad j = i. \end{cases}$$

Obviously, we have

$$|I - \Lambda \delta F(\hat{x}, [x])| d = |I - \Lambda \langle \underline{\delta F(\hat{x}, [x])} \rangle| d = \Lambda(\Lambda^{-1} - \tilde{M}) d.$$

If $\tilde{M}d \geq |F(\hat{x})|$, then we have

$$\begin{aligned} -\Lambda F(\hat{x}) + |I - \Lambda \delta F(\hat{x}, [x])| d &\leq d, \\ -\Lambda F(\hat{x}) - |I - \Lambda \delta F(\hat{x}, [x])| d &\geq -d. \end{aligned}$$

From these two inequalities, it follows that

$$\begin{aligned} \hat{x} - \Lambda F(\hat{x}) + |I - \Lambda \delta F(\hat{x}, [x])| d &\leq \hat{x} + d, \\ \hat{x} - \Lambda F(\hat{x}) - |I - \Lambda \delta F(\hat{x}, [x])| d &\geq \hat{x} - d. \end{aligned} \tag{3.4}$$

Noting the condition $[x] \cap [l, u] \neq \emptyset$, we have $\hat{x} + d \geq l$ and $\hat{x} - d \leq u$, which together with (3.4), yield

$$\begin{aligned} \overline{\Gamma(\hat{x}, [x], \Lambda)} &= \mathrm{median}\{l, u, \hat{x} - \Lambda F(\hat{x}) + |I - \Lambda \delta F(\hat{x}, [x])| d\} \leq \hat{x} + d, \\ \underline{\Gamma(\hat{x}, [x], \Lambda)} &= \mathrm{median}\{l, u, \hat{x} - \Lambda F(\hat{x}) - |I - \Lambda \delta F(\hat{x}, [x])| d\} \geq \hat{x} - d, \end{aligned}$$

so we have $\Gamma(x, [x], \Lambda) \subseteq [x]$. From Theorem 3.1 it follows that $x^* \in \Gamma(x, [x], \Lambda)$. ☐

Theorem 3.3. *Let Assumption 1.1 be fulfilled for* $[z]$*, let* $\tilde{M} = (\tilde{m}_{ij})$*, defined by (3.2), be an M-matrix, let* $\hat{x} \in [z]$*, and let* $d^* = \tilde{M}^{-1}e$*, where* $e = (1, \cdots, 1)^T$*, let* $\mathcal{I} := \{1, \ldots, n\}$*. Define*

$$\pi_l(\hat{x}) := \{i \in \mathcal{I} : \hat{x}_i < l_i\}, \quad \pi_u(\hat{x}) := \{i \in \mathcal{I} : \hat{x}_i > u_i\},$$

define

$$p_l(\hat{x}) := \begin{cases} 0 & \text{if} \quad \pi_l(\hat{x}) = \emptyset, \\ \max\left\{\dfrac{l_j - \hat{x}_j}{d_j^*} : j \in \pi_l(\hat{x})\right\} & \text{if} \quad \pi_l(\hat{x}) \neq \emptyset, \end{cases}$$

and

$$p_u(\hat{x}) := \begin{cases} 0 & \text{if} \quad \pi_u(\hat{x}) = \emptyset, \\ \max\left\{\dfrac{\hat{x}_j - u_j}{d_j^*} : j \in \pi_u(\hat{x})\right\} & \text{if} \quad \pi_u(\hat{x}) \neq \emptyset, \end{cases}$$

and define

$$\omega(\hat{x}) := \begin{cases} \max\{p_l(\hat{x}), p_u(\hat{x})\} & \text{if} \quad \pi_l(\hat{x}) \cup \pi_u(\hat{x}) \neq \emptyset, \\ \|F(\hat{x})\|_\infty & \text{if} \quad \pi_l(\hat{x}) \cup \pi_u(\hat{x}) = \emptyset. \end{cases} \tag{3.5}$$

Let $[x] := [\hat{x} - \omega(\hat{x})d^*, \hat{x} + \omega(\hat{x})d^*] \subseteq [z]$*, let* $\Gamma(\hat{x}, [x], \Lambda)$ *be defined as in (3.1), where* $\Lambda := diag((\gamma'_{ii})^{-1})$*,* γ'_{ii} *is given in Assumption 1.1 for* $i = 1, \ldots, n$*, and let* $\delta F(\hat{x}, [x])$ *be given by (3.3). Then* MCP(l, u, F) *has a solution* x^* *in* $\Gamma(\hat{x}, [x], \Lambda)$ *provided that*

$$\omega(\hat{x}) \geq \|F(\hat{x})\|_\infty.$$

If, moreover,

$$\pi_l(\hat{x}) \cup \pi_u(\hat{x}) \neq \emptyset,$$

then there is at least an index $k \in \pi_l(\hat{x}) \cup \pi_u(\hat{x})$ *such that* $[x]_k = l_k$ *or* $[x]_k = u_k$*. In this case, correspondingly at least one component* $x_k^* = l_k$ *or* $x_k^* = u_k$ *of* x^* *is identified.*

Proof. From the condition that $\tilde{M} = (\tilde{m}_{ij})$ is an M-matrix, it follows that d^* is well defined with $d^* \geq 0$ and $d^* \neq 0$. Note that $\omega(\hat{x})$ is well defined with $\omega(\hat{x}) \geq 0$. Then we have $d = \omega(\hat{x})d^* \geq 0$. The assumption of Theorem 3.3 that $\omega(\hat{x}) \geq \|F(\hat{x})\|_\infty$ implies that

$$\tilde{M}d = \omega(\hat{x})\tilde{M}d^* = \omega(\hat{x})e \geq |F(\hat{x})|.$$

We show $\hat{x} + d \geq l$ and $\hat{x} - d \leq u$. For the index i such that $l_i \leq \hat{x}_i \leq u_i$, we have $\hat{x}_i + d_i \geq l_i$ and $\hat{x}_i - d_i \leq u_i$ since $d_i \geq 0$. For the index $i \in \pi_l(\hat{x})$, we have $(l_i - \hat{x}_i)/d_i^* \leq \omega(\hat{x})$ and $\hat{x}_i \leq u_i$, from which it follows that $\hat{x}_i + d_i = \hat{x}_i + \omega(\hat{x})d_i^* \geq l_i$ and $\hat{x}_i - d_i \leq u_i$ as $d_i \geq 0$. We can show in the similar way that $\hat{x}_i + d_i \geq l_i$ and $\hat{x}_i - d_i \leq u_i$ for the index $i \in \pi_u(\hat{x})$. Then the conditions required in Theorem 3.2 are all verified to be valid, and we can conclude that MCP(l, u, F) has a solution $x^* \in \Gamma(x, [x], \Lambda)$ and $\Gamma(x, [x], \Lambda) \subseteq [x]$.

The remaining of the theorem can be shown in a similar manner as used for proving Theorem 2.2 in [17]. □

Remark 3.4. Theorem 3.3 gives an enclosure of a solution of MCP(l, u, F), which yields a natural error bound: $|\hat{x} - x^*| \leq d$. For the linear complementarity problem (when $F(x) = Mx + q$ for $M \in R^{n\times n}$ and $q \in R^n$), Assumptions 1.1 are fulfilled if M is an H-matrix with positive diagonals. Hence, Theorem 3.3 delivers the error bound

$$|\hat{x} - x^*| \ \leq \ \omega(\hat{x})\langle M\rangle^{-1}e. \tag{3.6}$$

In [4] Chen and Xiang gave the following error bound for the linear complementarity problem with $M = (m_{ij})$ being an H-matrix and its diagonal part $D = diag(m_{ii})$ being positive:

$$\|\hat{x} - x^*\|_\infty \le \| \max\{I, D\}\langle M\rangle^{-1}\|_\infty \| \min\{\hat{x}, M\hat{x} + q\}\|_\infty. \tag{3.7}$$

Although we are not in a position to compare these bounds theoretically, our error bound is in some case better than the one given by Chen et al. For example, we let

$$M = \begin{bmatrix} 1 & -\frac{1}{4} & & \\ -\frac{1}{4} & 1 & \ddots & \\ & \ddots & \ddots & -\frac{1}{4} \\ & & -\frac{1}{4} & 1 \end{bmatrix}, \qquad q = \begin{bmatrix} 1 \\ -1 \\ \vdots \\ -1 \\ 1 \end{bmatrix}.$$

Obviously, when $\hat{x} = -M^{-1}q$, we must have $\omega(\hat{x}) \ge \|M\hat{x} + q\|_\infty = 0$. Choose $\hat{x} \approx -M^{-1}q$ such that $\omega(\hat{x}) \ge \|M\hat{x} + q\|_\infty$ is fulfilled: for instance

$$\hat{x} = (1.4681, 1.8577, 1.9577, 1.9767, 1.9431, 1.8065, 1.2865, -0.6791)^T.$$

One can test that $\omega(\hat{x}) = 0.4638 > 0.0046 = \|M\hat{x} + q\|_\infty$. The error bound by Chen et al. reads 1.3493, while our bound reads $\|\omega(\hat{x})\langle M\rangle^{-1}e\|_\infty = 0.9216$. Note that (3.6) is a componentwise error bound, whereas in (3.7) the norm of $\hat{x} - x^*$ is bounded.

Collorary 3.5. *Suppose that an interval extension $\delta F(\hat{x}, [x])$ of $F(x)$ over $[x]$ is available such that $\delta F(\hat{x}, [x]) \subseteq \delta F(\hat{x}, [z])$ defined by (3.3). Let $\Gamma(\hat{x}, [x], \Lambda)$ be defined by (3.1). If, moreover, $\pi_l(\hat{x}) \cup \pi_u(\hat{x}) \ne \emptyset$, then there is at least an index $k \in \pi_l(\hat{x}) \cup \pi_u(\hat{x})$ such that $(\Gamma(\hat{x}, [x], \Lambda))_k = l_k$ or $(\Gamma(\hat{x}, [x], \Lambda))_k = u_k$. In this case, correspondingly at least one component $x^*_k = l_k$ or $x^*_k = u_k$ of x^* is identified.*

Proof. The proof can be given by a simple computation, we omit the details. See [17]. □

Remark 3.6. Let $F(x) = 0$ have a solution $\tilde{x}$, and let $\{x^s\}_{s=0}^\infty \to \tilde{x}$ be a given sequence obtained via a certain numerical algorithm. It is obvious that, if $\tilde{x}$ is a solution of MCP(l, u, F), then a good approximation to $\tilde{x}$ can be selected from the sequence $\{x^s\}_{s=0}^\infty$; otherwise, if $\tilde{x}$ is not a solution of MCP(l, u, F), then $\pi(\tilde{x}) = \pi_l(\tilde{x}) \cup \pi_u(\tilde{x}) \ne \emptyset$ and $\omega(\tilde{x}) > 0 = \|F(\tilde{x})\|_\infty$. Then there must be an iterate x^s that is close to $\tilde{x}$ sufficiently, fulfilling

$$\pi(x^s) \ne \emptyset \quad \text{and} \quad \omega(x^s) \ge \|F(x^s)\|_\infty, \tag{3.8}$$

in this case, as indicated by Corollary 3.5, at least one component $x^*_k = l_k$ or $x^*_k = u_k$ of the solution x^* of $MCP(l, u, F)$ can be identified.

4 Algorithm for Validated Solution

We present in this section an algorithm for computing the validated solution of the MCP. The algorithm successively uses a procedure, which returns either a good approximation of the solution of the MCP, or determines at least one component of the solution. We describe the procedure as follows, it is based on the mathematical justification given in the preceding section.

Procedure 4.1. (Components Identification Algorithm)

Step 0. (Initialization)
Let $[l] = [\underline{l}, \overline{l}]$ and $[u] = [\underline{u}, \overline{u}]$ be the interval representation of l and u, respectively. Set $l := \underline{l}$ and $u = \overline{u}$. Choose a small floating number $\epsilon > 0$ as the error tolerance, set $s := 0$, $\mathcal{I} := \{1, \ldots, n\}$ and $\alpha(l, u, F) = \beta(l, u, F) = \emptyset$.

Step 1. (Stopping Criterion)
Compute the interval evaluation $\|\text{median}\{x^s - l, x^s - u, F(x^s)\}\|_\infty = [0, \sigma_s]$. If $\sigma_s < \epsilon$, then return the enclosure $[\check{x}] := [x^s]$ and return the approximate solution $\check{x} := m([x^s])$, and return the index sets $\alpha(l, u, F)$ and $\beta(l, u, F)$, and terminate this procedure.

Step 2. (Checking Assumption 1.1)
Let an approximate solution x^s of $F(x) = 0$ be given. Choose an interval $[z] = [x^s - d^s, x^s + d^s]$ with $d^s \in R^n$ and $d^s > 0$. For $[z]$ and $\hat{x} = x^s$ and for $i, j = 1, \ldots, n$, compute the intervals $[\gamma_{ij}]$ for bounding the parameters γ_{ij} required in Assumption 1.1, compute the interval matrix $[\tilde{M}] = ([\tilde{m}_{ij}])$ with

$$[\tilde{m}_{ij}] = \begin{cases} -[\gamma_{ij}] & \text{if} \quad j \neq i, \\ [\gamma_{ii}] & \text{if} \quad j = i. \end{cases}$$

And solve the solution $[d^*]$ of the interval linear system $[\tilde{M}][y] = [e]$, where $[d^*]$ is an interval vector, and $[e]$ is the interval representation of the vector e. If the lower bound of a $[d_i^*]$ is less than ϵ, then abort the procedure.

Step 3. (Checking conditions of Theorem 3.3)
Compute the interval evaluation $\|F(x^s)\|_\infty \in [\underline{\varsigma}, \overline{\varsigma}]$, compute $(l_j - x_j^s)/[d_j^*] = [\underline{\mu}_j, \overline{\mu}_j]$ for $j \in \pi_l(x^s) := \{i \in \mathcal{I} : x_i^s < l_i\}$ and $(x_j^s - u_j)/[d_j^*] = [\underline{\nu}_j, \overline{\nu}_j]$ for $j \in \pi_u(x^s) := \{i \in \mathcal{I} : x_i^s > u_i\}$, and compute

$$\omega(x^s) := \begin{cases} \max\{\max\{\overline{\mu}_i, \overline{\nu}_i\} : \ i \in \pi_l(x^s) \cup \pi_u(x^s)\} & \text{if} \quad \pi_l(x^s) \cup \pi_u(x^s) \neq \emptyset, \\ \overline{\varsigma} & \text{if} \quad \pi_l(x^s) \cup \pi_u(x^s) = \emptyset. \end{cases}$$

Compute $[x^{s,0}] = [x^s - \omega(x^s)\underline{d}^*, x^s + \omega(x^s)\overline{d^*}]$, where $\underline{d}^*$ and $\overline{d}^*$ are the lower and the upper bounds of $[d^*]$ respectively. If $\omega(x^s) < \underline{\varsigma}$ or $[x^{s,0}] \not\subseteq [z]$, then go to Step 6; otherwise, set $j = 0$, $\alpha^{s,j} = \beta^{s,j} = \emptyset$.

Step 4. (Updating Enclosure)
Let $x^{s,j} = m([x^{s,j}])$, compute $[x^{s,j+1}] := [x^{s,j}] \cap \Gamma(x^{s,j}, [x^{s,j}], \Lambda^{s,j})$, where $\Lambda^{s,j}$ is the inverse of the midpoint of the interval slope of F with respect to the interval vector $[x^{s,j}]$ and the vector $x^{s,j}$. Compute $\alpha^{s,j+1} = \{i \in \mathcal{I} : [x^{s,j+1}]_i \subset [l_i - \epsilon, l_i + \epsilon]\}$ and $\beta^{s,j+1} = \{i \in \mathcal{I} : [x^{s,j+1}]_i \subset [u_i - \epsilon, u_i + \epsilon]\}$.

Step 5. (Updating Index Sets)
If $\alpha^{s,j+1} = \alpha^{s,j}$ and $\beta^{s,j+1} = \beta^{s,j}$, then return $\check{x} = m([x^{s,j+1}])$ and the index sets $\alpha(l, u, F) = \alpha^{s,j+1}$ and $\beta(l, u, F) = \beta^{s,j+1}$, and terminate this procedure, otherwise, set $j := j + 1$, and go to Step 4.

Step 6. (Updating Iterate x^s)
Compute another approximate solution x^{s+1} to replace x^s, set $s := s + 1$ and go to Step 1.

Remark 4.2. (1) In Step 0, $[\underline{l}, \overline{l}]$ and $[\underline{u}, \overline{u}]$ are the floating number interval representations of the original data l and u. The setting $l := \underline{l}$ and $u = \overline{u}$ may give an MCP with a little larger domain, whose solution must be the one of the original MCP.

(2) In Step 1, σ_s is a floating number, and the comparison $\sigma_s < \epsilon$ can be carried out successfully.

(3) In Step 2, the vectors x^s and d^s should have the floating point representation, this can be done when we use in coding some interval data types provided in round-off tracking software to represent x^s and d^s. If the lower bound of a $[d_i^*]$ is greater than ϵ, then we can guarantee that $\tilde{M}$ is an M-matrix, therefore the Assumption 1.1 is validated.

(4) In Step 3, if $\omega(x^s) \geq \underline{\varsigma}$, then the condition $\omega(\hat{x}) \geq \|F(\hat{x})\|_\infty$ is validated reliably.

(5) In Step 4, we have the inclusion $\Gamma(x^{s,0}, [x^{s,0}], \Lambda^{s,0}) \subseteq [x^{s,0}]$, and the second part of Theorem 3.1 guarantees that $\Gamma(x^{s,j}, [x^{s,j}], \Lambda^{s,j}) \cap [x^{s,j}]$ contains a solution of the MCP.

Algorithm 4.1 delivers a vector $\check{x}$ and two index sets $\alpha(l,u,F)$ and $\beta(l,u,F)$. If $\check{x}$ is not a good approximation of the solution of MCP(l,u,F), then we have

$$\alpha(l,u,F) \cup \beta(l,u,F) \neq \emptyset,$$

by which we can determine exactly the component $x_k^* = l_k$ for $k \in \alpha(l,u,F)$ and/or $x_k^* = u_k$ for $k \in \beta(l,u,F)$.

Denote $\tau = \alpha(l,u,F) \cup \beta(l,u,F)$, and denote its complement by $\bar{\tau}$. Denote $l_\tau = (l_i)_{i\in\tau}$, $l_{\bar{\tau}} = (l_i)_{i\in\bar{\tau}}$, $u_\tau = (u_i)_{i\in\tau}$, $u_{\bar{\tau}} = (u_i)_{i\in\bar{\tau}}$, $x_\tau^* = (x_i^*)_{i\in\tau}$ and $x_{\bar{\tau}}^* = (x_i^*)_{i\in\bar{\tau}}$, denote by $F_{\bar{\tau}} = (F_i(x))_{i\in\bar{\tau}}$. We know that x_τ^* can be determined by applying Algorithm 4.1 to the original problem MCP(l,u,F). Obviously, $x_{\bar{\tau}}^*$ is the solution of the problem MCP$(l_{\bar{\tau}}, u_{\bar{\tau}}, F_{\bar{\tau}})$. It can be seen that Assumption 1.1 holds still for $F_{\bar{\tau}}$. Hence, if $\check{x}$ can not be accepted as an approximate solution of MCP(l,u,F), then $\tau \neq \emptyset$ and we can apply Algorithm 4.1 to the problem MCP$(l_{\bar{\tau}}, u_{\bar{\tau}}, F_{\bar{\tau}})$, which is of the dimension $|\bar{\tau}|$, where $|\bar{\tau}|$ denotes the cardinality of $\bar{\tau}$ and obviously $|\bar{\tau}| = n - |\tau| < n$. Therefore, by applying Algorithm 4.1 to at most n reduced MCPs from the original one, we can get a good approximate solution of the problem MCP(l,u,F). We summarize the procedure of the application of Algorithm 4.1 to the reduced MCPs in Algorithm 4.3.

Algorithm 4.3. (Dimension-Reduced Algorithm)

Step 0. Set $\alpha := \emptyset$, $\beta := \emptyset$ and $\kappa := \mathcal{I} - \alpha \cup \beta$.

Step 1. Apply Procedure 4.1 to MCP$(l_\kappa, u_\kappa, F_\kappa)$. If Procedure 4.1 is aborted, then we call the function "verifynlss.m" provided in INTLAB to compute the verified solution of the nonlinear system $F_\kappa(x) = 0$; otherwise Procedure 4.1 returns an interval vector $[\check{x}_\kappa]$, a vector $\check{x}_\kappa$ and the index sets $\alpha(l_\kappa, u_\kappa, F_\kappa)$ and $\beta(l_\kappa, u_\kappa, F_\kappa)$.

Step 2. Compute the interval evaluation $\|\text{median}\{\check{x}_\kappa - l_\kappa, \check{x}_\kappa - u_\kappa, F_\kappa(\check{x}_\kappa)\}\|_\infty = [0, \sigma_s]$. If $\sigma_s < \epsilon$, then set the enclosure $[\mathbf{x}]$of the solution of the MCP:

$$[\mathbf{x}_i] = \begin{cases} l_i & \text{if } i \in \alpha, \\ u_i & \text{if } i \in \beta, \\ [\check{x}_i] & \text{if } i \notin \alpha \cup \beta, \end{cases}$$

and set the approximate solution $\mathbf{x}$ of the MCP:

$$\mathbf{x}_i = \begin{cases} l_i & \text{if } i \in \alpha, \\ u_i & \text{if } i \in \beta, \\ \check{x}_i & \text{if } i \notin \alpha \cup \beta. \end{cases}$$

Step 3. Set $\alpha = \alpha \cup \alpha(l_\kappa, u_\kappa, F_\kappa)$ and $\beta = \beta \cup \beta(l_\kappa, u_\kappa, F_\kappa)$, and set $\kappa := \mathcal{I} - \alpha \cup \beta$, then go to Step 1.

Remark 4.4. Algorithm 4.3 is an extension of the algorithm proposed in [3] for solving the MCP with an almost linear function. It, however, can be applied in a quite general setting if Assumption 1.1 is fulfilled.

5 Numerical Experiments

In this section we study the numerical performance of Algorithm 4.3 by using two examples.

5.1 Application to simulation of free boundary problem

Consider a model arising from the simulation of the free boundary problems of the form:

$$\begin{cases} \triangle u &= f(s,t,u) = -\frac{1}{2} + \frac{3}{2s+t+2} + \arctan(u) + 2u & (s,t) \in D_+, \\ u &= g(s,t) = 5\sin(s) - 3\cos(2t) - 5, & (s,t) \in \partial([0,1]^2). \end{cases}$$

where the set $D_+ := \{(s,t) \in (0,1)^2 : u(s,t) > 0\}$ is unknown.

This problem was studied in [3], where, by imposing grid $(s_j, t_m) = (jh, mh)$ over $[0,1]^2$, $j, m = 1, \dots, k$, $h = 1/(k+1)$, and by using the so-called Mehrstellenverfahren (see [6], Table III, p.538, second to the last line) to discretize the Laplace operator, a complementarity problem MCP(l, u, F) is formulated with $l_i = 0$ and $u_i = +\infty$ for $i = 1, \dots, n$, and $F(x) = Mx + \varphi(x)$. Its solution $x^* = (x_i^*) \in R^n$ can offer an approximation of a solution of the free boundary problem over the grid, i.e., $x_i^* = u_{jm} \approx u(s_j, t_m)$ for $i = (j-1)k + m$. Here the matrix M reads

$$M = \frac{1}{h^2} \begin{pmatrix} H & -I & & \\ -I & H & \ddots & \\ & \ddots & \ddots & -I \\ & & -I & H \end{pmatrix} \in R^{n \times n}, \tag{5.1}$$

where

$$H = \begin{pmatrix} 4 & -1 & & \\ -1 & 4 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 4 \end{pmatrix} \in R^{k \times k}, \tag{5.2}$$

and the i-th component of the nonlinear part $\varphi(x)$ has the form

$$\begin{aligned} \varphi_i(x) = \frac{1}{12} h^2 [& f(s_{j-1}, t_m, x_{i-k}) + f(s_j, t_{m-1}, x_{i-1}) + 20 f(s_j, t_m, x_i) \\ & + f(s_j, t_{m+1}, x_{i+1}) + f(s_{j+1}, t_m, x_{i+k})]. \end{aligned} \tag{5.3}$$

It is easy to verify that Assumption 1.1 are fulfilled with the matrix $\tilde{M} = (\tilde{m}_{ij})$, where

$$\tilde{m}_{ij} = \begin{cases} -1 - \frac{1}{4}h^2 & \text{if } \; j = i - k \\ -1 - \frac{1}{4}h^2 & \text{if } \; j = i - 1 \\ 4 + \frac{10}{3}h^2 & \text{if } \; j = i \\ -1 - \frac{1}{4}h^2 & \text{if } \; j = i + 1 \\ -1 - \frac{1}{4}h^2 & \text{if } \; j = i + k \\ 0 & \text{otherwise,} \end{cases}$$

$i = 1, \dots, n$. One can see that $\tilde{M}$ is an M-matrix.

Table 1: Numerical results for Algorithm 4.3

$n=9$		$n=25$		$n=36$		$n=64$		$n=100$	
$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ
9	3	25	3	36	4	64	2	100	3
7	3	21	3	32	2	63	2	98	1
6	2	19	2	29	1	57	1	97	4
4	5	14	1	21	4	52	4	89	3
–	–	11	7	18	5	46	3	81	5
–	–	–	–	15	7	43	2	78	3
–	–	–	–	–	–	38	1	75	1
–	–	–	–	–	–	36	4	70	2
–	–	–	–	–	–	33	11	67	3
–	–	–	–	–	–	–	–	62	4
–	–	–	–	–	–	–	–	48	8

We test the performance of Algorithm 4.3. The algorithm is performed in MATLAB with the support of the toolbox INTLAB (Rump [14]), which is used to track the rounding errors. We choose ϵ in Algorithm 4.1 as the floating point relative accuracy in Matlab setting, it reads about

$$\epsilon = 2.220446049250313e-016.$$

The main computational cost for Algorithm 4.3 is for computing the sequence $\{x^s\}$ required in Algorithm 4.1, for which many methods can be adopted, here the Newton's method is used. We report in Table 1 the numbers (abbreviated by n_κ) of Newton iteration in Algorithm 4.1 for each reduced problem MCP$(l_\kappa, u_\kappa, F_\kappa)$ associated with the index subset κ. The cardinality $|\kappa|$ of the index subset κ, which is just the dimension of the problem MCP$(l_\kappa, u_\kappa, F_\kappa)$, is also reported.

5.2 Application to obstacle problem

Consider a model arising from the obstacle problem. This problem consists of finding the equilibrium position of an elastic membrane under tension. We formulate at first its mathematical model.

Let $\Omega \subset R^2$ be a bounded open set with piecewise smooth boundary $\partial\Omega$. Denote by $H_0^1(\Omega)$ the space of functions with compact support set in Ω such that for every $v \in H_0^1(\Omega)$, v and $\|\nabla v\|_2$ belong to the square integrable class $L^2(\Omega)$. Here v represents the position of the membrane. Given two obstacle functions: $v_l, v_u : \bar{\Omega} \to R$ and a force $f \in L^2(\Omega)$. Then the obstacle problem can be modeled by the minimization of the membrane energy

$$\min_{v\in\mathcal{D}} \left\{ \frac{1}{2}\int_\Omega \|\nabla v\|_2^2 d\Omega - \int_\Omega v f(v) d\Omega \right\},$$

where

$$\mathcal{D} := \{v \in H_0^1(\Omega) : \ v_l \le v \le v_u \ a.e. \text{ on } \Omega\}.$$

It can be shown that the energy functional has a unique minimizer in $\mathcal{D}$. Refer to [5, Chapter 5.1] for the physical interpretation of the mathematical formulation.

Let $\Omega = (0,1) \times (0,1)$, and again impose grid $(s_j, t_m) = (jh, mh)$ over $[0,1]^2$. Denote $n = k^2$ and denote by $x \in R^n$ the approximation of v over the gird points, namely $x_i = v_{jm} \approx v(s_j, t_m)$ for $i = (j-1)k + m$ and $j, m = 1, \ldots, k$. Then, the discretization of the functional by the Mehrstellenverfahren together with the optimality condition yields an MCP(l, u, F) with $F(x) = Mx - \varphi(x)$, where M is defined by (5.1) and (5.2). The function φ is determined by the choice of the force function f. Here we take $f = f_0 + \lambda e^v$, f_0 is a constant force dependent only on the position where it is exerted, λ is a small positive constant, and so $\varphi(v) = \lambda e^v$. Then we have

$$\varphi_i(x) = \frac{\lambda}{12} h^2 [\exp(x_{i-k}) + \exp(x_{i-1}) + 20 \exp(x_i) + \exp(x_{i+1}) + \exp(x_{i+k})].$$

Here we take $\lambda = 0.08$ and take the obstacle: $v_l(s,t) = -0.2$ and $v_u(s,t) = 1/(1 + s^2 + t^2)$. Their values at the mesh points give the vectors l and u.

Now we check Assumption 1.1. Given an interval $[z]$ involved in Assumption 1.1 with $[z_i] = [\underline{z}_i, \overline{z}_i]$, it is easy to verify that Assumption 1.1 are fulfilled with the matrix $\tilde{M} = (\tilde{m}_{ij})$, where

$$\tilde{m}_{ij} = \begin{cases} -1 - \frac{1}{12}\lambda h^2 \exp(\overline{z}_{i-k}) & \text{if} \quad j = i - k \\ -1 - \frac{1}{12}\lambda h^2 \exp(\overline{z}_{i-1}) & \text{if} \quad j = i - 1 \\ \;\;4 - \frac{5}{3}\lambda h^2 \exp(\overline{z}_i) & \text{if} \quad j = i \\ -1 - \frac{1}{12}\lambda h^2 \exp(\overline{z}_{i+1}) & \text{if} \quad j = i + 1 \\ -1 - \frac{1}{12}\lambda h^2 \exp(\overline{z}_{i+k}) & \text{if} \quad j = i + k \\ \;\;0 & \text{otherwise,} \end{cases}$$

$i, j = 1, \ldots, n$. Note that $\tilde{M} = M + \frac{1}{12}\lambda h^2 \Delta M$, where

$$(\Delta M)_{ij} = \begin{cases} -\exp(\overline{z}_{i-k}) & \text{if} \quad j = i - k \\ -\exp(\overline{z}_{i-1}) & \text{if} \quad j = i - 1 \\ -20 \exp(\underline{z}_i) & \text{if} \quad j = i \\ -\exp(\overline{z}_{i+1}) & \text{if} \quad j = i + 1 \\ -\exp(\overline{z}_{i+k}) & \text{if} \quad j = i + k \\ \;\;0 & \text{otherwise.} \end{cases}$$

One can see that M is an M-matrix, and so is $\tilde{M}$ when λh^2 is small enough. This follows from the perturbation property of the M-matrices, see [18].

We test the performance of Algorithm 4.3 in the same computational settings as stated for the previous example, and report the numerical results in Table 2. In (a) of Figure 1 we plot the surface given by the approximate values of $v(s_j, t_m)$ at the mesh points which are returned by the algorithm, and plot in (b) the subset of $\mathcal{D}$ where the lower obstacle is not attained by the numerical solution, namely the set

$$\{(s,t) \in \mathcal{D} : \; v(s,t) > l(s,t)\}.$$

Then the empty domain gives an approximation of the region where the membrane touches the lower obstacle, it is of practical importance and not known in advance.

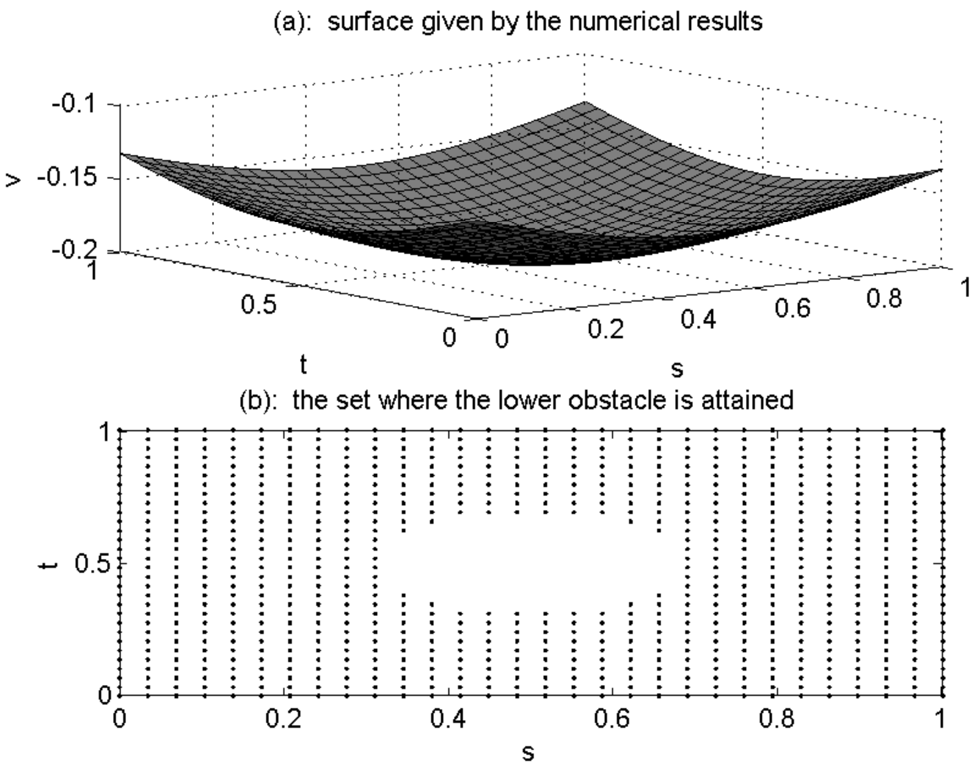
5.3 Concluding remarks

The numerical experiments show that Algorithm 4.3 performs quite well for the test problems. It can exactly identify a large part of the components of the solution which is equal to l_i or u_i, and deliver an interval vector bounding the rest of the components of the solution, the vector covers all the possible error arising in the practical computation. The exact identification of the components of the solution is based on the validation of the inclusion $\Gamma(\hat{x}, [x], \Lambda) \subseteq [x]$. Applying Procedure 4.1 to the discretized obstacle problem returns the

Table 2: Numerical results for Algorithm 4.3

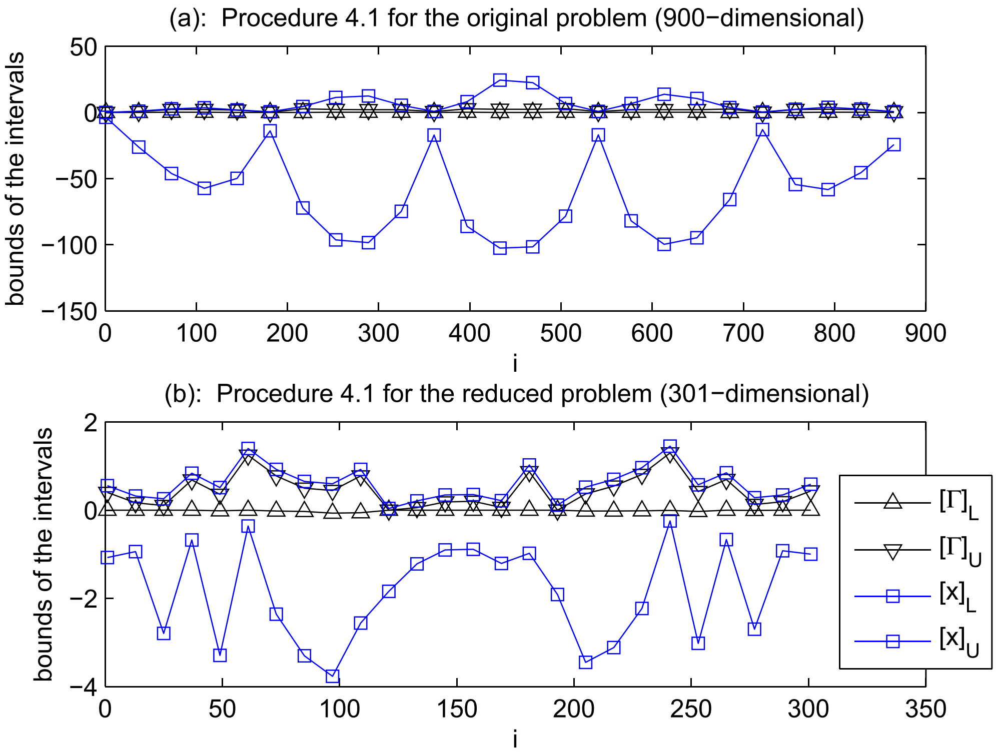
$n=25$		$n=100$		$n=225$		$n=400$		$n=900$	
$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ	$\|\kappa\|$	n_κ
25	3	100	2	225	4	400	2	900	3
5	4	68	3	132	3	204	3	301	3
–	–	24	4	108	3	156	3	269	3
–	–	–	–	106	3	144	4	263	3
–	–	–	–	103	6	–	–	260	2
–	–	–	–	–	–	–	–	256	3
–	–	–	–	–	–	–	–	240	2
–	–	–	–	–	–	–	–	238	5

Figure 1: Numerical results for $v(s,t)$



bounds of the interval vectors $[x]$ and $\Gamma(\hat{x},[x],\Lambda)$. Here we denote by $[\Gamma]_L$ and $[\Gamma]_U$ the lower and the upper bounds of $\Gamma(\hat{x},[x],\Lambda)$, and denote by $[x]_L$ and $[x]_U$ the lower and upper bounds of $[x]$. Clearly $[\Gamma]_L$, $[\Gamma]_U$, $[x]_L$ and $[x]_U$ are vectors of the same sizes. We first apply Procedure 4.1 to the discretized obstacle problem with $k=30$, namely $n=900$. In (a) of Figure 2 we plot the values of the above four vectors $[\Gamma]_L$, $[\Gamma]_U$, $[x]_L$ and $[x]_U$, the numerical results indicate that the inclusion is fulfilled, which rigorously ensures the existence of the solution in the interval vector. We then apply Procedure 4.1 to the reduced problem of the original MCP, which is a 301-dimensional MCP. In (b) of Figure 2 we plot the values of the four vectors, which rigorously validate the existence of the solution in the returned interval vector.

Figure 2: Numerical results for $[x]$ and $\Gamma(\hat{x}, [x], \Lambda)$



Besides, in each call of Algorithm 4.1, except for the last one, a system of nonlinear equations of reduced dimension is solved under a low precision, for which quite small computational cost is needed. These phenomena can be illustrated by the numerical results. For example, we notice in Table 1 that for the 100-dimensional problem, 52 components of the solution which are equal to 0 are exactly identified. For the identification, ten systems of nonlinear equations (of the dimension $|\kappa| = 100$, 97, 92, 89, 83, 80, 77, 71, 65 and 48, respectively) are solved. The first nine systems of equations are solved with just one or two iterations ($n_\kappa = 1$ or $n_\kappa = 2$). For the last system (of dimension $|\kappa| = 48$), nine iterations are needed ($n_\kappa = 9$), which is larger, because we use the solution of this system to approximate the 48 components of x^*. The other 52 components of x^* have been determined during calling Algorithm 4.1 for the first nine problems of the form $\mathrm{MCP}(l_\kappa, u_\kappa, F_\kappa)$.

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