

VERIFICATION OF FUNCTIONAL A POSTERIORI ERROR ESTIMATES FOR OBSTACLE PROBLEM IN 1D

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We verify functional a posteriori error estimate for obstacle problem proposed by Repin. Simplification into 1D allows for the construction of a nonlinear benchmark for which an exact solution of the obstacle problem can be derived. Quality of a numerical approximation obtained by the finite element method is compared with the exact solution and the error of approximation is bounded from above by a majorant error estimate. The sharpness of the majorant error estimate is discussed.

Keywords: obstacle problem, a posteriori error estimate, functional majorant, finite element method, variational inequalities, Uzawa algorithm

Classification: 34B15, 65K15, 65L60, 74K05, 74M15, 74S05

1. INTRODUCTION

Obstacle problems are one of the key problems in continuum mechanics. Their mathematical models based on variational inequalities are well established (we refer to classical works [11, 12, 13]). Numerical treatment of a obstacle problem is obtained by the finite element method and a solution of a quadratic minimization problems with constrains. It was traditionally tackled by the Uzawa method, the interior point method, the active set method with gradient splitting and the semi-smooth Newton method among others [8, 23].

A priori analysis providing asymptotic estimates of the quality of finite elements approximations converging toward the exact solution was studied for obstacle problems e. g. in [5, 9]. For the survey of the most important techniques in a posteriori analysis (such as residual, gradient averaging or equilibration methods) we refer to the monographs [1, 2, 3]. Particular a posteriori estimates for variational inequalities including a obstacle problem are reported e. g. in [4, 7, 25] among others.

Our goal is to verify guaranteed functional a posteriori estimates expressed in terms of functional majorants derived by Repin [16, 20]. The functional majorant upper bounds are essentially different with respect to known a posteriori error estimates mentioned above. The estimates are obtained with the help of variational (duality) method which was developed in [17, 18] for convex variational problems. The method was applied to various nonlinear models including those associated with variational inequalities [19], in particular problems with obstacles [6], problems generated by plasticity theory [10, 22]

and problems with nonlinear boundary conditions [21].

The obstacle problem is formulated and analyzed in two dimensions, however numerical experiments are considered in one dimension only. Then, we are easily able to construct an analytical benchmark with an exact solution of the nonlinear obstacle problem and evaluate integrals in numerical tests exactly.

Outline of the paper is as follows. In Section 2, we formulate a constrained minimization problem and introduce a perturbed minimization problem including its basic properties. A derivation and further analysis of error estimates in term of a functional majorant is explained in Section 3. A method of majorant minimization is also included there. A benchmark with known analytical solution is discussed in Section 4. Numerical tests performed in Matlab are reported in Section 5.

2. FORMULATION OF OBSTACLE PROBLEM

Let $\Omega \subset \mathbb{R}^2$ is a bounded domain with Lipschitz continuous boundary $\partial\Omega$. Let V stands for the standard Sobolev space $H^1(\Omega)$ and V_0 denote its subspace $H_0^1(\Omega)$, consisting of functions whose trace on $\partial\Omega$ is zero. We consider the obstacle problem, described by the following minimization problem:

Problem 1. (Minimization problem) Find $u \in K$ satisfying

$$J(u) = \inf_{v \in K} J(v),$$

where the energy functional reads

$$J(v) := \frac{1}{2} \int_{\Omega} \nabla v \cdot \nabla v \, dx - \int_{\Omega} f v \, dx \tag{1}$$

and the admissible set is defined as

$$K := \{v \in V_0 : v(x) \geq \phi(x) \text{ a.e. in } \Omega\},$$

where $f \in L^2(\Omega)$ and $\phi \in V$ such that $\phi \notin V_0$ and $\phi(x) < 0$ a.e. in (Ω) .

Problem 1 is a quadratic minimization problem with a convex constrain and the existence of its minimizer is guaranteed by the Lions- Stampacchia Theorem [15]. It is equivalent to the following variational inequality: Find $u \in K$ such that

$$\int_{\Omega} \nabla u \cdot \nabla(v - u) dx \geq \int_{\Omega} f(v - u) dx \quad \text{for all } v \in K. \tag{2}$$

The convex constrain $v \in K$ can be transformed into a linear term containing a new (Lagrange) variable in

Problem 2. (Perturbed problem) Let $W := \{v + t\phi : v \in V_0 \text{ and } t \in \mathbb{R}\} \subset V$. For given

$$\mu \in \Lambda := \{\mu \in W^* : \langle \mu, v - \phi \rangle \geq 0 \text{ for all } v \in K\} \tag{3}$$

find $u_{\mu} \in V_0$ such that

$$J_{\mu}(u_{\mu}) = \inf_{v \in V_0} J_{\mu}(v), \tag{4}$$

where $\langle \cdot, \cdot \rangle$ denote the duality pairing of W and W^* and the perturbed functional J_μ is defined as

$$J_\mu(v) := J(v) - \langle \mu, v - \phi \rangle. \quad (5)$$

Problems 1 and 2 are related and it obviously holds

$$J_\mu(u_\mu) \leq J(u) \quad \text{for all } \mu \in \Lambda. \quad (6)$$

Lemma 2.1. (Existence of optimal multiplier) There exists $\lambda \in \Lambda$ such that

$$u_\lambda = u \quad (7)$$

and

$$J_\lambda(u) = J(u). \quad (8)$$

Proof. Let $w \in W$ is arbitrary. We decompose

$$w = v + t\phi, \quad (9)$$

where $v \in V_0$ and $t \in \mathbb{R}$ and this decomposition can be shown to be unique. Now, we define a functional λ as follows:

$$\langle \lambda, w \rangle := \int_\Omega \nabla u \cdot \nabla v \, dx - \int_\Omega f v \, dx + t \left[\int_\Omega \nabla u \cdot \nabla u \, dx - \int_\Omega f u \, dx \right]. \quad (10)$$

We assert that the functional defined by (10) has required properties (7) and (8). Apparently, λ is a linear functional on W . The functional λ is also continuous. It is a consequence of continuity of decomposition (9), which can be proved as follows. Let $w \in W$ is arbitrary and $w_n \rightarrow w$ in W , where $w_n \in W$. With respect of (9), we can write $w_n = v_n + t_n\phi$ and $w = v + t\phi$, where $v_n, v \in V_0$ and $t_n, t \in \mathbb{R}$. If we use the unique orthogonal decomposition of element $\phi \in V$, we infer that

$$|t_n - t| \|\phi^\perp\|_V \leq \|w_n - w\|_V, \quad (11)$$

where ϕ^\perp is the component of ϕ orthogonal to subspace V_0 . Moreover, it follows from the triangle inequality that

$$\|v_n - v\|_V \leq \|w_n - w\|_V + |t_n - t| \|\phi\|_V. \quad (12)$$

As a consequence of (11) and (12), $t_n \rightarrow t$ and $v_n \rightarrow v$ in W . Thus, the decomposition (9) is continuous. Now, if we restrict the space W to the origin V_0 , we obtain

$$\langle \lambda, w \rangle := \int_\Omega \nabla u \cdot \nabla w \, dx - \int_\Omega f w \, dx \quad \text{for all } w \in V_0, \quad (13)$$

which is equivalent to $\inf_{w \in V_0} J_\lambda(w) = J_\lambda(u)$, i. e., the property (7) is fulfilled. Furthermore, if we take $w = u - \phi$, it follows from (10) that

$$\langle \lambda, u - \phi \rangle = \langle \lambda, u \rangle - \langle \lambda, \phi \rangle = 0$$

and consequently the property (8) is fulfilled. Finally, we should verify the condition of nonnegativity from definition (3). Let $v \in K$ is arbitrary. It follows from (2) and (10) that

$$\langle \lambda, v - \phi \rangle = \langle \lambda, v - u \rangle \geq 0.$$

□

Remark 2.2. (Existence of optimal multiplier in the case $\phi \in V_0$) In the case of a nonpositive obstacle $\phi \in V_0$, the existence of optimal multiplier could be proved as follows. Once again, the relation (13) defines a linear continuous functional λ in V_0 such that u minimizes the perturbed functional J_μ defined by (5) with $\mu = \lambda$. Since $\phi \in K$, we can apply the inequality (2) to $v = \phi$ and $v = 2u - \phi$. Consequently, we obtain that $\langle \lambda, u - \phi \rangle = 0$. Subsequently, it follows from (5) that the property (8) is fulfilled. The condition of nonnegativity from definition (3) is also fulfilled. It follows from the inequality (2) if we put $v = u + w$, where $w \in V_0, w \geq 0$ a.e. in (Ω) .

Remark 2.3. (Representation of (10) by a nonnegative function $\lambda \in L^2(\Omega)$)

If u has a higher regularity,

$$u \in V_0 \cap H^2(\Omega), \tag{14}$$

then integration by parts yields

$$\langle \lambda, w \rangle = - \int_{\Omega} \Delta u v dx - \int_{\Omega} f v dx + t \left[- \int_{\Omega} \Delta u u dx - \int_{\Omega} f u dx \right] = \int_{\Omega} \lambda v dx + t \int_{\Omega} \lambda u dx$$

for all $w \in W$, where

$$\lambda = -(\Delta u + f). \tag{15}$$

We show additionally that

$$\lambda \geq 0 \text{ a.e. in } \Omega \tag{16}$$

by choosing $w \in V_0, w \geq 0$ a.e. in Ω . Then $v := u + w \in K$ and inequality (2) rewrites as

$$\int_{\Omega} \lambda w dx = \int_{\Omega} \nabla u \cdot \nabla w dx - \int_{\Omega} f w dx \geq 0,$$

which implies (16).

3. FUNCTIONAL A POSTERIORI ERROR ESTIMATE

We are interested in analysis and numerical properties of the a posteriori error estimate in the energetic norm

$$\|v\|_E := \left(\int_{\Omega} \nabla v \cdot \nabla v dx \right)^{\frac{1}{2}}.$$

This section is based on results of S. Repin et al. [6, 16, 19]. It is simple to see that

$$J(v) - J(u) = \frac{1}{2} \int_{\Omega} \nabla(v - u) \cdot \nabla(v - u) dx + \int_{\Omega} \nabla u \cdot \nabla(v - u) dx - \int_{\Omega} f(v - u) dx \tag{17}$$

for all $v \in K$ and (2) implies the energy estimate

$$\frac{1}{2} \|v - u\|_E^2 \leq J(v) - J(u) \quad \text{for all } v \in K. \tag{18}$$

Remark 3.1. (Sharpness of estimate (18)) It is clear from (17), the estimate (18) turns into equality if

$$\langle \lambda, v - u \rangle = \int_{\Omega} \nabla u \cdot \nabla(v - u) \, dx - \int_{\Omega} f(v - u) \, dx = 0 \quad \text{for all } v \in K. \tag{19}$$

This situation always occurs if $\lambda = 0$. Then, (13) implies that u is a solution of Problem 1 in the whole space V_0 . This corresponds to a linear problem without any obstacle. However, the estimate (18) can turn into equality also for the active obstacle. We discuss it further in Section 4.

Estimate (18) can only be tested for problems with known exact solution $u \in K$. By using (6), we obtain the estimate

$$J(v) - J(u) \leq J(v) - J_{\mu}(u_{\mu}) \quad \text{for all } \mu \in \Lambda. \tag{20}$$

In practical computations, $u_{\mu} \in V_0$ will be approximated by $u_{\mu,h} \in V_{0,h}$ from some finite dimensional subspace $V_{0,h} \subset V_0$ (see Section 5 for details). Therefore, it holds

$$J_{\mu}(u_{\mu,h}) \geq J_{\mu}(u_{\mu})$$

and $J_{\mu}(u_{\mu,h})$ can not replace $J(u)$ in (20) so that the inequality holds. To avoid this difficulty, we establish the following dual problem:

Problem 3. (Dual perturbed problem) Find $\tau_{\mu}^* \in Q_{f\mu}^* \subset [L^2(\Omega)]^2$ such that

$$J_{\mu}^*(\tau_{\mu}^*) = \sup_{q^* \in Q_{f\mu}^*} J_{\mu}^*(q^*),$$

where

$$J_{\mu}^*(q^*) = -\frac{1}{2} \int_{\Omega} q^* \cdot q^* \, dx + \langle \mu, \phi \rangle$$

and

$$Q_{f\mu}^* := \left\{ q^* \in [L^2(\Omega)]^2 : \langle \mu, v \rangle = \int_{\Omega} q^* \cdot \nabla v \, dx - \int_{\Omega} f v \, dx \quad \text{for all } v \in V_0 \right\}.$$

Lemma 3.2. It holds

$$\sup_{q^* \in Q_{f\mu}^*} J_{\mu}^*(q^*) = J_{\mu}^*(\nabla u_{\mu}) = J_{\mu}(u_{\mu}).$$

Proof. As a consequence of (4), it holds that $\nabla u_{\mu} \in Q_{f\mu}^*$. Let $w \in Q_{f\mu}^*$ is arbitrary. Since

$$J_{\mu}^*(w) = J_{\mu}^*(\nabla u_{\mu}) - \int_{\Omega} \nabla u_{\mu} \cdot (w - \nabla u_{\mu}) \, dx - \frac{1}{2} \int_{\Omega} (w - \nabla u_{\mu}) \cdot (w - \nabla u_{\mu}) \, dx$$

and $\int_{\Omega} \nabla u_{\mu} \cdot (w - \nabla u_{\mu}) \, dx = 0$ in consequence of $\nabla u_{\mu}, w \in Q_{f\mu}^*$, we deduce that $J_{\mu}^*(\nabla u_{\mu})$ is supremum of dual perturbed functional J_{μ}^* . Finally, it is not difficult to verify that $J_{\mu}^*(\nabla u_{\mu}) = J_{\mu}(u_{\mu})$. □

Corollary 3.3. If we choose

$$\mu = \lambda,$$

it holds

$$J_\lambda(u) = \inf_{v \in V_0} J_\lambda(v) = \sup_{q^* \in Q_{f\lambda}^*} J_\lambda^*(q^*) = J_\lambda^*(\nabla u) = J(u).$$

It follows from Lemma 3.2, we can replace inequality (20) by

$$J(v) - J(u) \leq J(v) - \sup_{q^* \in Q_{f\mu}^*} J_\mu^*(q^*) \leq J(v) - J_\mu^*(q^*), \tag{21}$$

where $q^* \in Q_{f\mu}^*$ is arbitrary. The practical limitation of estimate (21) is to satisfy the constrain $q^* \in Q_{f\mu}^*$. From now, we consider a special case of the multiplier defined as

$$\langle \mu, w \rangle := \int_\Omega \mu w \, dx, \tag{22}$$

where

$$\mu \in \Lambda := \{ \mu \in L^2(\Omega) : \mu \geq 0 \text{ a.e. in } \Omega \}. \tag{23}$$

S. Repin transformed (21) in the so called majorant estimate

$$J(v) - J(u) \leq \mathcal{M}(v, f, \phi; \beta, \mu, \tau^*), \tag{24}$$

where the right-hand side of (24) denotes the functional majorant

$$\begin{aligned} \mathcal{M}(v, f, \phi; \beta, \mu, \tau^*) := & \frac{1 + \beta}{2} \int_\Omega (\nabla v - \tau^*) \cdot (\nabla v - \tau^*) \, dx \\ & + \frac{1}{2} \left(1 + \frac{1}{\beta} \right) C_\Omega^2 \|\operatorname{div} \tau^* + f + \mu\|_{L^2(\Omega)}^2 + \int_\Omega \mu(v - \phi) \, dx, \end{aligned} \tag{25}$$

where a constant $C_\Omega > 0$ originates from the Friedrichs inequality

$$\int_\Omega u^2 \, dx \leq C_\Omega^2 \int_\Omega \nabla u \cdot \nabla u \, dx \quad \forall u \in V_0.$$

Estimate (24) is valid for $\beta > 0$, $\mu \in \Lambda$ and $\tau^* \in H(\Omega, \operatorname{div})$, where

$$H(\Omega, \operatorname{div}) := \{ \tau^* \in [L^2(\Omega)]^2 : \operatorname{div} \tau^* \in L^2(\Omega) \}.$$

Lemma 3.4. (Optimal majorant parameters) Suppose (22)–(23) and, let the assumption (14) is fulfilled. If we choose $\tau^* = \nabla u$, $\mu = \lambda \in L^2(\Omega)$ and $\beta \rightarrow 0$, then, the inequality in (24) changes to equality, i.e. the majorant on right-hand side of (24) defines the difference of energies $J(v) - J(u)$ exactly.

Proof. If $\mu = \lambda$ and $\tau^* = \nabla u$, it is consequence of (15) that the second term on the right-hand side of (25) vanishes. Moreover, the last term can be written as

$$\int_{\Omega} \lambda(v - \phi)dx = \int_{\Omega} \lambda(v - u)dx = \int_{\Omega} \nabla u \cdot \nabla(v - u)dx - \int_{\Omega} f(v - u)dx$$

and consequently, if $\beta = 0$, it follows from (17) that the majorant with optimal parameters estimates the difference of energies $J(v)$ and $J(u)$ exactly. □

Practically, optimal parameters are unknown. For given solution approximation v , loading f and the obstacle ϕ , the majorant \mathcal{M} represents a convex functional in each of variables β, μ, τ^* . Our goal is to find, at least approximately, such variables $\beta_{\text{opt}}, \mu_{\text{opt}}$ and τ_{opt}^* that minimize the majorant \mathcal{M} .

Problem 4. (Majorant minimization problem) Let $v \in K, f \in L^2(\Omega), \phi < 0$ be given. Find optimal $\beta_{\text{opt}} > 0, \mu_{\text{opt}} \in \Lambda$ and $\tau_{\text{opt}}^* \in H(\Omega, \text{div})$ such that

$$(\beta_{\text{opt}}, \mu_{\text{opt}}, \tau_{\text{opt}}^*) = \underset{\beta, \mu, \tau^*}{\text{argmin}} \mathcal{M}(v, f, \phi; \beta, \mu, \tau^*).$$

To this end, we use the following minimization algorithm:

Algorithm 1. (Majorant minimization algorithm) Let $k := 0$ and let $\beta_k > 0$ and $\mu_k \in \Lambda$ be given. Then:

(i) find $\tau_{k+1}^* \in H(\Omega, \text{div})$ such that

$$\tau_{k+1}^* = \underset{\tau^* \in H(\Omega, \text{div})}{\text{argmin}} \mathcal{M}(v, f, \phi; \beta_k, \mu_k, \tau^*),$$

(ii) find $\mu_{k+1} \in \Lambda$ such that

$$\mu_{k+1} = \underset{\mu \in \Lambda}{\text{argmin}} \mathcal{M}(v, f, \phi; \beta_k, \mu, \tau_{k+1}^*),$$

(iii) find $\beta_{k+1} > 0$ such that

$$\beta_{k+1} = \underset{\beta > 0}{\text{argmin}} \mathcal{M}(v, f, \phi; \beta, \mu_{k+1}, \tau_{k+1}^*),$$

(iv) set $k := k + 1$ are repeat (i) – (iii) until convergence.

Remark 3.5. (Functional majorant in 1D) The goal is to verify the majorant error estimate for obstacle problem in 1D. In this simplified case, the former domain Ω reduces to one-dimensional interval $(0, 1)$. We set $V := H^1(0, 1)$ and $V_0 := H_0^1(0, 1)$, the energy functional (1) reads

$$J(v) = \frac{1}{2} \int_0^1 (v')^2 dx - \int_0^1 f v dx$$

and the admissible set is defined as

$$K := \{v \in V_0 : v(x) \geq \phi(x) \text{ a.e. in } (0, 1)\},$$

where $f \in L^2(0, 1)$ and $\phi \in V$ such that $\phi \notin V_0$ and $\phi(x) < 0$ a.e. in $(0, 1)$. Then, the functional majorant \mathcal{M} takes the form

$$\begin{aligned} \mathcal{M}(v, f, \phi; \beta, \mu, \tau^*) &= \frac{1 + \beta}{2} \int_0^1 (v' - \tau^*)^2 dx \\ &\quad + \frac{1}{2} \left(1 + \frac{1}{\beta}\right) \|(\tau^*)' + f + \mu\|_{L^2(0,1)}^2 + \int_0^1 \mu(v - \phi) dx, \end{aligned}$$

where $\beta > 0$, $\tau^* \in V$ and $\mu \in \Lambda = \{\mu \in L^2(0, 1) : \mu \geq 0 \text{ a.e. in } (0, 1)\}$.

Remark 3.6. (Majorant minimization in 1D) In 1D case, the minimization in step (i) is equivalent to the following variational equation : Find $\tau_{k+1}^* \in V$ such that

$$\begin{aligned} (1 + \beta_k) \int_0^1 \tau_{k+1}^* w dx + \left(1 + \frac{1}{\beta_k}\right) \int_0^1 (\tau_{k+1}^*)' w' dx \\ = (1 + \beta_k) \int_0^1 v' w dx - \left(1 + \frac{1}{\beta_k}\right) \int_0^1 (f + \mu_k) w' dx \end{aligned} \quad (26)$$

for all $w \in V$. The minimization in step (ii) is equivalent to the variational inequality: Find $\mu_{k+1} \in \Lambda$ such that

$$\begin{aligned} \int_0^1 \left[\left(1 + \frac{1}{\beta_k}\right) [\mu_{k+1} + (\tau_{k+1}^*)' + f] + v - \phi \right] (w - \mu_{k+1}) dx \geq 0 \quad \text{for all } w \in \Lambda. \\ \beta_{k+1} = \frac{\|(\tau_{k+1}^*)' + f + \mu_{k+1}\|_{L^2(0,1)}}{\|v' - \tau_{k+1}^*\|_{L^2(0,1)}}. \end{aligned}$$

4. 1D BENCHMARK WITH KNOWN ANALYTICAL SOLUTION

We derive an exact solution of Problem 1 – modified to 1D problem (see Remark 3.5) – assuming negative constant functions f and ϕ . The resulting solution is displayed in Figure 1 for the case of active obstacle. A mechanical intuition suggests that for small values (considered in absolute value) of acting force f , there will be no contact with the obstacle and there will be a contact on a subset of interval $(0, 1)$ located symmetrically around the value $x = 1/2$ for higher values of f . The solution of Problem 1 with inactive obstacle reads

$$u(x) = \frac{f}{2}(x - x^2).$$

The minimal value of u on interval $(0,1)$ is attained at $x = 1/2$ and the inactive obstacle condition $u(1/2) > \phi$ is satisfied for

$$|f| < 8|\phi|. \tag{27}$$

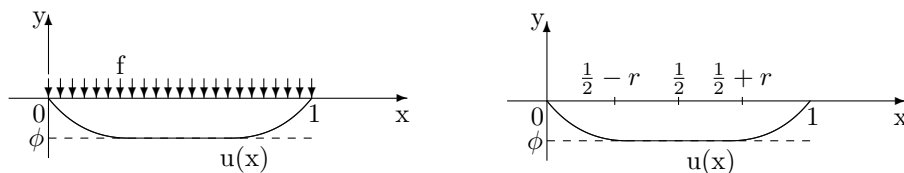


Fig. 1. Benchmark setup: Constant forces f pressing continuum against a constant lower obstacle ϕ , exact displacement u (left) and construction of exact displacement u in detail (right).

Then, the corresponding energy reads

$$J(u) := -\frac{f^2}{24}.$$

The obstacle is active if

$$|f| \geq 8|\phi|, \quad (28)$$

and the solution has the following form

$$u(x) = \begin{cases} -\frac{f}{2}x^2 + \frac{\phi + \frac{f}{2}(\frac{1}{2}-r)^2}{\frac{1}{2}-r}x & \text{if } x \in [0, \frac{1}{2}-r) \\ \phi & \text{if } x \in [\frac{1}{2}-r, \frac{1}{2}+r] \\ -\frac{f}{2}(x-1)^2 - \frac{\phi + \frac{f}{2}(\frac{1}{2}-r)^2}{\frac{1}{2}-r}(x-1) & \text{if } x \in (\frac{1}{2}+r, 1] \end{cases}$$

for unknown parameter $r \in [0, \frac{1}{2}]$. The parameter r determines the active contact set $[\frac{1}{2}-r, \frac{1}{2}+r]$ and its value can be determined from the minimum of energy

$$J(u) = \frac{[\phi + \frac{f}{2}(\frac{1}{2}-r)^2]^2}{\frac{1}{2}-r} - 2[\phi + \frac{f}{2}(\frac{1}{2}-r)^2]f(\frac{1}{2}-r) + \frac{2f^2}{3}(\frac{1}{2}-r)^3 - 2fr\phi$$

over all value of $r \in [0, \frac{1}{2}]$. The minimal energy

$$J(u) = f\phi\left(\frac{4}{3}\sqrt{\frac{2\phi}{f}} - 1\right)$$

is achieved for the argument

$$r = \frac{1}{2} - \sqrt{\frac{2\phi}{f}}.$$

Therefore, the solution of the problem with the active obstacle reads

$$u(x) = \begin{cases} -\frac{f}{2}x^2 - \sqrt{2\phi f}x & \text{if } x \in \left[0, \sqrt{\frac{2\phi}{f}}\right) \\ \phi & \text{if } x \in \left[\sqrt{\frac{2\phi}{f}}, 1 - \sqrt{\frac{2\phi}{f}}\right] \\ -\frac{f}{2}(x-1)^2 + \sqrt{2\phi f}(x-1) & \text{if } x \in \left(1 - \sqrt{\frac{2\phi}{f}}, 1\right] \end{cases} \quad (29)$$

Figure 2 provides few numerical approximations of u , see Section 5 for details. The first-order derivative

$$u'(x) = \begin{cases} -fx - \sqrt{2\phi f} & \text{if } x \in \left[0, \sqrt{\frac{2\phi}{f}}\right) \\ 0 & \text{if } x \in \left[\sqrt{\frac{2\phi}{f}}, 1 - \sqrt{\frac{2\phi}{f}}\right] \\ -f(x-1) + \sqrt{2\phi f} & \text{if } x \in \left(1 - \sqrt{\frac{2\phi}{f}}, 1\right] \end{cases}$$

is continuous everywhere. It is not difficult to show that

$$u''(x) = \begin{cases} -f & \text{if } x \in \left(0, \sqrt{\frac{2\phi}{f}}\right) \\ 0 & \text{if } x \in \left(\sqrt{\frac{2\phi}{f}}, 1 - \sqrt{\frac{2\phi}{f}}\right) \\ -f & \text{if } x \in \left(1 - \sqrt{\frac{2\phi}{f}}, 1\right) \end{cases}$$

is the second-order weak derivative of (29). With respect to (15), the optimal multiplier for our 1D benchmark problem reads

$$\lambda(x) = \begin{cases} 0 & \text{if } x \in \left(0, \sqrt{\frac{2\phi}{f}}\right) \\ -f & \text{if } x \in \left(\sqrt{\frac{2\phi}{f}}, 1 - \sqrt{\frac{2\phi}{f}}\right) \\ 0 & \text{if } x \in \left(1 - \sqrt{\frac{2\phi}{f}}, 1\right) \end{cases}$$

so that it is a piecewise constant function.

Remark 4.1. (Sharpness of estimate (18) for 1D benchmark) It is easy to show that the estimate (18) can turn into equality for the active obstacle. Indeed, in our 1D benchmark, the condition (19) rewrites as

$$\langle \lambda, v - u \rangle = -f \int_{\sqrt{\frac{2\phi}{f}}}^{1 - \sqrt{\frac{2\phi}{f}}} (v - u) dx = 0,$$

if the contact zone of an approximate solution $v \in K$ includes whole contact zone $\left[\sqrt{\frac{2\phi}{f}}, 1 - \sqrt{\frac{2\phi}{f}}\right]$ of exact solution u .

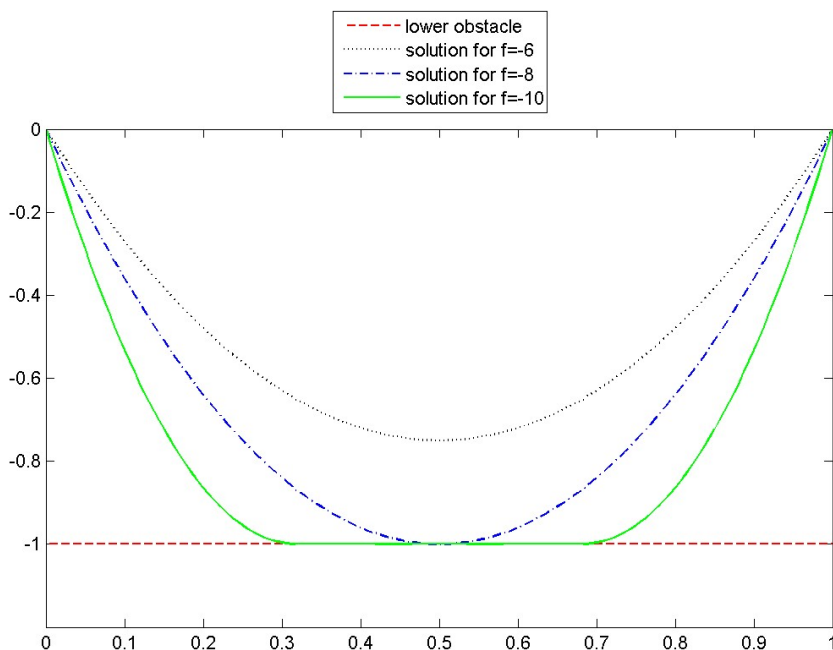


Fig. 2. Solutions for problems with loadings $f \in \{-6, -8, -10\}$ and $\phi = -1$.

5. NUMERICAL EXPERIMENTS

A MATLAB software is available as a package *Obstacle problem in 1D and its a posteriori error estimate* at Matlab Central under <http://www.mathworks.com/matlabcentral/fileexchange/authors/37756>.

Assuming the interval partition \mathcal{T} with n nodes

$$0 = x_1 < x_2 < \dots < x_n = 1,$$

we define $V_h \subset V$ as the finite dimensional space of nodal linear functions with a basis ψ_j , $j = 1 \dots n$ and its subspace $V_{0,h}$ of functions satisfying homogeneous Dirichlet boundary conditions. Using these basis functions, a stiffness matrix $A = (a_{ij})$ and a mass matrix $M = (m_{ij})$ are defined as

$$a_{ij} := \int_0^1 \psi'_i \psi'_j dx \quad m_{ij} = \int_0^1 \psi_i \psi_j dx.$$

A numerical approximation $v \in V_{0,h}$ of the exact solution $u \in V_0$ is constructed by the Uzawa algorithm.

Algorithm 2. (Uzawa algorithm)

1. Set the initial Lagrange multiplier $\mu_0 = 0$.
2. Start of the loop: for $k = 1, 2, \dots$ do until convergence:
3. Find an approximation $v_k \in V_{0,h}$ such that $J_{\mu_k}(v_k) \rightarrow \min$.
4. Set a Lagrange multiplier $\mu_k = (\mu_{k-1} + \rho(v_k - \phi))^+$.
5. End of the loop.
6. Output $v = v_k$ and $\mu = \mu_k$.

The approximation $v_k = \sum_{j=2}^{n-1} v_{k,j} \psi_j$ in step 3. of Algorithm 2 is computed from the equivalent variational equation

$$\int_0^1 v'_k w' dx = \int_0^1 (f + \mu_k) w dx \quad \text{for all } w \in V_{0,h}$$

leading to a linear system of equations for coefficients $v_{k,2}, \dots, v_{k,n-1}$. The convergence of Algorithm 2 depends on the choice of the scalar parameter ρ and it can be shown, see e.g. [11], that it always converges for $\rho \in (0, \rho_1)$ for some $\rho_1 > 0$. Some iterations of Algorithm 2 with $\rho = 10$ are displayed in Figure 3. Algorithm 2 converges slowly and therefore lower number of its iterations provides a poor approximation v of the exact solution u . In the following, we consider three particular sets of approximations v obtained by Algorithm 2 with different numbers of iterations:

- a) 100 iterations, b) 1000 iterations, c) 10000 iterations.

The sets of solutions a), b), c) will be constructed for the uniform mesh \mathcal{T} with 641 nodes (which corresponds to 6 uniform refinements of an initial uniform mesh with 10 elements) and for various loadings

$$f \in \{-5, -6, \dots, -17, -18\}.$$

It follows from (27) and (28), the obstacle is inactive for $f \in \{-5, \dots, -7\}$ and active for $f \in \{-8, \dots, -18\}$. Therefore, Algorithm 2 converges in a continuous setup for $f \in \{-5, \dots, -7\}$ after one iteration and approximations a), b), c) coincide. A verification of the energy estimate (18) is reported in Tables 1, 2, 3. We notice that the gap between the energy error $\frac{1}{2} \|v - u\|_E^2$ and the difference of energies $J(v) - J(u)$ is very small for approximations c) and becomes larger for approximations b) and a). In the case of inactive contact, the gap is apparently zero, see Remark 3.1.

For the verification of the majorant estimate (24), we run a discretized version of Algorithm 1. The minimal argument $\tau_{k+1}^* \in V_h$ in step (i) of Algorithm 1 is searched in the form $\tau_{k+1}^* = \sum_{j=1}^n y_j \psi_j$, where coefficients $y = (y_1, \dots, y_n) \in R^n$ follow (see (26)) from a linear system of equations

$$\left[(1 + \beta_k)M + \left(1 + \frac{1}{\beta_k}\right)A \right] y = (1 + \beta_k)b - \left(1 + \frac{1}{\beta_k}\right)c,$$

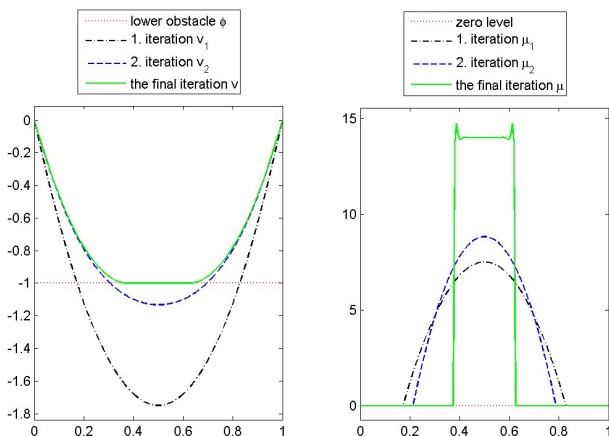


Fig. 3. The first, the second and the final (the 10000th) iterations of the Uzawa algorithm run on an uniform mesh with 641 nodes for the loading $f = -14$ and the obstacle $\phi = -1$.

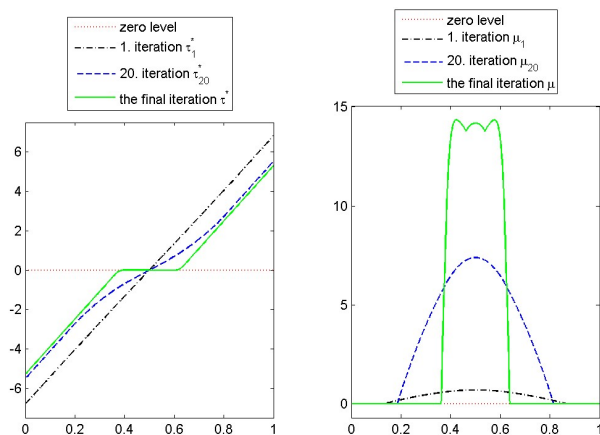


Fig. 4. The first, the twentieth and the final (the 10000th) iterations of the majorant minimization algorithm run on an uniform mesh with 641 nodes for the loading $f = -14$ and the obstacle $\phi = -1$. We assume the initial setup $\beta_0 = 1, \mu_0 = 0$ and the approximation v obtained after 100 iterations of the Uzawa algorithm.

where b and c are n - dimensional vectors defined as

$$b_i = \int_0^1 v' \psi_i dx, \quad c_i = \int_0^1 (f + \mu_k) \psi_i' dx$$

for $i, j = 1 \dots n$. The minimal argument $\mu_{k+1} \in \Lambda_h$ in step (ii) of Algorithm 1 is searched in the finite dimensional space $\Lambda_h \subset \Lambda$ of piecewise constant functions on \mathcal{T} . Then, under the assumption of $\phi \in V_h, f \in \Lambda_h$ with given values

$$\phi(x_j), \phi(x_{j+1}), \quad v(x_j), v(x_{j+1}), \quad f(x_{j+\frac{1}{2}}), \quad (\tau_{k+1}^*)'(x_{j+\frac{1}{2}})$$

for $j = 1 \dots n - 1$, we obtain the formula

$$\mu_{k+1}(x_{j+\frac{1}{2}}) = \left(-(\tau_{k+1}^*)'(x_{j+\frac{1}{2}}) - f(x_{j+\frac{1}{2}}) - \frac{v(x_j) + v(x_{j+1}) - \phi(x_j) - \phi(x_{j+1}))}{2 \left(1 + \frac{1}{\beta_k}\right)} \right)^+,$$

where $(\cdot)^+ = \max\{0, \cdot\}$. Some iterations of Algorithm 1 are displayed in Figure 4. We use a high (10000 in all experiments) number of iterations in order to achieve the sharpest possible estimate (24). Algorithm 1 provides a high quality approximations $\tau^* \in V_h$ and $\lambda \in \Lambda_h$ in accordance with Remark 3.4. We note that Algorithm 1 provides a sharp estimate (24) for all types a), b), c) of approximations $v \in V_{0,h}$. It corresponds to values around 1.00 in the last column of Tables 1, 2, 3.

f	$\frac{1}{2} \ v - u\ _E^2$	$J(v) - J(u)$	$\sqrt{\frac{J(v) - J(u)}{\frac{1}{2} \ v - u\ _E^2}}$	$\mathcal{M}(v, \dots)$	$\sqrt{\frac{\mathcal{M}(v, \dots)}{J(v) - J(u)}}$
-5	2.54e-006	2.54e-006	1.00	2.55e-006	1.00
-6	3.66e-006	3.66e-006	1.00	3.67e-006	1.00
-7	4.98e-006	4.98e-006	1.00	4.99e-006	1.00
-8	6.51e-006	6.51e-006	1.00	6.52e-006	1.00
-9	2.27e-005	2.27e-005	1.00	2.39e-005	1.03
-10	6.49e-005	6.86e-005	1.03	7.41e-005	1.04
-11	8.25e-005	9.91e-005	1.10	1.06e-004	1.04
-12	8.57e-005	9.99e-005	1.08	1.07e-004	1.04
-13	8.42e-005	1.13e-004	1.16	1.20e-004	1.03
-14	8.73e-005	3.69e-004	2.06	3.75e-004	1.01
-15	8.86e-005	6.44e-004	2.70	6.51e-004	1.00
-16	1.02e-004	9.91e-004	3.11	9.98e-004	1.00
-17	1.13e-004	1.26e-003	3.34	1.27e-003	1.00
-18	1.24e-004	1.54e-003	3.53	1.55e-003	1.00
-19	1.36e-004	1.73e-003	3.57	1.74e-003	1.00
-20	1.56e-004	1.98e-003	3.55	1.99e-003	1.00

Tab. 1. Verification of majorant and energy estimates for problems with various f computed on an uniform mesh with 641 nodes. Discrete solutions v is computed by 100 iterations of the Uzawa algorithm.

Remark 5.1. (Update of β) The experiments showed that the update of β in the step (iii) of Algorithm 1 should not be called in every iteration. It turns out useful to call steps (i) and (ii) repeatedly and run step (iii) only after variables τ^* and μ stabilize. We updated β during the 5000th and the final 10000th iterations.

f	$\frac{1}{2}\ v-u\ _E^2$	$J(v)-J(u)$	$\sqrt{\frac{J(v)-J(u)}{\frac{1}{2}\ v-u\ _E^2}}$	$\mathcal{M}(v, \dots)$	$\sqrt{\frac{\mathcal{M}(v, \dots)}{J(v)-J(u)}}$
-5	2.54e-006	2.54e-006	1.00	2.55e-006	1.00
-6	3.66e-006	3.66e-006	1.00	3.67e-006	1.00
-7	4.98e-006	4.98e-006	1.00	4.99e-006	1.00
-8	6.51e-006	6.51e-006	1.00	6.52e-006	1.00
-9	9.04e-006	9.49e-006	1.02	9.83e-006	1.02
-10	1.00e-005	2.36e-005	1.53	2.39e-005	1.01
-11	1.19e-005	2.72e-005	1.51	2.76e-005	1.01
-12	1.33e-005	2.90e-005	1.48	2.94e-005	1.01
-13	1.53e-005	3.96e-005	1.61	4.01e-005	1.01
-14	1.73e-005	4.79e-005	1.66	4.85e-005	1.01
-15	1.88e-005	5.61e-005	1.73	5.69e-005	1.01
-16	2.07e-005	5.51e-005	1.63	5.59e-005	1.01
-17	2.24e-005	6.01e-005	1.64	6.10e-005	1.01
-18	2.48e-005	6.94e-005	1.67	7.03e-005	1.01
-19	2.70e-005	9.06e-005	1.83	9.17e-005	1.01
-20	2.91e-005	8.52e-005	1.71	8.63e-005	1.01

Tab. 2. Verification of majorant and energy estimates for problems with various f computed on an uniform mesh with 641 nodes. Discrete solutions v is computed by 1000 iterations of the Uzawa algorithm.

f	$\frac{1}{2}\ v-u\ _E^2$	$J(v)-J(u)$	$\sqrt{\frac{J(v)-J(u)}{\frac{1}{2}\ v-u\ _E^2}}$	$\mathcal{M}(v, \dots)$	$\sqrt{\frac{\mathcal{M}(v, \dots)}{J(v)-J(u)}}$
-5	2.54e-006	2.54e-006	1.00	2.54e-006	1.00
-6	3.66e-006	3.66e-006	1.00	3.66e-006	1.00
-7	4.98e-006	4.98e-006	1.00	4.98e-006	1.00
-8	6.51e-006	6.51e-006	1.00	6.51e-006	1.00
-9	7.78e-006	8.05e-006	1.02	8.10e-006	1.00
-10	9.11e-006	9.79e-006	1.04	9.88e-006	1.00
-11	1.05e-005	1.10e-005	1.02	1.11e-005	1.00
-12	1.20e-005	1.29e-005	1.04	1.30e-005	1.00
-13	1.35e-005	1.42e-005	1.03	1.44e-005	1.00
-14	1.51e-005	1.60e-005	1.03	1.61e-005	1.00
-15	1.68e-005	1.78e-005	1.03	1.79e-005	1.00
-16	1.84e-005	2.01e-005	1.04	2.03e-005	1.01
-17	2.02e-005	2.16e-005	1.03	2.18e-005	1.00
-18	2.20e-005	2.39e-005	1.04	2.42e-005	1.01
-19	2.39e-005	2.55e-005	1.03	2.57e-005	1.00
-20	2.58e-005	2.80e-005	1.04	2.83e-005	1.01

Tab. 3. Verification of majorant and energy estimates for problems with various f computed on an uniform mesh with 641 nodes. Discrete solutions v is computed by 10000 iterations of the Uzawa algorithm.

CONCLUSIONS

A new minimization majorant algorithm providing an optimal value of the functional majorant \mathcal{M} that bounds the difference of energies $J(v) - J(u)$ was described. Numerical experiments in 1D show that the bound can be computed sharply for both low and high quality approximation v assuming a high number of the algorithm iterations. An analysis of a nonlinear benchmark with known analytical solution indicates, that $J(v) - J(u)$ provides the exact value of the error of approximation $\frac{1}{2}\|v - u\|_E^2$ in situations when contact zone of the discrete solution v covers whole contact zone of the exact solution u .

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REFERENCES

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- [1] M. Ainsworth and J. T. Oden: *A Posteriori Error Estimation in Finite Element Analysis*. Wiley and Sons, New York 2000.
 - [2] I. Babuška and T. Strouboulis: *The Finite Element Method and its Reliability*. Oxford University Press, New York 2001.
 - [3] W. Bangerth and R. Rannacher: *Adaptive Finite Element Methods for Differential Equations*. Birkhäuser, Berlin 2003.
 - [4] D. Braess, R. H. W. Hoppe, and J. Schöberl: A posteriori estimators for obstacle problems by the hypercircle method. *Comp. Visual. Sci.* 11 (2008), 351–362.
 - [5] F. Brezi, W. W. Hager, and P. A. Raviart: Error estimates for the finite element solution of variational inequalities I. *Numer. Math.* 28 (1977), 431–443.
 - [6] H. Buss and S. Repin: A posteriori error estimates for boundary value problems with obstacles. In: *Proc. 3rd European Conference on Numerical Mathematics and Advanced Applications*, Jyväskylä 1999, World Scientific 2000, pp. 162–170.
 - [7] C. Carstensen and C. Merdon: A posteriori error estimator completion for conforming obstacle problems. *Numer. Methods Partial Differential Equations* 29 (2013), 667–692.
 - [8] Z. Dostál: *Optimal Quadratic Programming Algorithms*. Springer 2009.
 - [9] R. S. Falk: Error estimates for the approximation of a class of variational inequalities. *Math. Comput.* 28 (1974), 963–971.

- [10] M. Fuchs and S. Repin: A Posteriori Error Estimates for the Approximations of the Stresses in the Hencky Plasticity Problem. *Numer. Funct. Anal. Optim.* *32* (2011), 610–640.
- [11] R. Glowinski, J. L. Lions, and R. Trémolieres: *Numerical Analysis of Variational Inequalities*. North-Holland 1981.
- [12] I. Hlaváček, J. Haslinger, J. Nečas, and J. Lovíšek: *Solution of Variational Inequalities in Mechanics*. Applied Mathematical Sciences *66*, Springer-Verlag, New York 1988.
- [13] N. Kikuchi and J. T. Oden: *Contact Problems in Elasticity: A Study of Variational Inequalities and Finite Element Methods*. SIAM 1995.
- [14] J. Kraus and S. Tomar: Algebraic multilevel iteration method for lowest-order Raviart-Thomas space and applications. *Internat. J. Numer. Meth. Engrg.* *86* (2011), 1175–1196.
- [15] J. L. Lions and G. Stampacchia: Variational inequalities. *Comm. Pure Appl. Math.* *XX(3)* (1967), 493–519.
- [16] P. Neittaanmäki and S. Repin: *Reliable Methods for Computer Simulation (Error Control and a Posteriori Estimates)*. Elsevier 2004.
- [17] S. Repin: A posteriori error estimation for variational problems with uniformly convex functionals. *Math. Comput.* *69(230)* (2000), 481–500.
- [18] S. Repin: A posteriori error estimation for nonlinear variational problems by duality theory. *Zapiski Nauchn. Semin. POMI* *243* (1997), 201–214.
- [19] S. Repin: Estimates of deviations from exact solutions of elliptic variational inequalities. *Zapiski Nauchn. Semin. POMI* *271* (2000), 188–203.
- [20] S. Repin: *A Posteriori Estimates for Partial Differential Equations*. Walter de Gruyter, Berlin 2008.
- [21] S. Repin and J. Valdman: Functional a posteriori error estimates for problems with nonlinear boundary conditions. *J. Numer. Math.* *16* (2008), 1, 51–81.
- [22] S. Repin and J. Valdman: Functional a posteriori error estimates for incremental models in elasto-plasticity. *Cent. Eur. J. Math.* *7* (2009), 3, 506–519.
- [23] M. Ulbrich: *Semismooth Newton Methods for Variational Inequalities and Constrained Optimization Problems in Function Spaces*. SIAM 2011.
- [24] J. Valdman: Minimization of functional majorant in a posteriori error analysis based on $H(\text{div})$ multigrid-preconditioned CG method. *Advances in Numerical Analysis* (2009).
- [25] Q. Zou, A. Veese, R. Kornhuber, and C. Gräser: Hierarchical error estimates for the energy functional in obstacle problems. *Numer. Math.* *117* (2012), 4, 653–677.

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