A Posteriori Estimators for the Obstacle Problem by the Hypercircle Method

Introduction

Elliptic obstacle problems lead to the minimization of a quadratic functional:

$$J(v) = \frac{1}{2}a(v, v) - (f, v)_0,$$

over a convex set

$$K = \{v \in V : v \geq \psi \text{ a.e. in } \Omega\}.$$

Goal: Derive reliable and efficient a posteriori estimators for obstacle problems using a Prager–Synge-type approach.

The Model Problem

We consider the Poisson equation with homogeneous Dirichlet conditions:

$$a(u, v) = \int_\Omega \nabla u \cdot \nabla v \, dx, \qquad V = H_0^1(\Omega),$$

Minimize J over

$$K = \{v \in V : v \geq \psi \text{ a.e.}\}.$$

Then $u \in K$ satisfies the variational inequality:

$$a(u, v - u) \geq (f, v - u)_0, \qquad \forall v \in K.$$

Lagrange Multiplier

Define the multiplier $\lambda \in V'$ by:

$$\langle \lambda, v \rangle = a(u, v) - (f, v)_0.$$

For all $w \in V_+ := \{v \geq 0\}$:

$$\langle \lambda, u - \psi \rangle = 0, \qquad \langle \lambda, w \rangle \geq 0.$$

The energy error satisfies

$$J(v) - J(u) = \frac{1}{2}\|\nabla v - \nabla u\|_0^2 + \langle \lambda, v - u \rangle. \tag{1}$$

Dual Problem: Fenchel duality

Suppose we want to solve the following minimization problem:

$$\min_{v \in V} \{ G(\Lambda v) + F(v) = J(v, \Lambda v) \}$$

by using Fenchel duality. Then we need to do:

1. define $\Phi(v, q)$ such that $\Phi(u, 0) = J(u)$. We usually take

$$\Phi(v, q) = G(\Lambda v - q) + F(v)$$

2. Compute $\Phi^*(v^*, q^*)$ the conjugate function of Φ.
3. the dual problem is defined as:

$$\begin{aligned} \sup\{-\Phi^*(0, q^*)\} &= \sup\{-J^*(\Lambda^* q^*, -q^*)\} \\ &= \sup\{-G^*(q^*) - F^*(\Lambda^* q^*)\} \end{aligned}$$

Dual Problem for the obstacle problem

1. $V^* = H^{-1}(\Omega)$.
2. $J(v, \Lambda v) = \frac{1}{2}\int_\Omega |\nabla v|^2 - \int_\Omega fv + I_K(v), \quad (\Lambda = -\nabla).$
$$J(v, \Lambda v) = G(\nabla v) + F(v)$$
3. $G(p) = \frac{1}{2}\int_\Omega p^2, \quad F(v) = -\int_\Omega fv + I_K(v).$ Then
$$G^*(p^*) = \frac{1}{2}\int_\Omega (p^*)^2,$$
$$F^*(v^*) = \int (v^* + f)\psi \text{ if } v^* + f \leq 0 \text{ and } +\infty \text{ otherwise}$$
4. The dual problem:
$$\sup_{\text{div } \tau + f \leq 0} \{-G^*(\tau) - F^*(\text{ div } \tau)\} = \sup_{\text{div } \tau + f \leq 0} \{-\frac{1}{2}\|\tau\|^2 - (\operatorname{div} \tau + f, \psi)\}$$

Dual Problem for the obstacle problem

The dual functional is

$$J^*(\tau) = -\frac{1}{2}\|\tau\|_0^2 - (\operatorname{div}\tau + f, \psi)_0,$$

maximized over

$$F = \{\tau \in H(\operatorname{div}) : \operatorname{div}\tau + f \leq 0\}.$$

Proposition

There is no duality gap, i.e,

$$J(u) = J^*(\nabla u).$$

Proof.

Let

$$\sigma = -\Lambda u = \nabla u.$$

Then $\sigma \in H_{\mathrm{div}}(\Omega)$ and

$$\mathrm{div}\, \sigma + f = \Delta u + f = -\lambda \leq 0.$$

Thus $\sigma \in F$, so ∇u is dual feasible.

$$J(u) = \frac{1}{2}\|\nabla u\|_0^2 - (f, u)_0,$$

and

$$J^*(\nabla u) = -\frac{1}{2}\|\nabla u\|_0^2 - (\Delta u + f, \psi)_0.$$

Then

$$J(u) - J^*(\nabla u) = \left(\tfrac{1}{2}\|\nabla u\|_0^2 - (f,u)_0\right) - \left(-\tfrac{1}{2}\|\nabla u\|_0^2 - (\Delta u + f, \psi)_0\right)$$
$$= \|\nabla u\|_0^2 - (f,u)_0 + (\Delta u + f, \psi)_0.$$

Use integration by parts:

$$\|\nabla u\|_0^2 = (\nabla u, \nabla u)_0 = -(\Delta u, u)_0.$$

Thus

$$\begin{aligned} J(u) - J^*(\nabla u) &= -(\Delta u, u)_0 - (f,u)_0 + (\Delta u + f, \psi)_0 \\ &= (\Delta u + f, \psi - u)_0 \\ &= 0 \end{aligned}$$

Theorem

For all $\tau \in F$:

$$J^*(\nabla u) - J^*(\tau) = \frac{1}{2}\|\nabla u - \tau\|_0^2 - (\operatorname{div}\tau + f, u - \psi)_0. \tag{2}$$

Proof. Define

$$g(t) = J^*(\tau + t(\nabla u - \tau)) \to g(1) - g(0) = J^*(\nabla u) - J^*(\tau)$$

we have,

$$\begin{aligned} g(t) &= -\frac{1}{2}\Big(\|\tau\|^2 + 2t(\tau, \nabla u - \tau) + t^2\|\nabla u - \tau\|^2\Big) \\ &\quad - \Big((\operatorname{div}\tau + f, \psi) + t\,(\operatorname{div}(\nabla u - \tau), \psi)\Big) \\ &= -\frac{1}{2}\|\tau\|^2 - (\operatorname{div}\tau + f, \psi) \\ &\quad - t\Big[(\tau, \nabla u - \tau) + (\operatorname{div}(\nabla u - \tau), \psi)\Big] - \frac{1}{2}t^2\|\nabla u - \tau\|^2. \end{aligned}$$

Caracterisation of σ

Let us find the variational inequality for σ

$$\sigma =: \arg \min_{\tau \in H_{div}; F(\tau) \leq 0} - J^*(\tau), \quad F(\tau) = \text{ div } \tau + f$$

1. Define the Lagrangian:

$$\mathscr{L}(\tau, q) = -J^*(\tau) + (q, F(\tau)),$$

2. (σ, p) is a saddle point for $\mathscr{L}$, i.e,

$$\forall q \in L^2(\Omega), \quad \mathscr{L}(\sigma, q) \leq \mathscr{L}(\sigma, p) \leq \mathscr{L}(\tau, p), \quad \forall \tau \in H_{div}(\Omega)$$

$$\mathscr{L}(\tau, q) = \frac{1}{2}\|\tau\|^2 + (\mathrm{div}\,\tau + f, \psi + q)$$

The optimality conditions imlpy:

$$\begin{aligned} \langle \mathscr{L}_\tau(\sigma, p), \tau\rangle &= 0, \quad \forall \tau \in V \\ F(\sigma) &\leq 0 \\ (F(\sigma), p) &= 0 \\ p &\geq 0 \end{aligned}$$

$$\begin{aligned} \mathscr{L}(\sigma + \tau, p) &= \frac{1}{2}\|\sigma + \tau\|^2 + (\mathrm{div}\,(\sigma + \tau) + f, \psi + p) \\ &= \mathscr{L}(\sigma, p) + \int_\Omega \sigma \cdot \tau + (\mathrm{div}\,\tau, \psi + p) + \frac{1}{2}\|\tau\|^2 \end{aligned}$$

Hence,

$$\langle \mathscr{L}_\tau(\sigma, p), \tau\rangle = \int_\Omega \sigma \cdot \tau + (\mathrm{div}\,\tau, \psi + p)$$

Optimality conditions

We have,

$$\begin{aligned} F(\sigma) &\leq 0 \\ (F(\sigma), p) &= 0 \\ (F(\sigma), -q) &\geq 0, \quad \forall q \geq 0 \end{aligned}$$

Then, the problem is to find $(\sigma, p) \in H_{div}(\Omega) \times \Lambda$

$$\begin{cases} \int_\Omega \sigma\tau + \int_\Omega p \operatorname{div} \tau = -\int_\Omega \psi \operatorname{div} \tau, \quad \forall \tau \in H_{div}(\Omega) \\ \int_\Omega (p-q) \operatorname{div} \sigma \geq -\int_\Omega f(p-q), \quad \forall q \in L^2(\Omega), q \geq 0 \end{cases} \tag{3}$$

Uzawa Algorithm

$$\min_{F(v) \leq 0} J(v)$$

1. Define the Lagrangian:

$$\mathscr{L}(v, \mu) = J(v) + (\mu, F(v))$$

2. Initialize λ_k,
3. Compute u_k as

$$u_k = \text{arg min } \mathscr{L}(v, \lambda_k)$$

4. Compute λ^*_{k+1} as

$$\lambda^*_{k+1} = \lambda_k + \alpha F(u_k), \quad \alpha > 0$$

5. Take the projection on Λ

$$\mathcal{P}_\Lambda(\lambda^*_{k+1}) = \lambda_{k+1},$$

Uzawa Algorithm

$$\min_{\mathcal{F}(\tau)\leq 0} \mathcal{G}(\tau)$$

1. Define the Lagrangian:

$$\mathscr{L}(\tau, q) = \mathcal{G}(\tau) + (q, \mathcal{F}(\tau))$$

2. Initialize p_k,
3. Compute σ_k as

$$\sigma_k = \text{arg min } \mathscr{L}(\tau_k, p_k)$$

4. Compute p^*_{k+1} as

$$p^*_{k+1} = p_k + \alpha\mathcal{F}(\sigma_k), \quad \alpha > 0.$$

5. Take the projection on Λ

$$\mathcal{P}_\Lambda(p^*_{k+1}) = p_{k+1}$$

Prager-Synge Identity for Obstacle Problems

Theorem

For $v \in \mathcal{K}$ and $\tau \in \mathcal{F}$,

$$[J(v) - J(u)] + [J^*(\nabla u) - J^*(\tau)] = \frac{1}{2}\|\nabla v - \tau\|_0^2 + (\operatorname{div}\tau + f, \psi - v)_0. \tag{4}$$

If the complementarity condition:

$$(\operatorname{div}\tau + f, v - \psi)_0 = 0, \tag{5}$$

holds, then

$$\|\nabla u - \nabla v\|_0^2 + \|\nabla u - \tau\|_0^2 \leq \|\nabla v - \tau\|_0^2. \tag{6}$$

Proof

$$\|\nabla v - \tau\|^2 = \|\nabla v - \nabla u\|^2 + \|\nabla u - \tau\|^2 + 2(\nabla u - \tau, \nabla v - \nabla u)$$

Since $(v-u) \in H_0^1(\Omega)$, we have

$$\begin{aligned}(\nabla u - \tau, \nabla v - \nabla u) =& (\nabla u, \nabla v - \nabla u) + (\operatorname{div} \tau, v-u) \\ =& (\nabla u, \nabla v - \nabla u) - (f, v-u) + (\operatorname{div} \tau + f, v-u) \\ =& \langle \lambda, v-u \rangle + (\operatorname{div} \tau + f, v-u)\end{aligned}$$

Now, we have,

$$\begin{aligned}\|\nabla v - \tau\|^2 &= \|\nabla v - \nabla u\|^2 + \|\nabla u - \tau\|^2 + 2\langle \lambda, v-u \rangle + 2(\operatorname{div} \tau + f, v-u) \\ &= 2[J(v) - J(u)] + 2\,[J^*(\nabla u) - J^*(\tau)] + 2(\operatorname{div} \tau + f, v-\psi)\end{aligned}$$

Hence, (4) holds true. The inequality (6) follows from the fact that $< \lambda, v - \psi > + (\operatorname{div} \tau + f, \psi - u) \geq 0$, when $v \in \mathcal{K}$ and $\tau \in \mathcal{F}$.

Remark

We emphasize that the assumption $\tau \in H\,(\text{div})$ may be dropped in Prager and Synge's theorem, if we set

$$\langle \text{ div } \tau, w\rangle = -(\tau, \nabla w) \text{ for } w \in H^1.$$

In particular, if τ belongs to the broken $H\,(\text{div})$ space, we have

$$\langle \text{div}\, \tau, w\rangle = \sum_T (\text{div}\, \tau, w)_{0,T} - \sum_e \int_e [\tau \cdot n] w \, ds$$

Remark on RT element

For the Raviart–Thomas element in two dimensions, only the normal component of the vector field is continuous across edges, not the whole vector field.

More precisely, the Raviart–Thomas space RT_k is an $H(\mathrm{div})$-conforming finite element space. Therefore, for any interior edge e shared by two elements K^+ and K^-, the normal component satisfies

$$[\mathbf{v}_h \cdot \mathbf{n}]_e := (\mathbf{v}_h|_{K^+} \cdot \mathbf{n}^+) + (\mathbf{v}_h|_{K^-} \cdot \mathbf{n}^-) = 0,$$

so the jump of the normal flux across the edge is zero.

However, the tangential component is, in general, discontinuous:

$$[\mathbf{v}_h \cdot \mathbf{t}]_e \neq 0,$$

where $\mathbf{t}$ denotes a unit tangent vector along e.

Thus, the Raviart–Thomas finite element does *not* enforce continuity of the whole vector field across edges, but only continuity of the normal component.

The Lagrange multiplier for the finite element solution

The discretization of the obstacle problem means that the linear space is replaced by a finite element space V_h, which will be here the space of linear elements on a triangulation $\mathcal{T}_h$ of $\Omega \subset \mathbb{R}^2$. As usual, Ω is assumed to be a polygonal domain, and the obstacle is given by a piecewise linear function $\psi \in V_h$.

The corresponding Lagrange multiplier λ_h is defined by

$$\langle \lambda_h, w \rangle = a\,(u_h, w) - (f, w)_0 \text{ for } w \in V_h. \tag{7}$$

Since the right-hand side is defined for all $w \in V$, we obtain an extension of λ_h to V' by (7). Partial integration yields the representation

$$\langle \lambda_h, w \rangle = -\sum_T (f, w)_{0,T} + \sum_e \left(\left[\frac{\partial u_h}{\partial n} \right], w \right)_{0,e}.$$

It shows that this extension of the Lagrange multiplier contains also the information on the residues outside the coincidence set.
From a computational point of view, it is given by the nonnegative residues of the finite element equations in the contact zone.
Let $\phi_i \in V_h$ be the nodal basis function associated with the nodal point x_i. Then

$$\lambda_{h,i} := \langle \lambda_h, \phi_i \rangle \geq 0 \text{ for all } i,$$

is the residue in the finite element inequalities and

$$\lambda_{h,i} = 0, \quad \text{if } u_h(x_i) - \psi(x_i) > 0.$$

Therefore, the discrete complementarity condition

$$\langle \lambda_h, u_h - \psi \rangle = 0 \tag{8}$$

holds and

$$\langle \lambda_h, w_h \rangle = \sum_i \lambda_{h,i} w_h(x_i), \quad w_h \in V_h. \tag{9}$$

The support of ϕ_i is the patch

$$\omega_i := \bigcup \{ \bar{T} \in \mathcal{T}_h \mid x_i \in \partial T \}.$$

The coincidence set (active set)

$$\mathcal{A}_h := \{x \in \Omega \mid u_h(x) = \psi(x)\}$$

is called regular, if it is the closure of its interior. This means that each nodal point $x_i \in \mathcal{A}_h$ lies on the boundary of a triangle T which is contained in the coincidence set $\mathcal{A}_h$.

Equilibration

The main task in the determination of the a posteriori error estimate is the construction of a function σ_h in the space,

$$RT_{-1} := \left\{ \tau \in L_2(\Omega) \mid \tau(x) = a_T + b_T x \text{ with } a_T \in \mathbb{R}^2, b_T \in \mathbb{R} \right\}.$$

that satisfies $\operatorname{div} \sigma_h \leq -f$ and moreover the complementarity condition (5) whenever possible. More precisely, the resulting σ_h will satisfy

$$\begin{cases} \operatorname{div} \sigma_h + \bar{f} \leq 0, \\ \quad [\sigma_h \cdot n] \geq 0, \end{cases} \tag{10}$$

where $\bar{f}$ is the L_2 projection of f in the space of piecewise constant functions.

In addition, the complementarity conditions

$$\begin{aligned} \left(-\operatorname{div}\sigma_h - \bar{f}, u_h - \psi\right)_{0,T} &= 0 \\ ([\sigma_h \cdot n], u_h - \psi)_{0,e} &= 0 \end{aligned} \tag{11}$$

will be satisfied at least outside a neighborhood of the coincidence set. We recall that the finite element functions in the Raviart-Thomas space

$$RT := RT_{-1} \cap H(\mathrm{div}),$$

are specified by their normal components on the edges of the grid. Similarly the functions in the broken Raviart-Thomas space RT_{-1} are given, if the normal components are known on both sides of the edges. Obviously, ∇u_h is a broken Raviart-Thomas function with zero divergence in each triangle.

The required σ will be obtained by a correction that eliminates the jumps of the normal components on the edges. Specifically, the correction

$$\sigma^{\Delta} := \tau - \nabla u_h$$

shall satisfy the following properties:

$$\left[\sigma^{\Delta} \cdot n\right] \geq -\left[\frac{\partial u_h}{\partial n}\right] \qquad \text{on each edge } e$$

The desired σ^{Δ}, in turn, will be computed as a sum of local corrections with support in the patches ω_i,

$$\sigma^{\Delta} = \sum_i \sigma_{\omega_i} \text{ with } \operatorname{supp} \sigma_{\omega_i} = \omega_i \tag{12}$$

and

$$\begin{cases} [\sigma_{\omega_i} \cdot n] \geq -\frac{1}{2}\left[\frac{\partial u_h}{\partial n}\right], & e \in \omega_i \\ \operatorname{div} \sigma_{\omega_i} \leq -f_{T,i}, & T \subset \omega_i \\ \sigma_{\omega_i} \cdot n = 0 & \text{on } \partial\omega_i \backslash \partial\Omega \end{cases} \tag{13}$$

where

$$f_{T,i} := \frac{1}{|T|} \int_T f \phi_i dx$$

Reliability

Theorem

Let each σ_{ω_i} be determined as described above and σ^Δ by (12). Then we have the a posteriori error estimate

$$
\begin{aligned}
\|\nabla u - \nabla u_h\|_0^2 \leq & J(u_h) - J(u) \\
& \leq \left\|\sigma^\Delta\right\|_0^2 + ch^2\|f - \bar{f}\|_0^2 + 2\left(\operatorname{div}\sigma^\Delta + \bar{f}, \psi - u_h\right)_0 \\
& \quad + 2\left(\left[\sigma^\Delta \cdot n\right], u_h - \psi\right)_{0,\cup e}.
\end{aligned}
$$

Relation to residual estimators

Theorem

Assume that $u_h = \psi$ holds in at least one triangle of a patch ω_i if $u_h - \psi$ vanishes at the central node in ω_i. Then the Prager-Synge error estimator is equivalent to the residual error estimator, i.e.,

$$\eta_{PS,i} \approx \sum_{T \subset \omega_i} \eta_{T,i} + \sum_{e \subset \omega_i} \eta_{e,i}.$$

Effeciency

Next we refer to the lower bounds of the error that result from the local Dirichlet problems on elements or edges and their neighborhood

$$\mathcal{E}_{D,T} := \sup_{\substack{v \in H_0^1(T) \\ v \geq \psi - u_h}} J(u_h) - J(u_h + v)$$

$$\mathcal{E}_{D,e} := \sup_{\substack{v \in H_0^1(\omega_e) \\ v \geq \psi - u_h}} J(u_h) - J(u_h + v)$$

In particular,

$$\sum_T \mathcal{E}_{D,T} + \sum_e \mathcal{E}_{D,e} \leq c \{J(u_h) - J(u)\} .$$

Effeciency

Theorem

There exists a constant c such that the area portion of the estimator η_{PS} satisfies

$$\eta_T \leq c\mathcal{E}_{D,T}.$$

Effeciency

Theorem

There exists a constant c such that the edge portion of the estimator η_{PS} satisfies

$$\eta_e \leq c\chi_e\mathcal{E}_{D,e}.$$

with the efficiency measure χ_e defined as

$$\chi_e = 1 \text{ unless}$$
$$\left[\frac{\partial u_h}{\partial n}\right] < 0 \text{ and } h_T^2 f_T < -\overline{u_h - \psi}$$

and

$$\chi_e = \max\left\{1, \max_{T\subset\omega_e} \min\left\{\frac{hf_T}{\left[\frac{\partial u_h}{\partial n}\right]}, \frac{h^2\left|f_T\right|}{\overline{u_h - \psi}}\right\}\right\}.$$