ERROR ESTIMATES FOR FINITE ELEMENT APPROXIMATIONS OF SUBGRADIENTS OF OBJECTIVE FUNCTIONS IN OPTIMAL CONTROL OF THE OBSTACLE PROBLEM *

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Abstract. We derive and present error estimates for a FEM-based approximation of a particular Clarke subgradient for the reduced objective function arising in optimal control of the obstacle problem. This Clarke subgradient for the reduced objective function can be computed by using an adjoint state that solves a Dirichlet problem on the complement of the strictly active set. Using finite element solutions of the obstacle problem, we construct discrete and convergent inner and outer approximations of this set. To show that our approximations are suitable and convergent, a detailed study of the topological structure of the strictly active set under appropriate assumptions is necessary. Based on the inner approximation, we solve the Dirichlet problem and obtain an upper bound for the error using the outer approximation. This upper bound converges to zero. We present numerical examples to test our estimates.

Key words. obstacle problem, variational inequalities, error estimates, free boundaries, generalized derivatives, Bouligand generalized differential, optimal control, nonsmooth optimization

AMS subject classifications. 35R35, 49J40, 49J52, 58E35, 65N15

1. Introduction.

For $\zeta := f(u) \in H^{-1}(\Omega)$, we consider the obstacle problem

$$\text{(COP)} \qquad \text{Find } y \in K_\psi : \quad \langle -\Delta y - \zeta, z - y\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} \geq 0 \quad \forall\, z \in K_\psi .$$

Here, K_ψ is the admissible set

$$K_\psi := \{z \in H_0^1(\Omega) \mid z \geq \psi \text{ q.e. in } \Omega\}$$

and $\psi \in H^1(\Omega)$ is a given obstacle. The usage of the operator $f\colon U \to H^{-1}(\Omega)$ allows for more general control spaces than $H^{-1}(\Omega)$ and our assumptions on f ensure that generalized derivatives for the solution operator of (COP) are available, see [39, 42, 41, 40]. We will recall these assumptions in subsection 2.2. It is well known that for every $\zeta = f(u) \in H^{-1}(\Omega)$ the problem (COP) has a unique solution. We denote the solution operator by $S\colon U \to H_0^1(\Omega)$. Let $J\colon H_0^1(\Omega) \times U \to \mathbb{R}$ be continuously differentiable. We are interested in the optimal control problem with respect to the obstacle problem (COP) and the objective function J

$$\text{(OCP)} \qquad \min_{(y,u)\in H_0^1(\Omega)\times U} J(y, u) \quad \text{s.t. } y = S(u)$$

and study the reduced objective function

$$\hat{J}(u) := J(S(u), u). \tag{1.1}$$

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In this article, we construct an error estimate for Clarke subgradients of $\hat{J}$ that result from computing only discrete solutions of (COP). Here, we make use of the construction of generalized derivatives of S as in [39, 42, 41, 40] and the corresponding Clarke subgradients of $\hat{J}$.

As we will recall, these generalized derivatives (in a fixed point u) depend on the active $A(\zeta)$ and strictly active set $A_{\mathrm{s}}(\zeta)$ w.r.t. $\zeta := f(u) \in H^{-1}(\Omega)$. More precisely, the domain, on which the generalized derivative is computed, is a quasi-open set between the inactive set $I(\zeta) := \Omega \setminus A(\zeta)$ and the complement of the strictly active set $\Omega \setminus A_{\mathrm{s}}(\zeta)$. When computing a discrete solution of the obstacle problem (COP), only approximations of the active sets are known and available. We construct discrete approximations of the strictly active sets and study the influence/ effects of these sources of inexactness on the resulting inexact generalized derivatives. Here, we use results on discrete approximations of the inactive sets and estimates of the distances of the relative free boundaries to the continuous free boundary as analyzed in [5, 38]. Crucial for our investigation is a nondegeneracy condition which is a condition on $-\Delta\psi - \zeta$ and which ensures a quadratic growth property of $S(u) - \psi$ away from the active set. The formulation of this condition we use is taken from [38] and it originally goes back to [12].

Finding suitable discrete approximations of Clarke subgradients of $\hat{J}$ and estimating the corresponding errors is a relevant task when, e.g., computing a subgradient in a bundle method as in [29]. Moreover, our error estimates might be useful in the context of semi-smooth Newton methods, see also [16], where the Newton differentiability of the solution operator of the obstacle problem is derived.

The results in this manuscript are based on the dissertation [39, Ch. 7].

This paper is organized as follows. In section 2, we state a short collection of results concerning regularity of the solution of the continuous obstacle problem and recall the relevant results on Clarke subgradients for the reduced objective function $\hat{J}$. The discrete obstacle problem is introduced in section 3 and existing L^∞-error estimates for the discrete solutions are discussed. In section 4, we present a formula for an inexact Clarke subgradient of $\hat{J}$. Here, inexactness arises since the inactive set or the complement of the strictly active set, the domains where the generalized derivatives are computed, are replaced by abstract approximations obtained from discrete solutions of the obstacle problem. Conditions on the approximations are derived to ensure the convergence of the inexact Clarke subgradients and to ensure a computable and convergent upper estimate for the error. We investigate existing approximations of the inactive set based on L^∞-error estimates for the solution of the discrete obstacle problem in section 5. In section 6, assuming a nondegeneracy condition, we recall a result from [38] estimating the distance of the boundaries of the approximations of the inactive set and the boundaries of the exact inactive set. Still assuming the nondegeneracy condition, we justify that suitable approximations of the inactive set are hard to construct analyze topological properties of the strictly active set that can be exploited in the sequel. We present our construction of sub- and superset approximations of $\Omega \setminus A_{\mathrm{s}}(\zeta)$ in section 7 and verify the previously determined requirements for their usage in the error estimates for the Clarke subgradients of $\hat{J}$. In section 8, we summarize our results and formulate the main theorem on error estimates of the generalized derivatives. The paper concludes with some numerical examples in section 9.

Notation. We denote by $\Omega \subseteq \mathbb{R}^d$ an open and bounded domain. Throughout this paper, $\langle \cdot, \cdot \rangle$ denotes the dual pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$ and $\langle \cdot, \cdot \rangle_{X^*,X}$

is the dual pairing between a specific Banach space X and its dual space X^*. We use the notation $(\cdot,\cdot)$ for the scalar product in $L^2(\Omega)$. For a set $E \subseteq \mathbb{R}^d$, we denote by $\overline{E}$ its closure w.r.t. the usual topology in $\mathbb{R}^d$ and by $\operatorname{int}(E)$ its interior.

2. Properties of the continuous problem. In this section, we collect known facts about the continuous obstacle problem (COP) which are important for the analysis in this paper. In particular, we address relevant properties concerning regularity of the continuous solution of the obstacle problem and recall characterizations of Clarke subgradients of the reduced objective function $\hat{J}$ as defined in (1.1).

Let us first recall the notation for the active set $A(\zeta) = \{\omega \in \Omega \mid S(u)(\omega) = \psi(\omega)\}$ and the inactive set $I(\zeta) = \Omega \setminus A(\zeta)$. Moreover, we use the notation $A_{\mathrm{s}}(\zeta)$ for the strictly active set, the fine support of the measure associated with $-\Delta S(u) - \zeta \in H^{-1}(\Omega)_+$, cf. subsection 6.1. Note that $A_{\mathrm{s}}(\zeta)$ is a quasi-closed subset of $A(\zeta)$. $A(\zeta)$ is quasi-closed and defined up to a set of capacity zero and the complement $I(\zeta)$ is quasi-open.

2.1. Regularity results for the solution of the continuous obstacle problem. A certain smoothness of the solution of the obstacle problem is required to obtain error estimates for Clarke subgradients of the reduced objective function associated with the optimal control problem in (OCP) based on discrete solutions of the obstacle problem. Thus, the purpose of this short subsection is to summarize a collection of already established regularity results for the solution of the obstacle problem under assumptions on the data $\zeta(u)$, ψ and Ω. We are not aiming for a complete presentation of the results, but mention only a short selection of results that are sufficient for the presentation in this paper. In particular, the presented selection of results shows that the assumptions on the solution of (COP) we have in this chapter can be fulfilled and can be guaranteed a priori by requiring the appropriate regularity of the data. Of course, in the literature, many authors are concerned with regularity results for solutions of obstacle problems. Among many others, we mention [13], [24], [25], [31] and [43].

Let us collect the following results on regularity of the solution $y = S(u)$ of (COP), which are taken from [43, Cor. 5:2.3] and [31, Thm. IV 2.3].

LEMMA 2.1.
1. *Assume $\zeta \in L^2(\Omega)$ and $\psi \in H^2(\Omega)$. If Ω is a convex domain or if $\partial\Omega$ is sufficiently smooth, the solution of* (COP) *satisfies $S(u) \in H^2(\Omega)$.*
2. *Let Ω be an open connected domain with sufficiently smooth boundary $\partial\Omega$. Assume there is a number s with $d < s < \infty$ and suppose $\zeta \in L^s(\Omega)$ and $\max(-\Delta\psi - \zeta, 0) \in L^s(\Omega)$. Then, the solution $S(u)$ of* (COP) *is in $H^{2,s}(\Omega) \cap C^{1,\beta}(\overline{\Omega})$ for $\beta = 1 - \frac{d}{s}$.*

In the remainder of this paper, we often assume that the obstacle ψ and the solution $y = S(u)$ of (COP) are continuous functions. Under the assumptions in Lemma 2.1, this can be guaranteed (in space dimension $d = 2, 3$). There are more statements establishing continuity of y under rather mild assumptions on the data ζ, ψ and Ω. Exemplary, we mention also [43, Thm. 5:2.7].

On the active set $A(\zeta)$, the solution $S(u)$ inherits the smoothness of the obstacle ψ. On the inactive set $I(\zeta)$, regularity theory for the Poisson problem is eligible, when $\zeta \in L^2(\Omega)$. Nevertheless, the presence of the obstacle implies that the regularity of the solution $S(u)$ is, in general, limited, regardless of the smoothness of the data. Indeed, the following results states that optimal regularity of the obstacle problem is $C^{1,1}$. We refer to [7, Thm. 1] and mention also the references [24] and [25].

LEMMA 2.2. *Assume $\zeta \in C^1(\overline{\Omega})$ and $\psi \in C^2(\overline{\Omega})$. Suppose Ω has a smooth boundary $\partial\Omega$. Then the solution of (COP) satisfies $S(u) \in C^{1,1}(\Omega)$.*

In the formulation of the above regularity result in [7], the admissible set of Lipschitz functions v on Ω which satisfy $v \geq \psi$ on Ω and $v = 0$ on $\partial\Omega$ is considered instead of K_ψ in (COP). This is a convex subset of K_ψ. Since under the regularity assumptions in Lemma 2.2 the solution $S(u)$ of (COP) is Lipschitz continuous, see Lemma 2.1, $S(u)$ is a solution of the problem considered in [7].

2.2. Clarke subgradients for the reduced objective function. Recently, generalized derivatives for the solution operator S of (COP) have been obtained, see [39, 40, 42, 41]. From the representation one easily obtains Clarke subgradients for the reduced objective function $\hat{J}$ as in (1.1). In this subsection, we state and recall the corresponding results which are relevant for the analysis in this paper.

The following theorem describes how two generalized derivatives of $\hat{J}$ as in (1.1) can be obtained. We refer to [20] for the definition of a Clarke subgradient.

THEOREM 2.3. *Let U be a partially ordered and separable Banach space. We assume that there is a partially ordered Banach space V embedded into U such that the positive cone in V has nonempty interior and such that the embedding is dense and increasing. We further assume that the order relation $\geq_V$ in V has the property that for all $v, w \in V$ with $v \geq_V w$ it holds $v + z \geq_V w + z$ for all $z \in V$ and $tv \geq_V tw$ for all $t \geq 0$. Suppose that $f : U \to H^{-1}(\Omega)$ is increasing and continuously differentiable. Let $u \in U$ be arbitrary and denote, as usual in this paper, $\zeta := f(u)$. For $D := I(\zeta)$, respectively $D := \Omega \setminus A_{\mathrm{s}}(\zeta)$, denote by $q_{I(\zeta)}$, respectively $q_{\Omega\setminus A_{\mathrm{s}}(\zeta)}$, the unique solution of the variational equation*

$$\text{(2.1)} \qquad \text{Find } q \in H_0^1(D): \quad \langle -\Delta q, v\rangle = \langle J_y\left(S(u), u\right), v\rangle \quad \forall\, v \in H_0^1(D).$$

Then the elements

$$f'(u)^* q_{I(\zeta)} + J_u(S(u), u), \quad f'(u)^* q_{\Omega\setminus A_{\mathrm{s}}(\zeta)} + J_u(S(u), u)$$

are Clarke subgradients of $\hat{J}$ in u.

The assertion concerning the subgradient based on $q_{I(\zeta)}$ can be found in [40, Thm. 5.7]. For the assertion concerning the subgradient based on $q_{\Omega\setminus A_{\mathrm{s}}(\zeta)}$ we refer to [41, Cor. 6.3]. Here, a related statement is contained for the bilateral obstacle problem. The entire statement of Theorem 2.3 is also contained in [39, Thm. 4.21]. For the special example where $U = H^{-1}(\Omega)$ and f is the identity mapping, the statement in Theorem 2.3 is a corollary of [42, Thm. 4.3].

The following remarks are in order concerning the preceding theorem.

Remark 2.4.
1. The sets $H_0^1(I(\zeta))$ and $H_0^1(\Omega\setminus A_{\mathrm{s}}(\zeta))$ are Sobolev spaces on quasi-open domains, which are determined up to a set of capacity zero (which gives a unique Sobolev space). For a quasi-open set $O \subseteq \Omega$, the space $H_0^1(O)$ is defined as $H_0^1(O) := \{v \in H_0^1(\Omega) \mid v = 0 \text{ q.e. outside } O\}$ and represents a closed subset of $H_0^1(\Omega)$. The definition coincides with the usual definition for open domains if O is an open subset of Ω, see, e.g., [28, Thm. 4.5].
2. It might also be of interest to use the estimates established in this paper or the employed techniques in the context of mesh independence for semismooth Newton methods in function spaces. Indeed, in [16], the Newton differentiability of the solution operator of the obstacle problem is established.

To obtain the subgradients of $\hat{J}$ in u as suggested in Theorem 2.3, the knowledge of $S(u)$ and of $I(\zeta)$ or $A_s(\zeta)$ is required. In practice, one obtains only discrete approximations of $S(u)$ by solving a discrete version of the obstacle problem (COP). In the following subsection, we will introduce such a discrete version of the obstacle problem. Afterwards, we will discuss the influence of a discrete solution of the obstacle problem on the quality of a possible approximation of the Clarke subgradients proposed in Theorem 2.3.

3. Properties of the discrete problem. In this section, we formulate a discrete version of (COP) and give a short summary of available $L^\infty(\Omega)$-error estimates, which are relevant for the subsequent derivation of error estimates for generalized derivatives of $\hat{J}$.

3.1. Formulation of the discrete obstacle problem. We consider a family $(\mathcal{T}_h)_{h>0}$ of regular and quasi-uniform triangulations of Ω. For $h > 0$ we consider the discrete obstacle problem

$$\text{(DOP)} \qquad \text{Find } y_h \in K_h : \quad \langle -\Delta y_h - \zeta, z_h - y_h \rangle \geq 0 \quad \forall\, z_h \in K_h,$$

where

$$K_h := \{z_h \in \mathbb{V}_h^0 \mid z_h \geq \psi_h \text{ a.e. in } \Omega\}$$
$$\mathbb{V}_h := \{v \in C(\bar{\Omega}) \mid v|_T \text{ is affine for all } T \in \mathcal{T}_h\} \quad \text{and} \quad \mathbb{V}_h^0 := \mathbb{V}_h \cap H_0^1(\Omega).$$

In the definition of the admissible set K_h, the element $\psi_h = L_h \psi$ denotes the discrete obstacle and L_h is the Lagrange interpolation operator onto $\mathbb{V}_h$. We refer to [38] for this formulation.

It is well known that the discrete obstacle problem has a unique solution, see [25], [31], [38] and that $y_h \to y$ holds in $H_0^1(\Omega)$ as $h \to 0$ for a fixed $\zeta = f(u) \in L^2(\Omega)$ and the corresponding solutions $y_h = S_h(u)$ of (DOP), $y = S(u)$ of (COP), compare [18, Thm. 9.2]. Here and in the sequel, we denote by S_h the solution operator of (DOP).

If Ω is not polyhedral, we could consider triangulations of Ω_h instead, where $\Omega_h \subseteq \Omega$ is polyhedral. Then $z_h \geq \psi_h$ is prescribed only on Ω_h and for the elements in $\mathbb{V}_h$ we demand $v|_{\bar{\Omega}\setminus\Omega_h} = 0$.

3.2. L^∞-estimates for the solution of the discrete obstacle problem. In this section, we will review various types of L^∞-error estimates for the obstacle problems very briefly. Here and in most parts of the paper, we assume that $y = S(u)$ is continuous.

The goal of this paper is to control the error in the generalized derivative when it is derived based on a discrete solution of the obstacle problem. It can be seen from the variational equation (2.1) for the generalized derivative that, for a given $u \in U$, it depends on the solution $S(u)$ of the obstacle problem through the equation itself, but also through the domain $D \subseteq \Omega$ which, in the context of Theorem 2.3, can be chosen as either $I(\zeta)$ or $\Omega \setminus A_s(\zeta)$. Because of this dependance, it is important to control the error between $y = S(u)$ and the discrete version $y_h = S_h(u)$. Since the inactive set $I(\zeta) = \{y > \psi\}$ is defined via the pointwise behavior of y, the L^∞-error between y and y_h is very advantageous when trying to control the discrepancy in the discrete and continuous inactive sets leading to an error in the corresponding discrete and continuous generalized derivatives.

In this paper, we do not rely on a specific L^∞-error estimate. Instead, we usually assume there is a bound ε_h with $\varepsilon_h \to h$ as $h \to 0$ such that

$$\|y - y_h\|_{L^\infty(\Omega)} \leq \varepsilon_h.$$

In practice, ε_h depends on h, and on the norms of ζ and ψ in appropriate spaces. By requiring the appropriate assumptions, any of the L^∞-error estimates can be used.

Based on the discrete maximum principle of Raviart-Ciarlet, see [17] and [19], a priori L^∞-error estimates are established in the literature. Exemplary, we mention [35, 14, 4, 23, 32, 37].

To circumvent necessary assumptions on the triangulations, other approaches yield a priori L^∞-error estimates for the obstacle problem. Here, error estimates for $\|y - y_h\|_{H^1(\Omega)}$ can be used, see [9], [34]. Now, using inverse inequalities, a bound for $\|y - y_h\|_{L^\infty(\Omega)}$ can be obtained, see e.g. [36]. Note that this bound is, in general, not sharp.

A posteriori L^∞-error estimates for the obstacle problem are derived in [38]. Here, no restrictions in the choice of triangulations are required, since the continuous maximum principle is applied. The authors also use these estimates in the $L^\infty(\Omega)$ norm to control the error in the respective active sets. We will focus more on this detail in subsection 6.2.

4. Error estimates for approximate Clarke subgradients. In this section, we explain and derive an error estimate for the Clarke subgradients of the reduced objective function $\hat{J}$ as introduced in Theorem 2.3 and its discrete approximations.

We consider a continuously differentiable objective function $J\colon H_0^1(\Omega) \times U \to \mathbb{R}$ and fix $u \in U$. Using the discrete solution y_h of (DOP), we compute the solution q_h to

$$\text{Find } q_h \in H_0^1(D_h): \quad \langle -\Delta q_h, v_h \rangle = \langle J_y\left(y_h, u\right), v_h \rangle \quad \forall\, v_h \in H_0^1(D_h), \tag{4.1}$$

which is an analogous variational equation to (2.1). Note that D_h is an approximation of the quasi-open set D in Theorem 2.3 based on y_h which will be specified later on. The goal is to find a good estimate for the error $\|q - q_h\|_{H_0^1(\Omega)}$, where q denotes the solution of (2.1), and to choose D_h and D such that this error will be small when h is small.

An estimate for $\|q - q_h\|_{H_0^1(\Omega)}$ immediately yields an estimate for the Clarke subgradients and its approximations

$$\xi(u) := f'(u)^* q + J_u(y, u) \in \partial_{\mathrm{C}} \hat{J}(u) \quad \text{ and } \xi_h(u) := f'(u)^* q_h + J_u(y_h, u),$$

compare Theorem 2.3, via

$$\|\xi(u) - \xi_h(u)\|_{U^*} \leq \|f'(u)^*\|_{\mathcal{L}(H_0^1(\Omega), U^*)} \|q - q_h\|_{H_0^1(\Omega)} + \|J_u(y, u) - J_u(y_h, u)\|_{U^*}.$$

With a little abuse of language, we often call the solutions of (4.1) and (2.1) (inexact) generalized derivatives since the derivation of Clarke subgradients (or approximations thereof) is immediate.

In the sequel, we consider decreasing sequences $(h_n)_{n\in\mathbb{N}}$ of positive numbers with $h_n \to 0$ in the context of triangulations with mesh size h_n. This describes the situation of successively refined meshes with mesh sizes $h_n \to 0$. We fix the notation $y_n := y_{h_n}$ for the solution of (DOP), $q_n := q_{h_n}$ for the solution of (4.1), $\varepsilon_n := \varepsilon_{h_n}$ for an upper bound for $\|y - y_n\|_{L^\infty(\Omega)}$ and $D_n := D_{h_n}$ for a discrete approximation of the quasi-open set D as in Theorem 2.3. In the following sections, we always assume $D_n \subseteq D$.

We emphasize that it is sufficient to show Mosco convergence of $(H_0^1(D_n))_{n\in\mathbb{N}}$ to $H_0^1(D)$ for a suitable choice of sets D_n to obtain the convergence of the solutions

$(q_n)_{n\in\mathbb{N}}$ to q, see [33, Prop. 3.5] and [43, Thm. 4.1]. To use such approximate subgradients in, e.g., bundle methods, compare [29], it is useful to know an upper bound for $\|q_n - q\|_{H_0^1(\Omega)}$ which can be computed in each iteration of the bundle method and which gets arbitrarily small as $n \to \infty$.

Let us first recall the definition of Mosco convergence, cf. [43, Ch. 4:4].

DEFINITION 4.1. *A sequence $(C_n)_{n\in\mathbb{N}}$ of nonempty, closed, convex subsets of a Banach space X converges to a set $C \subseteq X$ in the sense of Mosco if the following conditions are satisfied.*

1. *For each $x \in C$ there exists a sequence $(x_n)_{n\in\mathbb{N}}$ with $x_n \in C_n$ for every $n \in \mathbb{N}$ and such that $(x_n)_{n\in\mathbb{N}}$ converges to x.*
2. *Let $(x_{n_k})_{k\in\mathbb{N}}$ be a subsequence of a sequence $(x_n)_{n\in\mathbb{N}}$ fulfilling $x_n \in C_n$ for all $n \in \mathbb{N}$. If for some $x \in X$ we have $x_{n_k} \rightharpoonup x$ in X, then the weak limit x is an element of C.*

Throughout this paper we consider the Mosco convergence of sets $(H_0^1(O_n))_{n\in\mathbb{N}}$ with quasi-open domains O_n, $n \in \mathbb{N}$. Let us note that the convergence of such sets in the sense of Mosco is equivalent to the γ-convergence of the capacitary measures obtained from O_n, cf. [10, Prop. 4.53, Rem. 4.5.4].

In the following lemma, we will first find an upper bound for the error $\|q-q_n\|_{H_0^1(\Omega)}$ which cannot immediately be computed without knowledge of the continuous solution y of (COP).

LEMMA 4.2. *Let D be a quasi-open set and, for $n \in \mathbb{N}$, let $D_n \subseteq D$ be quasi-open subsets. Denote by $q \in H_0^1(\Omega)$ the solution of (2.1) and for $n \in \mathbb{N}$ denote by q_n the solution of (4.1). Then*

$$\|q - q_n\|_{H_0^1(\Omega)} \le \| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(D)} + \|J_y(y_n, u) - J_y(y, u)\|_{H^{-1}(\Omega)} \tag{4.2}$$

holds. If $H_0^1(D_n) \to H_0^1(D)$ in the sense of Mosco, we additionally have $\| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(D)} \to 0$ as $n \to \infty$.

Proof. Let us note that $q - q_n \in H_0^1(D)$, but not necessarily $q - q_n \in H_0^1(D_n)$. We observe

$$\begin{aligned}
&\|q - q_n\|^2_{H_0^1(\Omega)} = (\nabla(q - q_n), \nabla(q - q_n)) \\
&= (\nabla q, \nabla(q - q_n)) - \langle J_y(y, u), q - q_n\rangle - (\nabla q_n, \nabla(q - q_n)) + \langle J_y(y, u), q - q_n\rangle \\
&= -(\nabla q_n, \nabla(q - q_n)) + \langle J_y(y, u), q - q_n\rangle \\
&= -(\nabla q_n, \nabla(q - q_n)) + \langle J_y(y_n, u), q - q_n\rangle + \langle J_y(y, u) - J_y(y_n, u), q - q_n\rangle \\
&= -\langle -\Delta q_n - J_y(y_n, u), q - q_n\rangle_{H^{-1}(D),H_0^1(D)} + \langle J_y(y, u) - J_y(y_n, u), q - q_n\rangle \\
&\le \left(\| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(D)} + \|J_y(y_n, u) - J_y(y, u)\|_{H^{-1}(\Omega)}\right) \|q - q_n\|_{H_0^1(\Omega)}.
\end{aligned}$$

This implies

$$\|q - q_n\|_{H_0^1(\Omega)} \le \| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(D)} + \|J_y(y_n, u) - J_y(y, u)\|_{H^{-1}(\Omega)}.$$

Assume the sequence $(H_0^1(D_n))_{n\in\mathbb{N}}$ converges to $H_0^1(D)$ in the sense of Mosco. Then, by [33, Prop. 3.5], we obtain $q_n \to q$ in $H_0^1(\Omega)$ as $n \to \infty$. Since also $y_n \to y$ in $H_0^1(\Omega)$ as $n \to \infty$ and since J is continuously differentiable we conclude

$$(-\Delta q_n - J_y(y_n, u)) \to (-\Delta q - J_y(y, u))$$

in $H^{-1}(\Omega)$. This implies $(-\Delta q_n - J_y(y_n, u)) \to (-\Delta q - J_y(y, u)) = 0$ in $H^{-1}(D)$ by (2.1). ∎

Without knowing the exact set D (e.g. $D = I(\zeta)$ or $D = \Omega \setminus A_s(\zeta)$, see Theorem 2.3) the $H^{-1}(D)$ norm in (4.2) cannot be evaluated and the error estimate is not computable. Let us establish the following tool.

LEMMA 4.3. *Let $p_n, p \in H^{-1}(\Omega)$ and let $D \subseteq \Omega$ be a quasi-open set. Assume that $p_n \to p$ in $H^{-1}(\Omega)$ and $p_n \to 0$ in $H^{-1}(D)$ as $n \to \infty$. If there is a sequence $(\tilde{D}_n)_{n\in\mathbb{N}}$ of quasi-open supersets of D with the property that $H_0^1(\tilde{D}_n) \to H_0^1(D)$ in the sense of Mosco, then $\|p_n\|_{H^{-1}(\tilde{D}_n)} \to 0$.*

Proof. For $p \in H^{-1}(\Omega)$ we fix $v_n \in H_0^1(\tilde{D}_n)$, $\|v_n\|_{H_0^1(\tilde{D}_n)} \leq 1$, $n \in \mathbb{N}$, with $\langle p, v_n\rangle_{H^{-1}(\tilde{D}_n),H_0^1(\tilde{D}_n)} \geq \|p\|_{H^{-1}(\tilde{D}_n)} - \frac{1}{n}$. Then, the sequence $(v_n)_{n\in\mathbb{N}}$ is bounded in $H_0^1(\Omega)$ and we can extract a weakly convergent subsequence $(v_{n_k})_{k\in\mathbb{N}}$. We denote the weak limit by v. Note that $\|v\|_{H_0^1(\Omega)} \leq 1$ by Mazur's lemma. By Mosco convergence of $H_0^1(\tilde{D}_n)$ to $H_0^1(D)$, the weak limit v is in $H_0^1(D)$. We have

$$\begin{aligned}\|p\|_{H^{-1}(D)} &\geq \langle p, v\rangle_{H^{-1}(D),H_0^1(D)} = \langle p, v\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} = \lim_{k\to\infty} \langle p, v_{n_k}\rangle_{H^{-1}(\Omega),H_0^1(\Omega)} \\ &= \lim_{k\to\infty} \langle p, v_{n_k}\rangle_{H^{-1}(\tilde{D}_{n_k}),H_0^1(\tilde{D}_{n_k})} \geq \lim_{k\to\infty} \left(\|p\|_{H^{-1}(\tilde{D}_{n_k})} - \frac{1}{n_k}\right).\end{aligned}$$

This, together with $\|p\|_{H^{-1}(D)} \leq \|p\|_{H^{-1}(\tilde{D}_{n_k})}$ for all $k \in \mathbb{N}$, which follows from the inclusion $H_0^1(D) \subseteq H_0^1(\tilde{D}_{n_k})$, implies that $\langle p, v\rangle_{H^{-1}(D),H_0^1(D)} = \|p\|_{H^{-1}(D)}$. By a subsequence-subsequence argument, we can conclude that $\left(\|p\|_{H^{-1}(\tilde{D}_n)}\right)_{n\in\mathbb{N}}$ converges to $\|p\|_{H^{-1}(D)}$.

Now, we can estimate

$$\begin{aligned}\|p_n\|_{H^{-1}(\tilde{D}_n)} &\leq \|p_n - p\|_{H^{-1}(\tilde{D}_n)} + \|p\|_{H^{-1}(\tilde{D}_n)} \\ &\leq \|p_n - p\|_{H^{-1}(\Omega)} + \|p\|_{H^{-1}(\tilde{D}_n)} \to \|p\|_{H^{-1}(D)}.\end{aligned}$$

On the other hand,

$$\begin{aligned}\|p_n\|_{H^{-1}(\tilde{D}_n)} &\geq \|p\|_{H^{-1}(\tilde{D}_n)} - \|p - p_n\|_{H^{-1}(\tilde{D}_n)} \\ &\geq \|p\|_{H^{-1}(\tilde{D}_n)} - \|p - p_n\|_{H^{-1}(\Omega)} \to \|p\|_{H^{-1}(D)}\end{aligned}$$

and we conclude that

$$\|p_n\|_{H^{-1}(\tilde{D}_n)} \to \|p\|_{H^{-1}(D)} = 0. \qquad \square$$

The following corollary uses an outer approximation of D, which will later on be computed based on y_n, to obtain a computable upper bound for $\|q - q_n\|_{H_0^1(\Omega)}$.

COROLLARY 4.4. *Let D be a quasi-open set and, for $n \in \mathbb{N}$, assume D_n, $\tilde{D}_n$ are quasi-open sets with*

$$D_n \subseteq D \subseteq \tilde{D}_n \tag{4.3}$$

and

$$H_0^1(D_n) \to H_0^1(D) \quad \text{and} \quad H_0^1(\tilde{D}_n) \to H_0^1(D) \tag{4.4}$$

in the sense of Mosco. Let q_n, q be the solutions of (4.1), (2.1), respectively. Then the error estimate

$$\|q - q_n\|_{H_0^1(\Omega)} \leq \| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(\tilde{D}_n)} + \|J_y(y_n, u) - J_y(y, u)\|_{H^{-1}(\Omega)} \overset{n\to\infty}{\to} 0$$

is valid.

Proof. Combining (4.2) with $H_0^1(D) \subseteq H_0^1(\tilde{D}_n)$ for all $n \in \mathbb{N}$, we derive

$$\|q - q_n\|_{H_0^1(\Omega)} \leq \| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(\tilde{D}_n)} + \|J_y(y_n, u) - J_y(y, u)\|_{H^{-1}(\Omega)}.$$

As argued in the proof of Lemma 4.2, we have $(-\Delta q_n - J_y(y_n, u)) \to (-\Delta q - J_y(y, u))$ in $H^{-1}(\Omega)$. By Lemma 4.2, it holds $\| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(D)} \stackrel{n\to\infty}{\to} 0$. Now, Lemma 4.3 implies that $\| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(\tilde{D}_n)} \stackrel{n\to\infty}{\to} 0$ and the conclusion follows. ∎

5. Discrete inner approximation of the inactive set. In this section, we take a look at approximations of the inactive set $I(\zeta)$ that can be constructed using only discrete solution of the obstacle problem y_n. These sets are introduced in the literature and based on an upper bound ε_n for the L^∞-error $\|y - y_n\|_{L^\infty(\Omega)}$. The definition yield subset approximations of $I(\zeta)$. In our analysis, these sets I_n will be the starting point to derive also approximations of $D := \Omega \setminus A_s(\zeta)$ in the upcoming sections. By Corollary 4.4, such approximations are useful in the construction of error estimates for generalized derivatives of $\hat{J}$.

The following result is a slight modification of [5, Thm. 1.1.] and introduces the approximations I_n.

LEMMA 5.1. *Let $\zeta \in L^2(\Omega)$ be fixed. Assume $y, \psi \in C(\overline{\Omega})$. Let $(\varepsilon_n)_{n\in\mathbb{N}}$ be such that*

$$\|y - y_n\|_{L^\infty(\Omega)} \leq \varepsilon_n \stackrel{n\to\infty}{\to} 0$$

holds for the solutions y, y_n of (COP) and (DOP). Define

$$I_n := I_n(\zeta) := \{\omega \in \Omega \mid y_n(\omega) > \psi(\omega) + \varepsilon_n\}. \tag{5.1}$$

Then we have $I_n \subseteq I(\zeta)$ for all $n \in \mathbb{N}$ and $\liminf_{n\to\infty} I_n = I(\zeta)$, i.e., $\bigcup_{n\in\mathbb{N}} \bigcap_{k\geq n} I_k = I(\zeta)$.

Proof. The first part of the proof can be found in the proof of [38, Thm. 4.1]. Using the obvious modifications, the subsequent part of the proof can be found in [5, Thm. 1.1]. Here, the set I_n is defined slightly different.

Remark 5.2. It is also possible to define an approximation of $I(\zeta)$ based on the discrete obstacle $\psi_n := \psi_{h_n}$, namely

$$J_n := \left\{y_n > \psi_n + \varepsilon_n + \|(\psi - \psi_n)_+\|_{L^\infty(\{y_n \leq \psi_n + \varepsilon_n + \|(\psi-\psi_n)_+\|_{L^\infty(\Omega)}\})}\right\}. \tag{5.2}$$

With this definition, the respective result in Lemma 5.1 can be shown aswell and also the upcoming construction of approximations of $\Omega \setminus A_s(\zeta)$ and the resulting error estimates for the Clarke subgradients stay valid (with suitable adaptations). For the details, see [39, Ch. 7.7].

For the approximations I_n introduced in Lemma 5.1, we will see that the Mosco convergence $H_0^1(I_n) \to H_0^1(I(\zeta))$ holds. As stated in Lemma 4.2, this property implies the convergence of the solutions of (4.1) with $D_n := I_n$ to the solution of (2.1) with $D := I(\zeta)$. In addition, the error estimate (4.2) for the Clarke subgradients holds.

Before we verify Mosco convergence, let us argue that the sets $\left(\bigcap_{k\geq n} I_k\right)_{n\in\mathbb{N}}$ are open. Thus, by Lemma 5.1, they are an open covering of $I(\zeta)$.

LEMMA 5.3. *Assume the conditions of Lemma 5.1 are fulfilled. Then the sets $\bigcap_{k\geq n} I_k$ are open for all $n \in \mathbb{N}$.*

Proof. Let $n \in \mathbb{N}$ and assume there is $\omega \in \bigcap_{k\geq n} I_k \subseteq I(\zeta)$, compare Lemma 5.1. Then we have

$$c := y(\omega) - \psi(\omega) > 0.$$

Since y and ψ are continuous, there is $C > 0$ such that

$$y(z) - \psi(z) > c/2$$

for all $z \in B_C(\omega)$. Let $n_0 \in \mathbb{N}$ be such that $\varepsilon_k \leq c/4$ for all $k \geq n_0$. Then it holds for all $k \geq n_0$ and for all $z \in B_C(\omega)$

$$y_k(z) - \psi(z) = y_k(z) - y(z) + y(z) - \psi(z) > -\varepsilon_k + c/2 \geq \varepsilon_k.$$

We conclude the ball $B_C(\omega)$ of radius C is a subset of $\bigcap_{k\geq n_0} I_k$. If $n < n_0$, $\bigcap_{k\geq n} I_k$ is the finite intersection of $\bigcap_{k\geq n_0} I_k$ and open sets and thus contains a ball $B_{\tilde{C}}(\omega)$ of radius $\tilde{C} \geq 0$. Since $\omega \in \bigcap_{k\geq n} I_k$ was arbitrary, we conclude that $\bigcap_{k\geq n} I_k$ is open. ◻

In the following theorem, we verify the Mosco convergence $H_0^1(I_n) \to H_0^1(I(\zeta))$.

THEOREM 5.4. *Assume the conditions of Lemma 5.1 are satisfied. Then the sequence $(H_0^1(I_n))_{n\in\mathbb{N}}$ converges to $H_0^1(I(\zeta))$ in the sense of Mosco.*

Proof. Let $v \in H_0^1(I(\zeta))$ be arbitrary. The family of sets $(\bigcap_{k\geq n} I_k)_{n\in\mathbb{N}}$ is an increasing covering of $I(\zeta)$, see Lemma 5.3 and Lemma 5.1. Thus, there exists a sequence $(v_n)_{n\in\mathbb{N}}$ with $v_n \to v$ in $H_0^1(I(\zeta))$ as $n \to \infty$ and such that $v_n \in H_0^1(\bigcap_{k\geq n} I_k)$ for each $n \in \mathbb{N}$, see [30, Thm. 2.10, Lem. 2.4]. In particular, $v_n \in H_0^1(I_n)$ since $\bigcap_{k\geq n} I_k \subseteq I_n$.

Suppose there is a sequence $(w_n)_{n\in\mathbb{N}}$ with $w_n \in H_0^1(I_n)$ and $w_{n_k} \rightharpoonup w$ in $H_0^1(\Omega)$ for some $w \in H_0^1(\Omega)$ and for a subsequence $(w_{n_k})_{k\in\mathbb{N}}$ of $(w_n)_{n\in\mathbb{N}}$. Since $I_n \subseteq I(\zeta)$ holds, see Lemma 5.1, we have $w_n \in H_0^1(I(\zeta))$ for all $n \in \mathbb{N}$. Then the weak limit w is also in $H_0^1(I(\zeta))$ by Mazur's lemma. ◻

6. Properties of the strictly and weakly active sets under a nondegeneracy condition.

In this section we will motivate the decision to approximate the set $\Omega \setminus A_s(\zeta)$ instead of the set $I(\zeta)$. Based on the inactive set one can also obtain a generalized derivative (see Theorem 2.3) and it probably appears to be more accessible, in particular because we already have the discrete approximations I_n at hand, compare section 5. As demonstrated in Corollary 4.4, to obtain a computable and convergent upper bound for the term $\|q - q_n\|_{H_0^1(\Omega)}$ an additional sequence $(\tilde{I}_n)_{n\in\mathbb{N}}$ of quasi-open supersets of $I(\zeta)$, such that $(H_0^1(\tilde{I}_n))_{n\in\mathbb{N}}$ converges to $H_0^1(I(\zeta))$, needs to be constructed. As will be discussed in subsection 6.3, the weakly active set $A_w(\zeta)$ can be thin and irregular. For this reason, it is very hard to approximate or predict the inactive set from the outside based only on the discrete numerics.

To construct D_n and $\tilde{D}_n$ as approximations of $\Omega \setminus A_s(\zeta)$, we make use of estimates for the distances of the free boundaries $\partial I(\zeta)$ and ∂I_n which are available in the literature. The validity of these estimates is ensured under the so-called nondegeneracy condition. Assuming this condition, we will also show that the weakly active set does not have interior points (Lemma 6.6) and that the strictly active set is the closure w.r.t. the fine topology of the interior of the active set (Corollary 6.9).

6.1. Definition of the strictly active set. In this subsection we recall known results concerning the strictly active set and its characterization and properties.

First, let us recall that any element $\xi \in H^{-1}(\Omega)_+$ can be identified with a regular Borel measure $\tilde{\xi}$ on Ω and for every Borel set $E \subseteq \Omega$ of capacity zero it holds $\tilde{\xi}(E) = 0$. Moreover, the quasi-continuous representative of some $v \in H_0^1(\Omega)$ is integrable with respect to $\tilde{\xi}$ and it holds $\langle \xi, v\rangle = \int_\Omega v \,\mathrm{d}\tilde{\xi}$, see [6, Thm. 6.54, Lem. 6.55, Lem. 6.56].

For elements in $H^{-1}(\Omega)_+$ or, equivalently, for the related regular Borel measures, the fine support can be defined as follows, see [45, App. A].

Lemma 6.1. *Let $\xi \in H^{-1}(\Omega)_+$. Then there exists a largest finely open set $O \subseteq \Omega$ with $\tilde{\xi}(O) = 0$ and we can define* $\text{f-supp}(\tilde{\xi}) := O^{\complement}$.

Lemma 6.1 uses the notion of the fine topology on $\mathbb{R}^d$, which is defined as the coarsest topology on $\mathbb{R}^d$ such that all sub-harmonic functions are continuous. For details, we refer to [1] and [28].

Usually, it is possible to circumvent the usage of the fine topology by using concepts from capacity theory, in particular the notions of quasi-open and quasi-closed sets. Note that the family of quasi-open subsets is not a topology. The fine topology, nevertheless, is compatible with most of the concepts related to quasi-open sets and quasi-continuous functions.

In our context, note that for any $u \in U$ the element $\xi := -\Delta S(u) - \zeta$ is in $H^{-1}(\Omega)_+$ and thus, can be identified with a regular Borel measure $\tilde{\xi}$ on Ω. The strictly active set is defined as $A_{\mathrm{s}}(\zeta) := \text{f-supp}(\tilde{\xi})$. Its complement $A_{\mathrm{w}}(\zeta) := \Omega \setminus A_{\mathrm{s}}(\zeta)$ is called the weakly active set.

6.2. Error estimate for the discrete and continuous free boundaries. The purpose of this subsection is to prepare the formulation of a result estimating the distance between I_n and the boundary of $I(\zeta)$, i.e., the free boundary $\partial A(\zeta)$. This topic has been discussed in the literature. As references, we mention, among other related references, [8, 21, 36, 38].

The following lemma states that the so called nondegeneracy condition implies a quadratic growth property of $y - \psi$ away from the active set, which is the basis for the estimates concerning the free boundaries. The formulation is taken from [38] and the proof is based on [25, Ch. 2, Lem. 3.1].

Lemma 6.2. *Let $\zeta \in L^2(\Omega)$ and let y, ψ be continuous. Suppose there is an open neighborhood $\mathcal{U} \subseteq \Omega$ of the active set $A(\zeta)$ and a positive number $\eta > 0$ such that the nondegeneracy condition*

$$\text{(ND)} \qquad \langle -\Delta\psi - \zeta, v\rangle \geq \eta \int_{\mathcal{U}} v \,\mathrm{d}\lambda^d \quad \forall\, v \in H_0^1(\mathcal{U})_+$$

holds. Then, for any $\omega_0 \in \overline{I(\zeta)}$ and any $r > 0$ such that $B_r(\omega_0) \subseteq \mathcal{U}$ it holds

$$\text{(QG)} \qquad \sup_{\omega \in B_r(\omega_0)} y(\omega) - \psi(\omega) \geq y(\omega_0) - \psi(\omega_0) + \frac{\eta r^2}{2d}.$$

Proof. Let us first consider the case $\omega_0 \in I(\zeta)$ and assume $B_r(\omega_0) \subseteq \mathcal{U}$. The function

$$w(x) = y(x) - \psi(x) - y(\omega_0) + \psi(\omega_0) - \frac{\eta}{2d}|x - \omega_0|^2$$

satisfies $w(\omega_0) = 0$ and also

$$\langle -\Delta w, v\rangle = \langle -\Delta y + \Delta\psi, v\rangle + \eta \frac{2d}{2d} \int_{\mathcal{U}} v \,\mathrm{d}\lambda^d = \langle \Delta\psi + \zeta, v\rangle + \eta \int_{\mathcal{U}} v \,\mathrm{d}\lambda^d \leq 0$$

for all $v \in H_0^1(\mathcal{U})_+ \cap H_0^1(I(\zeta))$. Here, we have used (ND) and $\langle -\Delta y - \zeta, v\rangle = 0$ due to $v = 0$ q.e. on $A_{\mathrm{s}}(\zeta)$, see Lemma 6.1 and subsection 6.1. In particular, $\langle -\Delta w, v\rangle \leq 0$ for all $v \in H_0^1(B_r(\omega_0) \cap I(\zeta))_+$. By the maximum principle [31, Thm. II 5.7], it holds

$$w(x) \leq \sup_{\omega \in \partial(B_r(\omega_0)\cap I(\zeta))} w(\omega)$$

in $B_r(\omega_0) \cap I(\zeta)$. Since $w < 0$ holds on $\partial I(\zeta)$, there must exist a point $\omega_1 \in \partial B_r(\omega_0) \cap I(\zeta)$ such that $w(x_1) \geq 0$ and (QG) follows.

For $\omega_0 \in \partial I(\zeta)$, let $(\omega^n)_{n\in\mathbb{N}} \subseteq I(\zeta)$ be a sequence with $\omega^n \to \omega_0$. Then (QG) is already shown for ω^n, $n \in \mathbb{N}$, and, using continuity arguments, we obtain the statement for ω_0. □

Note that the original strong formulation of nondegeneracy goes back to Caffarelli [12].

Now, let us state the following result on the distance of the free boundaries $\partial I(\zeta)$ and ∂I_n which is based on [38, Thm. 4.1].

LEMMA 6.3. *We assume that $\zeta \in L^2(\Omega)$, $y, \psi \in C(\bar{\Omega})$ and $\psi < 0$ on $\partial\Omega$. Suppose there exists a neighborhood $\mathcal{U}$ of $A(\zeta)$ and a positive number $\eta > 0$ such that the nondegeneracy condition (ND) holds on $\mathcal{U}$. Assume $(\varepsilon_n)_{n\in\mathbb{N}}$ is a family of upper bounds for the errors $\|y - y_n\|_{L^\infty(\Omega)}$ for the solutions y, y_n of (COP) and (DOP), which converges to 0 as $n \to \infty$. Set*

$$r_n := 2\sqrt{\frac{d\,\varepsilon_n}{\eta}}. \tag{6.1}$$

Then, if n is large enough, it holds

$$\{\omega \in \Omega \mid \operatorname{dist}(\omega, I_n) \geq r_n\} \subseteq A(\zeta).$$

Proof. Since $A(\zeta)$ and $\partial\Omega$ are compact and disjoint sets, it holds $\operatorname{dist}(\partial\Omega, A(\zeta)) > 0$. Thus, w.l.o.g., we can assume $\operatorname{dist}(\mathcal{U}, \partial\Omega) > 0$. Since y and ψ are continuous and since $\Omega \setminus \mathcal{U}$ is relatively compact, we find a constant $c > 0$ such that $y - \psi > c$ holds outside $\mathcal{U}$. By definition of I_n, this implies

$$I_n^{\complement} \subseteq \mathcal{U}$$

if $n \in \mathbb{N}$ is sufficiently large. Moreover, if n is large enough, we also have $r_n < \operatorname{dist}(\mathcal{U}, \partial\Omega)$. Let us assume that $n \in \mathbb{N}$ is sufficiently large in the sense of these two conditions.

Let $\omega \in \Omega$ with $\operatorname{dist}(\omega, I_n) \geq r_n$ and assume $\omega \in I(\zeta)$, i.e.,

$$y(\omega) > \psi(\omega).$$

In particular, we have $\omega \in I_n^{\complement} \subseteq \mathcal{U}$ and thus, $\overline{B_{r_n}(\omega)} \subseteq \Omega$. We even observe $\overline{B_{r_n}(\omega)} \subseteq I_n^{\complement} \subseteq \mathcal{U}$.

Now, Lemma 6.2 implies

$$\sup_{x \in B_{r_n}(\omega)} y(x) - \psi(x) > \frac{\eta r_n^2}{2d}.$$

This means, for some $x \in B_{r_n}(\omega)$ it holds

$$y_n(x) = y(x) + (y_n(x) - y(x)) > \psi(x) + \frac{\eta r_n^2}{2d} - \varepsilon_n = \psi(x) + \varepsilon_n$$

and this contradicts $\overline{B_{r_n}(\omega)} \subseteq I_n^{\complement}$. We conclude $\omega \in A(\zeta)$. □

Remark 6.4. Usually, the analysis concerning the Hausdorff distance between the exact and the approximate free boundary require regularity of $\partial A(\zeta)$, see, e.g., [8], [21], [36]. In contrast, the authors in [38] stress that the derivation of the error estimate in Lemma 6.3 does not require any regularity assumptions on the exact free boundary $\partial A(\zeta(u))$, see [38, Rem. 4.4].

6.3. Structure of the weakly and strictly active set under regularity assumptions. Under the nondegeneracy condition (ND), i.e., under the same assumptions that are required for the estimates relating the continuous and discrete free boundaries in the previous subsection, we now investigate the topological structures of the weakly and the strictly active set. This approach is not common in the classical literature, where the free boundary analysis and the investigation of topological structures is usually performed for the overall active set and its boundary and the distinction between strictly active and weakly active set is not drawn. Yet, as we will see, there are fundamental differences and the strictly active set often exhibits a considerably more regular structure than the overall active set.

Before we start, let us state the following auxiliary lemma.

LEMMA 6.5.
1. *Let $O \subseteq \Omega$ be quasi-open. Then there exists an element $v \in H_0^1(\Omega)_+$ satisfying $\{v > 0\} = O$ up to a set of zero capacity.*
2. *Let $A \subseteq \Omega$ be quasi-closed. Then there exists an element $\lambda \in H^{-1}(\Omega)_+$ such that* $\operatorname{f-supp}(\lambda) = A$.

For the proof of the first statement, we refer the reader to [27, Lem. 3.6] and [44, Prop. 2.3.14]. The proof of the second statement can be found in [42, Thm. 3.9]. In the above lemma, $\{v > 0\}$ refers to the set of points where the quasi-continuous representative of $v \in H_0^1(\Omega)$ is positive. This set is determined up to a set of capacity zero, cf. e.g. [22, Chap. 8, Thm. 6.1].

LEMMA 6.6. *Let $\zeta \in L^2(\Omega)$. Assume the nondegeneracy condition (ND) holds in a neighborhood $\mathcal{U}$ of the active set. Then the weakly active set does not have interior points.*

Proof. Let $v \in H_0^1(\Omega)_+$ with

$$\{v > 0\} = \operatorname{int}(A_{\mathrm{w}}(\zeta)), \tag{6.2}$$

see Lemma 6.5. This implies

$$\begin{aligned}\langle -\Delta\psi - \zeta, v\rangle &= \int_\Omega \nabla\psi^T \nabla v \,\mathrm{d}\lambda^d - (\zeta, v) = \int_{A_{\mathrm{w}}(\zeta)} \nabla y^T \nabla v \,\mathrm{d}\lambda^d - (\zeta, v)\\ &= \int_\Omega \nabla y^T \nabla v \,\mathrm{d}\lambda^d - (\zeta, v) = \langle -\Delta y - \zeta, v\rangle = 0.\end{aligned}$$

Here, we have used that $\nabla v = 0$ a.e. on $\Omega \setminus A_{\mathrm{w}}(\zeta)$ and $\nabla\psi = \nabla y$ a.e. on $A_{\mathrm{w}}(\zeta)$, see [3, Prop. 5.8.2]. In the last step, we use $v = 0$ q.e. on $A_{\mathrm{s}}(\zeta)$, see Lemma 6.1 and subsection 6.1. On the other hand, the nondegeneracy condition (ND) yields

$$\langle -\Delta\psi - \zeta, v\rangle \ge \eta \int_{\mathcal{U}} v \,\mathrm{d}\lambda^d.$$

Combining the two arguments, we conclude $\int_{\mathcal{U}} v \,\mathrm{d}\lambda^d = 0$ and thus $v = 0$ a.e. on $\mathcal{U}$. Observing $\operatorname{int}(A_{\mathrm{w}}(\zeta)) \subseteq \mathcal{U}$ and recalling (6.2), we conclude $\lambda^d(\operatorname{int}(A_{\mathrm{w}}(\zeta))) = 0$ and since this set is open we derive $\operatorname{int}(A_{\mathrm{w}}(\zeta)) = \emptyset$. ∎

Since we are interested in a topological description of the strictly active set, we will use the following notions related to the fine topology on $\mathbb{R}^d$. For a set $E \subseteq \mathbb{R}^d$ we denote the closure w.r.t. the fine topology by f-cl(E) and the interior w.r.t. the fine topology by f-int(E), compare also Lemma 6.1.

Let us state the following auxiliary lemma.

LEMMA 6.7. *Let $\xi \in H^{-1}(\Omega)_+$ and let $B \subseteq \Omega$ be a Borel measurable set. We consider the restriction $\xi|_B$ defined by*

$$\langle \xi|_B, v\rangle := \int_B v \, \mathrm{d}\tilde{\xi} = \int_\Omega v \, \mathrm{d}\tilde{\xi}|_B,$$

where $\tilde{\xi}$ is the Borel measure associated with ξ and $\tilde{\xi}|_B$ the trace measure or restricted measure w.r.t. B.

1. *We have $\xi|_B \in H^{-1}(\Omega)_+$.*
2. *Assume that ∂B has Lebesgue measure zero and suppose further $\xi \in L^2(\Omega)_+ \subseteq H^{-1}(\Omega)_+$. Then* f-supp$(\tilde{\xi}|_B) =$ f-cl$(\mathrm{int}(B) \cap \text{f-supp}(\tilde{\xi}))$.

Proof. 1. The operator $\xi|_B$ is well-defined and linear on $H_0^1(\Omega)$. Furthermore, we have

$$|\langle \xi|_B, v\rangle| \le \int_B |v| \, \mathrm{d}\tilde{\xi} \le \int_\Omega |v| \, \mathrm{d}\tilde{\xi} = \langle \xi, |v|\rangle,$$

thus, using $\||v|\|_{H_0^1(\Omega)} = \|v\|_{H_0^1(\Omega)}$, see [3, Cor. 5.8.1], we see that $\xi|_B$ is bounded. Since $\xi|_B$ can be identified with the trace measure $\tilde{\xi}|_B$, it is clear that $\xi|_B$ is nonnegative and we conclude $\xi|_B \in H^{-1}(\Omega)_+$.

2. Now, assume ∂B has Lebesgue measure zero and that $\xi \in L^2(\Omega)_+$. Let

$$O := \text{f-int}(\overline{B^\complement} \cup \text{f-supp}(\tilde{\xi})^\complement).$$

Using $\tilde{\xi}(E) = 0$ for every Borel set $E \subseteq \text{f-supp}(\tilde{\xi})^\complement$, cf. Lemma 6.1, we derive

$$\tilde{\xi}|_B(O) = \tilde{\xi}(B \cap O) \le \tilde{\xi}(B \cap \overline{B^\complement}) + \tilde{\xi}(B \cap \text{f-supp}(\tilde{\xi})^\complement) = 0$$

since $\tilde{\xi}$ is absolutely continuous w.r.t. the Lebesgue measure and using that $\lambda^d(\partial B) = 0$. Thus, f-supp$(\tilde{\xi}|_B) \subseteq$ f-cl$(\mathrm{int}(B) \cap \text{f-supp}(\tilde{\xi}))$.
On the other hand, let $O :=$ f-supp$(\tilde{\xi}|_B)^\complement$, i.e., O is the largest finely open set with $\tilde{\xi}|_B(O) = 0$. Then $O \cap \mathrm{int}(B)$ is finely open and $\tilde{\xi}(O \cap \mathrm{int}(B)) = 0$. This implies $O \cap \mathrm{int}(B) \subseteq$ f-supp$(\tilde{\xi})^\complement$. We conclude $O \subseteq \overline{B^\complement} \cup$ f-supp$(\tilde{\xi})^\complement$ and obtain $\mathrm{int}(B) \cap$ f-supp$(\tilde{\xi}) \subseteq$ f-supp$(\tilde{\xi}|_B)$. Since the set on the right-hand side is finely closed, we even have f-cl$(\mathrm{int}(B) \cap \text{f-supp}(\tilde{\xi})) \subseteq$ f-supp$(\tilde{\xi}|_B)$. ☐

For our further analysis of the strictly active set, we require additional regularity of the obstacle, namely $\psi \in H^2(\Omega)$. This implies $(-\Delta\psi - \zeta) \in L^2(\Omega)$ if $\zeta \in L^2(\Omega)$. We obtain the following result.

LEMMA 6.8. *Let $\zeta \in L^2(\Omega)$. Assume the nondegeneracy condition* (ND) *holds in a neighborhood $\mathcal{U}$ of the active set and, in addition, let $\psi \in H^2(\Omega)$. Denote $\xi_\psi := (-\Delta\psi - \zeta)_+ \in L^2(\Omega)_+$. Then* f-supp$(\tilde{\xi}_\psi) \supseteq A(\zeta)$ *holds.*

Proof. Assume $\emptyset \ne O \subseteq \mathcal{U}$ is finely open. Let $v \in H_0^1(O)_+$ with $\{v > 0\} = O$, compare Lemma 6.5 and note that finely open sets are quasi-open. We conclude

$$\int_\Omega (-\Delta\psi - \zeta)\, v \, \mathrm{d}\lambda^d = \langle -\Delta\psi - \zeta, v\rangle \ge \eta \int_{\mathcal{U}} v \, \mathrm{d}\lambda^d$$

by the nondegeneracy condition (ND). This means $\int_\Omega (-\Delta\psi - \zeta)\, v \,\mathrm{d}\lambda^d > 0$, since $v \in H_0^1(O)_+$ and since O has positive Lebesgue measure, see [2, Thm. 7.3.11, Cor. 7.2.4]. We have

$$\int_\Omega v \,\mathrm{d}\tilde{\xi}_\psi = \int_\Omega (-\Delta\psi - \zeta)_+ \, v \,\mathrm{d}\lambda^d \geq \int_\Omega (-\Delta\psi - \zeta)\, v \,\mathrm{d}\lambda^d > 0,$$

which implies

$$\tilde{\xi}_\psi(O) > 0.$$

Recalling Lemma 6.1, this shows

$$A(\zeta) \subseteq \mathcal{U} \subseteq \text{f-supp}(\tilde{\xi}_\psi). \qquad \square$$

Now, we can show that the strictly active set is the fine closure of its interior points.

Corollary 6.9. *Suppose Ω is convex or has a sufficiently regular boundary. Let $\zeta \in L^2(\Omega)$. Assume the nondegeneracy condition (ND) holds in a neighborhood $\mathcal{U}$ of the active set and additionally assume $\psi \in H^2(\Omega)$ and $\lambda^d(\partial A(\zeta)) = 0$. Denote $\xi := -\Delta S(u) - \zeta$. Then we have $A_{\mathrm{s}}(\zeta) = \text{f-supp}(\tilde{\xi}) = \text{f-cl}(\text{int}(A(\zeta)))$.*

Proof. Under the regularity assumptions we have $S(u) \in H^2(\Omega)$, see Lemma 2.1. Moreover,

$$-\Delta S(u) - \zeta = \begin{cases} -\Delta\psi - \zeta & \text{a.e. on } A(\zeta), \\ 0 & \text{a.e. on } I(\zeta), \end{cases} \tag{6.3}$$

cf. [15, Thm. 2.2], which is a consequence of the regularity and of $\nabla\psi = \nabla S(u)$ a.e. on $A(\zeta)$, see [3, Prop. 5.8.2]. Since ξ is nonnegative, we have $-\Delta S(u) - \zeta \geq 0$ a.e. on Ω and conclude that $-\Delta\psi - \zeta \geq 0$ a.e. on $A(\zeta)$. By (6.3), we have

$$\xi = \xi_\psi|_{A(\zeta)},$$

a.e. in Ω, where $\xi_\psi := (-\Delta\psi - \zeta)_+$ as in Lemma 6.8. We apply Lemma 6.7 and Lemma 6.8 and obtain

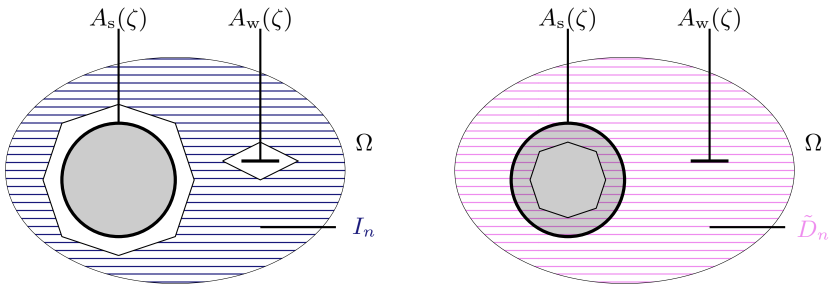
$$A_{\mathrm{s}}(\zeta) = \text{f-supp}(\tilde{\xi}) = \text{f-cl}(\text{int}(A(\zeta)) \cap \text{f-supp}(\tilde{\xi}_\psi)) = \text{f-cl}(\text{int}(A(\zeta))), \qquad \square$$

In the following, to ensure the topological property of the strictly active set derived in Corollary 6.9, we assume $\lambda^d(\partial A(\zeta)) = 0$. The following result from [25, Ch. 2, Thm. 3.5] shows that this assumption can be guaranteed a priori.

Lemma 6.10. *Let Ω have a smooth boundary $\partial\Omega$. Assume further $\zeta \in C^1(\overline{\Omega})$ and $\psi \in C^2(\overline{\Omega})$. Suppose the nondegeneracy condition (ND) holds. Then this implies $\lambda^d(\partial A(\zeta)) = 0$.*

7. Discrete approximations of the complement of the strictly active set. In this section, we will suggest and analyze particular choices of approximations D_n and $\tilde{D}_n$ of the set $\Omega \setminus A_{\mathrm{s}}(\zeta)$. By Theorem 2.3 and Corollary 4.4, a suitable construction will lead to an error estimate for the generalized derivative on the domain $D = \Omega \setminus A_{\mathrm{s}}(\zeta)$.

We will take advantage of the structure of the strictly and weakly active sets examined in subsection 6.3 and construct approximations of $\Omega \setminus A_{\mathrm{s}}(\zeta)$ from in- and outside based on the estimates for the distances of the free boundaries, cf. subsection 6.2. Since the verified structure is crucial for our construction and analysis, we collect the requirements for these results in the following assumption.



(a) Exemplary presentation of I_n (b) Exemplary presentation of $\tilde{D}_n$

Fig. 1: Construction of $\tilde{D}_n$ from I_n using the upper bound for the error $\tilde{r}_n$

ASSUMPTION 7.1. *Let $(h_n)_{n\in\mathbb{N}}$ be a sequence of mesh size parameters with $h_n \to 0$ as $n \to \infty$. Let Ω be convex or assume it has a sufficiently regular boundary. We assume that $\zeta \in L^2(\Omega)$, $y, \psi \in C(\bar{\Omega})$, $\psi \in H^2(\Omega)$ and $\psi < 0$ on $\partial\Omega$. Suppose there exists a neighborhood $\mathcal{U}$ of $A(\zeta)$ and a positive number $\eta > 0$ such that the nondegeneracy condition (ND) holds on $\mathcal{U}$. Let $(\varepsilon_n)_{n\in\mathbb{N}}$ be a sequence satisfying $\varepsilon_n \to 0$ as $n \to \infty$ as well as $\|y - y_n\|_{L^\infty(\Omega)} \le \varepsilon_n$ for all $n \in \mathbb{N}$. Moreover, we assume $\lambda^d(\partial A(\zeta)) = 0$.*

We suggest the superset approximations

$$\tilde{D}_n := \{\omega \in \Omega \mid \mathrm{dist}(\omega, I_n) < \tilde{r}_n\}, \tag{7.1}$$

of $\Omega \setminus A_s(\zeta)$ with $I_n = \{y_n - \psi > \varepsilon_n\}$ as in (5.1) and $\tilde{r}_n$ satisfying

$$\tilde{r}_n > r_n \quad \text{and} \quad \tilde{r}_n \overset{n\to\infty}{\to} 0$$

for $r_n = 2\sqrt{\frac{d\,\varepsilon_n}{\eta}}$ as in (6.1).

LEMMA 7.2. *Suppose the conditions in Assumption 7.1 are fulfilled. Let $\tilde{D}_n$ be defined as in (7.1). Then the inclusion*

$$\Omega \setminus A_s(\zeta) \subseteq \tilde{D}_n$$

holds for large enough $n \in \mathbb{N}$ and $H_0^1(\tilde{D}_n) \to H_0^1(\Omega \setminus A_s(\zeta))$ in the sense of Mosco.

Proof. Using Corollary 6.9 and Lemma 6.3 for large enough $n \in \mathbb{N}$, we observe

$$\Omega \setminus A_s(\zeta) = (\text{f-cl}(\mathrm{int}(A(\zeta))))^{\complement} \subseteq \overline{I(\zeta)} \subseteq \{\omega \in \Omega \mid \mathrm{dist}(\omega, I_n) \le r_n\} \subseteq \tilde{D}_n$$

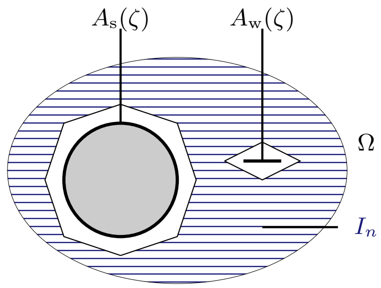
Assume $v \in H_0^1(\Omega \setminus A_s(\zeta))$. Then $v_n := v \in H_0^1(\tilde{D}_n)$ for $n \in \mathbb{N}$ large enough and $v_n \to v$ in $H_0^1(\Omega)$, which shows the first condition for Mosco convergence.

Suppose there is a sequence $(v_n)_{n\in\mathbb{N}}$ with $v_n \in H_0^1(\tilde{D}_n)$ and $v_{n_k} \rightharpoonup v$ for a subsequence $(v_{n_k})_{k\in\mathbb{N}}$ of $(v_n)_{n\in\mathbb{N}}$.

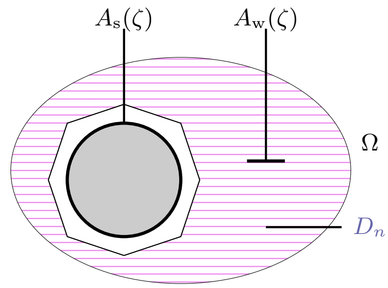
We can write

$$\mathrm{int}(A(\zeta)) = \bigcup_{m\in\mathbb{N}} A(\zeta)_m := \bigcup_{m\in\mathbb{N}} \{\omega \in A(\zeta) \mid \mathrm{dist}(\omega, \partial A(\zeta)) \ge m^{-1}\}.$$

By the inclusion $I_n \subseteq I(\zeta)$, see Lemma 5.1, and since $\tilde{r}_n \to 0$ as $n \to \infty$, there is $N_m \in \mathbb{N}$ such that $v_n(x) = 0$ for all $n \ge N_m$ and for quasi-all $x \in A(\zeta)_m$. Let



(a) Exemplary presentation of I_n and $\tilde{D}_n$



(b) Exemplary presentation of D_n

Fig. 2: Construction of D_n using connected components of $I_n^{\complement}$ and $\tilde{D}_n^{\complement}$

$\xi_m \in H^{-1}(\Omega)_+$ with f-supp$(\tilde{\xi}_m) = A(\zeta)_m$, see Lemma 6.5. Since $v_n = 0$ q.e. on f-supp$(\tilde{\xi}_m)$, we conclude $\langle \xi_m, |v_n| \rangle = 0$ for all $n \geq N_m$, see Lemma 6.1. This implies $\langle \xi_m, |v| \rangle = 0$ by the weak convergence $|v_n| \rightharpoonup |v|$. We thus have $v = 0$ q.e. on $A(\zeta)_m$, see Lemma 6.1. Repeating this argument for all $m \in \mathbb{N}$, we conclude that $v = 0$ q.e. on $\operatorname{int}(A(\zeta))$.

Since (a representative of) v is finely continuous quasi-everywhere, see [1, Thm. 6.4.5], $v = 0$ q.e. on f-cl$(\operatorname{int}(A(\zeta)))$ follows. Thus, $v = 0$ q.e. on $A_{\mathrm{s}}(\zeta)$, see Corollary 6.9, and we obtain $v \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$. ∎

The counterpart for the approximations $\tilde{D}_n$ as defined in (7.1) will be the subset approximations

$$D_n := \Big(\bigcup \{ C \mid C \text{ connected component of } I_n^{\complement} \text{ with } C \cap \tilde{D}_n^{\complement} \neq \emptyset \} \Big)^{\complement}. \tag{7.2}$$

of $\Omega \setminus A_{\mathrm{s}}(\zeta)$. Let us again verify the conditions from Corollary 4.4.

Lemma 7.3. *Suppose the conditions in Assumption 7.1 are fulfilled. Furthermore, assume that* $\operatorname{dist}(A_{\mathrm{w}}(\zeta), A_{\mathrm{s}}(\zeta)) > 0$ *and that we find a positive number* $\kappa > 0$ *such that* $B_\kappa(x) \subseteq A_{\mathrm{s}}(\zeta)$ *holds for at least one* x *in every connected component of* $A_{\mathrm{s}}(\zeta)$*. Let* D_n *be defined as in (7.2). Then it holds*

$$D_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta)$$

for $n \in \mathbb{N}$ *large enough and*

$$H_0^1(D_n) \to H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$$

in the sense of Mosco.

Proof. Let $\omega_0 \in A_{\mathrm{s}}(\zeta)$. First of all, we have $\omega_0 \in I_n^{\complement}$ since $I_n \subseteq I(\zeta)$, see Lemma 5.1. We show that the connected component C of $I_n^{\complement}$ containing ω_0 fulfills $C \cap \tilde{D}_n^{\complement} \neq \emptyset$.

Recall that by Corollary 6.9 it holds $A_{\mathrm{s}}(\zeta) = $ f-cl$(\operatorname{int}(A(\zeta)))$. Since the connected component of $A_{\mathrm{s}}(\zeta)$ including ω_0 and thus the component C contains a ball of radius κ, the center of this ball is contained in $\tilde{D}_n^{\complement}$ if $\tilde{r}_n < \kappa$, i.e., if n is large enough. This shows $\omega_0 \in D_n^{\complement}$ and we conclude $D_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta)$ for large enough $n \in \mathbb{N}$.

The family of sets $\left(\operatorname{int}\left(\bigcap_{k \geq n} D_k\right)\right)_{n \in \mathbb{N}}$ is increasing. We want to argue, that it is also a covering of $\Omega \setminus A_{\mathrm{s}}(\zeta)$. Using that the sets $\bigcap_{k \geq n} I_k$, $n \in \mathbb{N}$, are open, see Lemma 5.3, the inclusion $\bigcap_{k\geq n} D_k \supseteq \bigcap_{k\geq n} I_k$ implies $\operatorname{int}\left(\bigcap_{k\geq n} D_k\right) \supseteq \bigcap_{k\geq n} I_k$. From Lemma 5.1 we know that $\left(\bigcap_{k\geq n} I_k\right)_{n\in\mathbb{N}}$ covers $I(\zeta)$. Thus, it is clear that $\left(\operatorname{int}\left(\bigcap_{k\geq n} D_k\right)\right)_{n\in\mathbb{N}}$ covers $I(\zeta)$.

Assume $P \subseteq A_{\mathrm{w}}(\zeta)$ is of positive capacity and contained in one connected component of $A_{\mathrm{w}}(\zeta)$. Let $\mathcal{V}_{\mathrm{s}}$ and $\mathcal{V}_{\mathrm{w}}$ be open neighborhoods of $A_{\mathrm{s}}(\zeta)$ and $A_{\mathrm{w}}(\zeta)$, respectively, and assume $\mathcal{V}_{\mathrm{s}} \cap \mathcal{V}_{\mathrm{w}} = \emptyset$. This is possible, since $\operatorname{dist}(A_{\mathrm{w}}(\zeta), A_{\mathrm{s}}(\zeta)) > 0$ by assumption. Note that $\mathcal{V}_{\mathrm{s}}$ and $\mathcal{V}_{\mathrm{w}}$ have disjoint connected components.

Since y and ψ are continuous and since $\psi < 0$ on $\partial\Omega$, we have $y - \psi \geq c > 0$ outside $\mathcal{V} := \mathcal{V}_{\mathrm{s}} \cup \mathcal{V}_{\mathrm{w}}$ for some $c > 0$. This means, if n is big enough, it holds $I_n^{\complement} \subseteq \mathcal{V}$. In particular, any conncected component of $I_n^{\complement}$ is either contained in $\mathcal{V}_{\mathrm{s}}$ or in $\mathcal{V}_{\mathrm{w}}$.

Since $\tilde{D}_n^{\complement} \subseteq A_{\mathrm{s}}(\zeta)$ if n is large enough, this shows that $\mathcal{V}_{\mathrm{w}}$ contains only connected components C of $I_n^{\complement}$ with $C \cap \tilde{D}_n^{\complement} = \emptyset$. We conclude $\mathcal{V}_{\mathrm{w}} \subseteq \bigcap_{k\geq n} D_k$ and from this

$$P \subseteq \operatorname{int}\left(\bigcap_{k\geq n} D_k\right).$$

Thus, $\left(\operatorname{int}\left(\bigcap_{k\geq n} D_k\right)\right)_{n\in\mathbb{N}}$ is a quasi-covering of $\Omega \setminus A_{\mathrm{s}}(\zeta)$.

Let $v \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$. By [30, Thm. 2.10, Lem. 2.4], there exists a sequence $(v_n)_{n\in\mathbb{N}}$ with $v_n \to v$ in $H_0^1(\Omega)$ as $n \to \infty$ and such that $v_n \in H_0^1\left(\operatorname{int}\left(\bigcap_{k\geq n} D_k\right)\right)$ for each $n \in \mathbb{N}$. In particular, $v_n \in H_0^1(D_n)$ since $\operatorname{int}\left(\bigcap_{k\geq n} D_k\right) \subseteq D_n$.

It remains to show the weak limit property for the Mosco convergence. Suppose there is a sequence $(w_n)_{n\in\mathbb{N}}$ with $w_n \in H_0^1(D_n)$ and $w_{n_k} \rightharpoonup w$ in $H_0^1(\Omega)$ for a subsequence $(w_{n_k})_{k\in\mathbb{N}}$ of $(w_n)_{n\in\mathbb{N}}$ and some $w \in H_0^1(\Omega)$. Since

$$D_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta) \subseteq \tilde{D}_n$$

holds for all $n \in \mathbb{N}$ large enough, cf. Lemma 7.2, we have $w_n \in H_0^1(\tilde{D}_n)$ if $n \in \mathbb{N}$ is large enough. By the Mosco convergence of $H_0^1(\tilde{D}_n)$ to $H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$, see Lemma 7.2, we conclude $w \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$. ∎

Remark 7.4. The assumption in Lemma 7.3 that there is $\kappa > 0$ such that $B_\kappa(x) \subseteq A_{\mathrm{s}}(\zeta)$ holds for some x in any connected component of $A_{\mathrm{s}}(\zeta)$ is fulfilled if the strictly active set has only finitely many connected components, since $A_{\mathrm{s}}(\zeta) = \text{f-cl}(\operatorname{int}(A(\zeta)))$, see Corollary 6.9.

7.1. Alternative discrete inner approximation of the complement of the strictly active set. We suggest an alternative choice of the subset of approximations for $\Omega \setminus A_{\mathrm{s}}(\zeta)$. Here, we exploit the Lipschitz domain structure of the strictly active set, which we will assume in Lemma 7.8. For this approach it is not necessary that the strictly and weakly active set have a positive distance.

Let us state the following definitions in the context of cones and Lipschitz domains. The first two points in the following definition are based on [46, Def. 2.3].

Definition 7.5 (Cone property).

1. *For $x \in \mathbb{R}^d$, $\rho > 0$ and an open nonempty subset Σ of $S_\rho(x) := \{y \mid \|y - x\| = \rho\}$ we call the set*

$$C(x, \rho, \Sigma) = B_\rho(x) \cap \{\beta(y - x) \mid y \in \Sigma, \beta > 0\}$$

a cone with vertex in x.

2. *An open and set E of $\mathbb{R}^d$ has the cone property, if for each $x \in \overline{E}$ there is a cone C_x with vertex at x which is congruent to a fixed cone C_0 such that the subset C_x is contained in E. Here, the statement that C_x is congruent to C_0 means that C_x is a possibly translated and rotated copy of C_0.*
3. *Let $E \subseteq \mathbb{R}^d$ be a Lipschitz domain. Denote by $C_0 := C_0(x, \rho, \Sigma)$ a cone such that E has the cone property with cone C_0. Let $z \in \Sigma$ and let $B_r(z)$ be a ball such that $B_r(z) \cap S_\rho(x) \subseteq \Sigma$. We say that E has at least the interior angle $\alpha > 0$, if the convex cone induced by $B_r(z) \cap S_\rho(x)$, i.e., the cone*

$$\{\beta(y - x) \mid y \in B_r(z) \cap S_\rho(x), \beta > 0\}$$

has the angle α.

The next lemma can be found in [46, Thm. 2.1].

LEMMA 7.6. *Let E be a bounded Lipschitz domain. Then E has the cone property.*

The following statement shows a sufficient condition for a point to be a point where $\partial A(\zeta)$ is locally Lipschitz. It is based on [11].

LEMMA 7.7. *Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with sufficiently regular boundary and assume $\psi \in C^2(\Omega)$. Suppose that $\zeta \in L^2(\Omega)$ is bounded and locally Hölder continuous. If ω_0 is a point of positive Lebesgue density for $A(\zeta)$, i.e.,*

$$\lim_{r \to 0} \frac{\lambda^d(B_r(\omega_0) \cap A(\zeta))}{\lambda^d(B_r(\omega_0))} > 0,$$

then in a neighborhood of w_0, $\partial A(\zeta)$ can be represented as the graph of a Lipschitz function.

Proof. By [26, Thm. 4.3], the Poisson equation

$$-\Delta v = \zeta, \quad v = 0 \text{ on } \partial\Omega$$

has a unique solution $v \in C^2(\Omega) \cap C(\overline{\Omega})$. The obstacle problem with right hand side ζ as in (COP) is then equivalent to the problem

$$\text{Find } w \in K_{\psi - v}: \quad (\nabla w, \nabla(z - w)) \geq 0 \quad \forall\, z \in K_{\psi - v}$$

and it holds $w = y - v$. By Lemma 2.1, the solution w is in $C^{1,\beta}(\overline{\Omega})$ for any $\beta \in (0, 1)$. In particular, w is Lipschitz continuous. This shows that w is the solution to the problem considered in [11]. Noting that $\{w = \psi - v\} = \{y = \psi\}$, we can apply [11, Thm. 2] to deduce the statement. ∎

For $\gamma_n > 0$ specified below, we define

$$E_n := \{\omega \in \Omega \mid \operatorname{dist}(\omega, \tilde{D}_n^{\complement}) > \gamma_n\}. \tag{7.3}$$

In the following lemma, we verify that this choice of discrete approximation fulfills the conditions in Corollary 4.4.

LEMMA 7.8. *Suppose the conditions in Assumption 7.1 are fulfilled. Assume that $A_{\mathrm{s}}(\zeta)$ is a closed set with Lipschitz boundary that has at least the interior angle $\alpha > 0$ and let $(\gamma_n)_{n\in\mathbb{N}}$ be a sequence with $\gamma_n \to 0$ as $n \to \infty$ and*

$$\gamma_n \geq \frac{\tilde{r}_n}{\sin(\alpha/2)}.$$

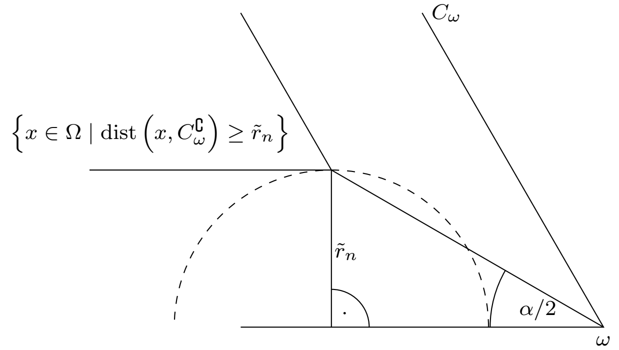


Fig. 3: Cone C_ω and the set of points in C_ω having a distance of at least $\tilde{r}_n$ to $\Omega \setminus C_\omega$

Let E_n be defined as in (7.3). Then it holds

$$E_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta)$$

for $n \in \mathbb{N}$ large enough and

$$H_0^1(E_n) \to H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$$

in the sense of Mosco.

Proof. Since $\operatorname{int}(A_{\mathrm{s}}(\zeta))$ has the cone property, see Lemma 7.6, we find a fixed cone C_0 with radius $\alpha > 0$, such that for each $x \in A_{\mathrm{s}}(\zeta)$ the set C_x is contained in $A_s(\zeta)$.

Let $n \in \mathbb{N}$ be fixed and let $\omega \in A_{\mathrm{s}}(\zeta)$ be arbitrary.

For $x \in A_{\mathrm{s}}(\zeta)$ we have

$$C_x \subseteq A_{\mathrm{s}}(\zeta) \subseteq I_n^{\complement}, \text{ i.e.,} \quad I_n \subseteq C_x^{\complement}.$$

This shows

$$\{x \in \Omega \mid \operatorname{dist}(x, I_n) \geq \tilde{r}_n\} \supseteq \{x \in \Omega \mid \operatorname{dist}(x, C_\omega^{\complement}) \geq \tilde{r}_n\}.$$

Using this and the trigonometry indicated in Figure 3, we estimate

$$\begin{aligned}\operatorname{dist}(\omega, \tilde{D}_n^{\complement}) &= \operatorname{dist}(\omega, \{x \in \Omega \mid \operatorname{dist}(x, I_n) \geq \tilde{r}_n\}) \\ &\leq \operatorname{dist}(\omega, \{x \in \Omega \mid \operatorname{dist}(x, C_\omega^{\complement}) \geq \tilde{r}_n\}) \leq \frac{\tilde{r}_n}{\sin(\alpha/2)} \leq \gamma_n.\end{aligned}$$

This shows $\omega \in E_n^{\complement}$. Since $\omega \in A_{\mathrm{s}}(\zeta)$ was arbitrary, we have shown $E_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta)$.

We want to show that the sets $\left(\operatorname{int}\left(\bigcap_{k \geq n} E_k\right)\right)_{n \in \mathbb{N}}$ are a quasi-covering of $\Omega \setminus A_{\mathrm{s}}(\zeta)$. Let $\omega \in \Omega \setminus A_{\mathrm{s}}(\zeta)$. Since $A_{\mathrm{s}}(\zeta)$ is closed, ω has a fixed distance > 0 to the set $A_{\mathrm{s}}(\zeta)$. If $n \in \mathbb{N}$ is sufficiently large, we find $c(n) > 0$ such that

$$B_{c(n)}(\omega) \subseteq \{x \in \Omega \mid \operatorname{dist}(x, A_{\mathrm{s}}(\zeta)) > \gamma_n\}$$

and thus, by $\tilde{D}_n^{\complement} \subseteq A_{\mathrm{s}}(\zeta)$, see Lemma 7.2,

$$B_{c(n)}(\omega) \subseteq \{x \in \Omega \mid \operatorname{dist}(x, \tilde{D}_n^{\complement}) > \gamma_n\} = E_n.$$

In particular, $\omega \in \operatorname{int}\left(\bigcap_{k\geq n} E_k\right)$ for some $n \in \mathbb{N}$ large enough. Thus, the family $\left(\operatorname{int}\left(\bigcap_{k\geq n} E_k\right)\right)_{n\in\mathbb{N}}$ is an increasing covering of $\Omega \setminus A_{\mathrm{s}}(\zeta)$.

To prove Mosco convergence, we proceed analogously to the proof of Lemma 7.3. Let $v \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$. By [30, Thm. 2.10, Lem. 2.4], there exists a sequence $(v_n)_{n\in\mathbb{N}}$ with $v_n \to v$ in $H_0^1(\Omega)$ as $n \to \infty$ and such that $v_n \in H_0^1\left(\operatorname{int}\left(\bigcap_{k\geq n} E_k\right)\right)$ for each $n \in \mathbb{N}$. In particular, $v_n \in H_0^1(E_n)$ since $\operatorname{int}\left(\bigcap_{k\geq n} E_k\right) \subseteq E_n$.

Now, we verify the second condition for Mosco convergence. Suppose that there is a sequence $(w_n)_{n\in\mathbb{N}}$ with $w_n \in H_0^1(E_n)$ and $w_{n_k} \rightharpoonup w$ in $H_0^1(\Omega)$ for a subsequence $(w_{n_k})_{k\in\mathbb{N}}$ of $(w_n)_{n\in\mathbb{N}}$. Since

$$E_n \subseteq \Omega \setminus A_{\mathrm{s}}(\zeta) \subseteq \tilde{D}_n$$

holds for all $n \in \mathbb{N}$ large enough, cf. Lemma 7.2, we have $w_n \in H_0^1(\tilde{D}_n)$ if $n \in \mathbb{N}$ is large enough. By the Mosco convergence of $H_0^1(\tilde{D}_n)$ to $H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$, see Lemma 7.2, we conclude $w \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$. ∎

Remark 7.9. In practice, the interior angle in $A_{\mathrm{s}}(\zeta)$ is unknown and this leads to a worse approximation of $\Omega \setminus A_{\mathrm{s}}(\zeta)$ and a slower Mosco convergence of $H_0^1(E_n) \to H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta))$ compared to the choice D_n in (7.2). Instead of setting $\gamma_n = \frac{\tilde{r}_n}{\sin(\alpha/2)}$ in (7.3), one then has to use, e.g.,

$$\gamma_n := \tilde{r}_n^{1-\kappa} \geq \frac{\tilde{r}_n}{\sin(\alpha/2)}$$

for some small $\kappa > 0$. The last inequality holds if n is large enough.

8. Main result. Now, we are in the position to state the main theorem of this paper.

Theorem 8.1. *Suppose the conditions of Theorem 2.3 on U and $f\colon U \to H^{-1}(\Omega)$ are satisfied. Assume the conditions in Assumption 7.1 are satisfied and let $\tilde{D}_n$ be defined as in (7.1). Denote by q the solution of*

$$\text{Find } q \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta)): \quad \langle -\Delta q, v\rangle = \langle J_y(y,u), v\rangle \quad \forall\, v \in H_0^1(\Omega \setminus A_{\mathrm{s}}(\zeta)),$$

i.e., $f'(u)^* q + J_u(y,u)$ is a Clarke generalized derivative for $\hat{J}$. In addition, consider one of the following cases.

1. *Suppose $\operatorname{dist}(A_{\mathrm{w}}(\zeta), A_{\mathrm{s}}(\zeta)) > 0$ and let $\kappa > 0$ be a positive number such that $B_\kappa(x) \subseteq A_{\mathrm{s}}(\zeta)$ holds for some x in every connected component of $A_{\mathrm{s}}(\zeta)$. Let D_n be defined as in (7.2) and denote by $(q_n)_{n\in\mathbb{N}}$ the solutions of*

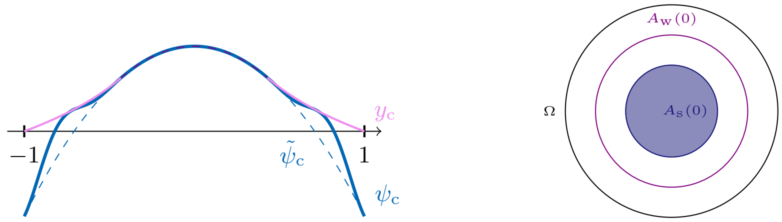
$$\text{(8.1)} \quad \text{Find } q_n \in H_0^1(D_n): \ \langle -\Delta q_n, v_n\rangle = \langle J_y(y_n,u), v_n\rangle \quad \forall\, v_n \in H_0^1(D_n).$$

2. *Suppose $A_{\mathrm{s}}(\zeta)$ is a closed set with Lipschitz boundary and let E_n be defined as in (7.3) with γ_n as in Lemma 7.8. Denote by $(q_n)_{n\in\mathbb{N}}$ the solutions of*

$$\text{Find } q_n \in H_0^1(E_n): \quad \langle -\Delta q_n, v_n\rangle = \langle J_y(y_n,u), v_n\rangle \quad \forall\, v_n \in H_0^1(E_n).$$

In both cases, $q_n \to q$ holds as $n \to \infty$ as well as

$$\text{(8.2)} \quad \begin{aligned} &\|q - q_n\|_{H_0^1(\Omega)} \\ &\leq \|-\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n)} + \|J_y(y_n,u) - J_y(y,u)\|_{H^{-1}(\Omega)} \overset{n\to\infty}{\to} 0. \end{aligned}$$



(a) Cross section of radial symmetric obstacle problem

(b) Corresponding active sets in Ω

Fig. 4: Visualisation of the obstacle problem considered in section 9

9. Numerical examples. In this section we present numerical results demonstrating our approximations of $\Omega \setminus A_s(\zeta)$ and the corresponding inexact generalized derivatives as well as the investigated error estimates.

We set $\Omega := B_1(0) := \{x \in \mathbb{R}^2 \mid x_1^2 + x_2^2 < 1\}$ and consider the radial symmetric obstacle

$$\psi(x) := \vartheta(x)\, y(x) + (1 - \vartheta(x))\, \tilde{\psi}(x) \quad (x \in B_1(0)).$$

for

$$\vartheta(x) := \begin{cases} 0 & \text{for } 0 \le |x| \le r, \\ \frac{1}{2}\left(1 - \cos\left(\frac{|x|-r}{\frac{1+r}{2}-r}\pi\right)\right) & \text{for } r < |x| \le 1 \end{cases} \quad \text{and} \quad \tilde{\psi}(x) := -x_1^2 - x_2^2 + \frac{1}{2}.$$

Note that ψ is a perturbation of the obstacle $\tilde{\psi}$ such that the violation of the strict complementarity condition can be achieved when considering the radial symmetric solution of the obstacle problem (COP) with $\zeta = 0$. It can be verified that for $r \in (0, 1)$ solving the equation $\ln(r) = -\frac{1}{4r^2} + \frac{1}{2}$ the function $y \in H_0^1(\Omega)$ with

$$y(x) = \begin{cases} \tilde{\psi}(x) & \text{for } |x| \le r, \\ -2r^2 \ln(|x|) & \text{for } r < |x| \le 1 \end{cases} \tag{9.1}$$

is the solution of (COP) in the given setting.

Denoting by $S_{\tilde{r}}$ the sphere with radius $\tilde{r}$ around the origin, the strictly active set is $A_s(0) = B_r(0)$ and the weakly active set is $A_w(0) = S_{\frac{1+r}{2}}(0)$, since

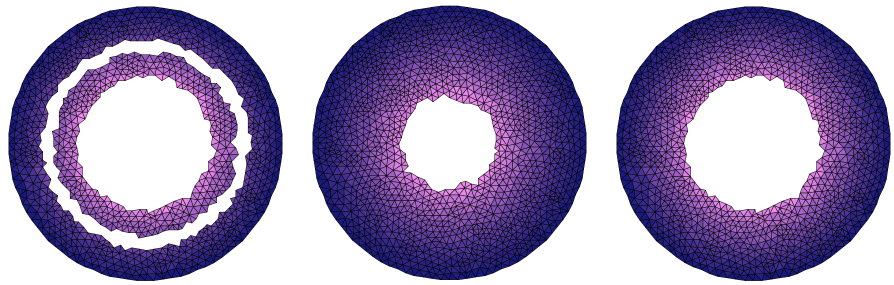
$$\{x \in \Omega \mid \vartheta(x) = 1\} = \left\{x \in \Omega \mid |x| = \frac{1+r}{2}\right\}.$$

Figure 4 shows the cross section of the obstacle and the solution as well as the respective two-dimensional weakly and strictly active set.

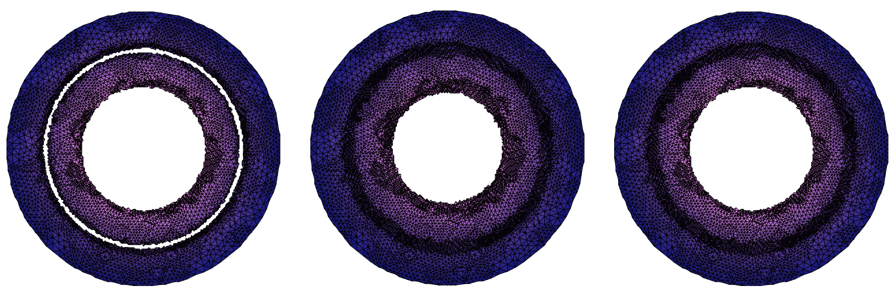
In our examples, we consider the objective function $J\colon H_0^1(\Omega) \times U \to \mathbb{R}$ given by $J(y, u) := \frac{1}{2}\left\|y - \frac{1}{4}\right\|_{L^2(\Omega)}^2$. For our demonstration, we do not need to specify U and f, let us just assume the conditions of Theorem 2.3 are satisfied.

Let us check that the conditions of Assumption 7.1 are satisfied. It is straightforward to verify the regularity assumptions on ζ, y and ψ. We observe $\lambda^2(\partial A(0)) = 0$ and $-\Delta\psi \ge 4$ on $A(0)$ as well as $-\Delta\psi \ge 3.8$ a.e. in a neighborhood of the active set. Thus, the nondegeneracy condition (ND) is satisfied.

Let us note that $\operatorname{dist}(A_w(0), A_s(0)) > 0$ and also $B_r(0) \subseteq A_s(0)$. Thus, the results from Theorem 8.1 are applicable.

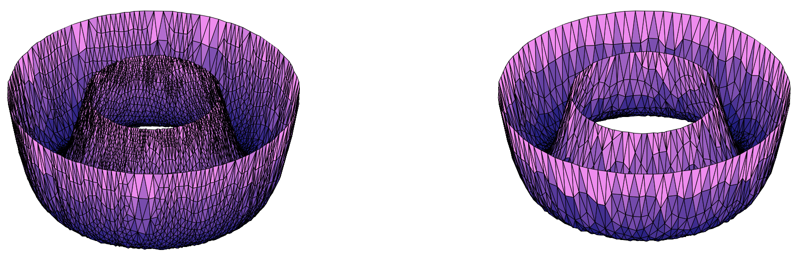


(a) I_0 (b) $\tilde{D}_0$ (c) D_0



(d) I_2 (e) $\tilde{D}_2$ (f) D_2

Fig. 5: Construction of the sets I_n, $\tilde{D}_n$ and D_n in Example 9.1 for $n = 0, 2$



(a) Numerical subgradient in iteration $n = 3$ for Example 9.1

(b) Numerical subgradient in iteration $n = 2$ for Example 9.2

Fig. 6: Numerical subgradients for Examples 9.1 and 9.2

Example 9.1. In a first experiment, we use the sets I_n as in (5.1), the sets $\tilde{D}_n$ as defined in (7.1) and the sets D_n as in (7.2). These approximations are based on the $L^\infty(\Omega)$-error estimates from [38]. and they are plotted in Figure 5. Knowing the solution y, cf. (9.1), we can even tighten the error estimate from [38] leading to more accurate approximations of the complement of the strictly active set and speeding up the convergence process. In practice, we use a possibly larger set $\tilde{D}_n$ for the error estimate and a possibly smaller set D_n as a domain for the computation of the subgradient for the assignment of the triangles in the mesh to either D_n, $\tilde{D}_n$ or their complements in Ω.

The generalized derivative q_3 is shown in Figure 6a. Moreover, Table 1 shows the contributions $\| - \Delta q_n - J_y(y_n, u)\|_{H^{-1}(\tilde{D}_n)}$ to the upper bounds for the error

Table 1: Terms $\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n)}$, $\tilde{r}_n$ and rate $\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n)}/\sqrt{\tilde{r}_n}$ in iteration n for Examples 9.1 and 9.2

	Example 9.1			Example 9.2		
Iteration	Error term for $\|q-q_n\|_{H_0^1(\Omega)}$	$\tilde{r}_n$	Ratio	Error term for $\|q-q_n\|_{H_0^1(\Omega)}$	$\tilde{r}_n^J$	Ratio
0	0.0152	0.0649	0.0597	0.0260	0.2225	0.0551
1	0.0118	0.0459	0.0551	0.0164	0.1394	0.0439
2	0.0090	0.0271	0.0547	0.0150	0.1292	0.0417
3	0.0074	0.0174	0.0561	0.0143	0.1183	0.0416
4	0.0062	0.0130	0.0544	0.0126	0.0955	0.0408
5	0.0049	0.0079	0.0551	0.0112	0.0736	0.0413
6	0.0041	0.0052	0.0569	0.0105	0.0650	0.0412
7	0.0032	0.0034	0.0549	0.0096	0.0539	0.0414
8	0.0027	0.0024	0.0551	0.0085	0.0414	0.0418

$\|q-q_n\|_{H_0^1(\Omega)}$, compare (8.2), as well as the considered radii $\tilde{r}_n$ for the construction of $\tilde{D}_n$ from I_n, see (7.1), and the ratio

$$\frac{\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n)}}{\sqrt{\tilde{r}_n}}.$$

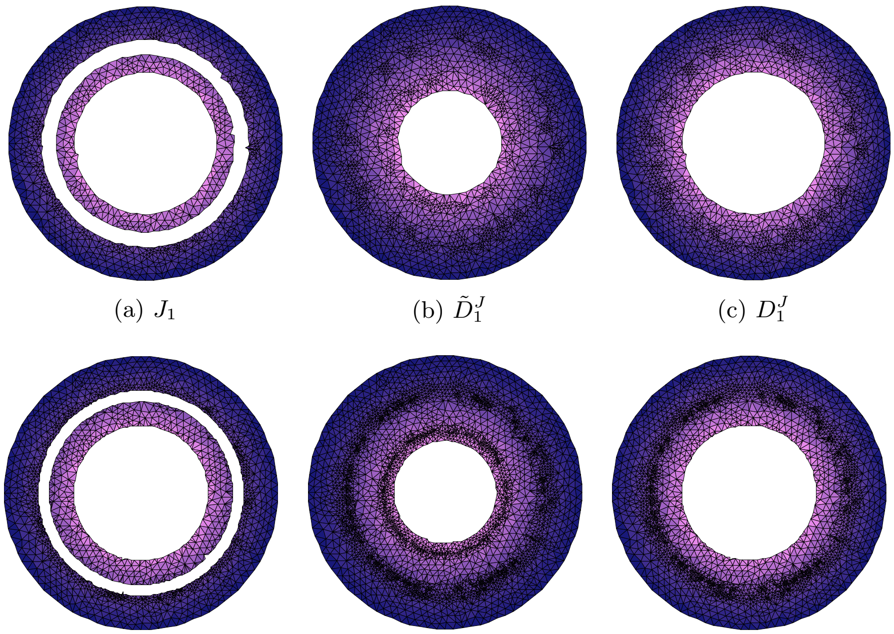
We observe that this ratio is approximately constant. Indeed, assuming sufficient regularity of the individual sets, one can theoretically derive an estimate of the form

$$\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n)} \le C\sqrt{\tilde{r}_n}$$

for some constant C.

Example 9.2. For a second example, we use the sets J_n mentioned in Remark 5.2. Since the boundaries of the sets J_n are level sets of piecewise affine functions, we can determine the boundary in each triangle accurately and the mesh is adjusted accordingly in each iteration. This results in a less serrated appearance of the boundary of the constructed sets $J_n, \tilde{D}_n^J$ and D_n^J compared to the sets based on I_n. This can be observed in Figure 7. Once again, we use the a posteriori $L^\infty(\Omega)$-error estimates from [38] for the construction of the sets J_n. The mesh is refined adaptively taking into account the error contribution for the $L^\infty(\Omega)$-error estimate ε_n and the quantity $\|(\psi-\psi_n)_+\|_{L^\infty(\{y_n\le\psi_n+\varepsilon_n+\|(\psi-\psi_n)_+\|_{L^\infty(\Omega)}\})}$ in each triangle separately. The resulting generalized derivative q_2 is shown in Figure 6b. For the first iterations, Table 1 shows the terms $\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n^J)}$ contributing to the upper bounds for the error $\|q-q_n\|_{H_0^1(\Omega)}$, see (8.2). Moreover, the used radii for the construction of $\tilde{D}_n^J$ from J_n, see (7.1), are recorded as well as the ratio $\frac{\| -\Delta q_n - J_y(y_n,u)\|_{H^{-1}(\tilde{D}_n^J)}}{\sqrt{\tilde{r}_n^J}}$.

Remark 9.3. In our numerical experiments, we have neglected the errors resulting from solving the Dirichlet problem (8.1) in the finite element spaces rather than in the function space setting.



(a) J_1 (b) $\tilde{D}_1^J$ (c) D_1^J

(d) J_3 (e) $\tilde{D}_3^J$ (f) D_3^J

Fig. 7: Construction of the sets J_n, $\tilde{D}_n^J$, D_n^J in Example 9.2 for $n = 1, 3$

Conclusion. We have developed an error estimate for inexact Clarke subgradients in optimal control problems with respect to the obstacle problem. Solving the obstacle problem on a discrete level using finite elements results in a defective description of the respective active and strictly active sets. To obtain a Clarke subgradient of the reduced objective function, a PDE has to be solved on a domain which depends on the (strictly) active set. Based on the discrete sets, we constructed a convergent sequence of sub- and supersets of the accurate complement of the strictly active set. This construction was based on error estimates for the distances of the (inexact) free boundaries established in [38]. The smaller sets were used to provide inexact Clarke subgradients and the larger sets were then used to control the error. We have presented numerical examples to test our error estimates.

The correct and convergent approximation of the accurate complement of the strictly active set relies on the nondegeneracy condition, which implies the error estimates as in [38] as well as topological structures of the (strictly) active sets. How the nondegeneracy condition can be avoided or relaxed remains subject of further research.

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