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Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

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Solving Non-Smooth Semi-Linear Optimal Control Problems with Abs-Linearization

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Abstract

We investigate optimization problems with a non-smooth partial differential equation as constraint, where non-smoothness is assumed to be caused by the functions abs(), min() and max(). For the efficient as well as robust solution of such problems, we propose a new optimization method based on abs-linearisation, i.e., a special handling of the non-smoothness without regularization. The key idea of this approach is the determination of stationary points by an appropriate decomposition of the original non-smooth problem into several smooth so-called branch problems. Each of these branch problems can be solved by classical means. The exploitation of corresponding optimality conditions for the smooth case identifies the next branch and thus yields a successive reduction of the objective value. This approach is able to solve the considered class of non-smooth optimization problems without any regularization of the non-smooth optimization problems without any regularization of the non-smooth optimization problems illustrate the proposed approach and its performance.

1 Introduction

Non-smooth optimization problems with a partial differential equation (PDE) as constraint that involves the non-differentiable functions abs(), min() and max() arise in many modern applications. For example, a corresponding semi-linear elliptic partial differential equation describes the deflection of a stretched thin membrane partially covered by water, see [8]. Furthermore, a similar non-smooth partial differential equation arises in free boundary problems for a confined plasma, see, e.g., [8, 10]. Even nowadays, the optimization of such problems is challenging. Therefore, often the non-smoothness is regularized to apply an algorithm suitable for smooth optimization or the semi-smooth Newton method is used. Here, we propose an alternative algorithm that is not based on the semi-smooth Newton method and that explicitly exploits the non-smoothness.

In the finite dimensional setting the unconstrained minimization of piecewise smooth functions by successive abs-linearization without any regularization for the non-smoothness was studied by Griewank, Walther and co-authors in [2, 3, 4] and related work. There, it is always assumed that the non-smoothness of the considered optimization problem stems from evaluations of the absolute value function only. Using well-known reformulations, this covers the maximum and the minimum functions as well as complementarity problems. The purpose of this paper is to extend the algorithmic idea of the approach in finite dimensions to the infinite dimensional case, i.e., to PDE-constrained optimization problems. However, it is not possible to transfer the results obtained to the PDE-constrained case directly. Here, one issue is that due to the lack of a chain rule in the non-smooth case, one cannot directly handle the reduced unconstrained formulation. Therefore, we propose here a penalty-based approach to treat the PDE constraint explicitly. Nevertheless, we follow the idea for the finite dimensional case in that the key idea of the optimization method under consideration is the location of stationary points by an appropriate decomposition of the original problem into several smooth so-called branch problems. Each of these branch problems can be

solved by classical methods for smooth PDE-constrained optimization. Then, the exploitation of standard optimality conditions for the smooth case determines the next branch problem and ensures the reduction of the target function value. In deriving necessary optimality conditions, the difficulty lies in the fact that while the solution domain of the PDE is compact, the number and location of the solutions is unknown. For this reason, a direct approach, i.e., first-discretize-then-optimize, is presented for the numerical solution of the optimization problems.

The paper is organized as follows. In Sec. 2, we introduce the considered problem class, discuss its properties and propose a reformulation of the first order necessary optimality conditions. The resulting smooth branch problems will presented in Sec. 3. This includes a solution approach involving a penalty term and an analysis of the corresponding optimality conditions. Sec. 4 summarizes the resulting optimization algorithm. Furthermore, the chosen discretization approach as well as the corresponding solution of the subproblems is discussed. Numerical results for a collection of test problems are presented and analysed in Sec. 5. Finally, a conclusion and an outlook are given in Sec. 6.

2 The Problem Class, its Properties and a Reformulation

In this paper we focus on real valued functions defined on a Lipschitz domain $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$. As a model problem we consider the following class of PDE constrained optimization problems

$$\min_{\substack{(y,u)\in H_0^1(\Omega)\times L^2(\Omega)}} \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2$$
s.t. $-\Delta y + \ell(y) - u = 0$ in Ω
(1)

with a convex and twice continuously Fréchet differentiable objective functional and a semi-linear elliptic PDE constraint.

The special and at the same time challenging feature of Eq. (1) is the non-smoothness in the state equation which is given by the non-smooth operator $\ell : H_0^1(\Omega) \to L^2(\Omega)$. For the exact definition of the operator ℓ we refer to Assumption 2.1 below.

It should be noted that the algorithm proposed in this paper is not limited to this class of semilinear PDE or this kind of objective functionals. Instead, the arguments can easily be adapted to more general cases with, for example, a general linear elliptic differential operator of second order instead of the Laplacian operator. Therefore, Sec. 5 presents also numerical results for other differential operators. However, to illustrate the idea of the algorithm we restrict ourselves here to this class of semi-linear elliptic PDEs.

Throughout the paper, we assume that the model problem (1) has the following properties:

Assumptions 2.1.

- (a) The operator $\ell : H_0^1(\Omega) \to L^2(\Omega)$ is bounded and measurable in $x \in \Omega$ for every fixed y, strictly monotone in y for almost every $x \in \Omega$ and locally Lipschitz-continuous. This means in particular, that $\ell(0)$ is bounded and measurable.
- (b) It is assumed that ℓ can be expressed as composition of the absolute value function and other Fréchet-differentiable functions.
- (c) The control function $u \in L^2(\Omega)$ is sufficiently smooth.

In addition to these assumptions on the non-smooth PDE, it can easily be observed that the objective functional $\mathcal{J} : H_0^1(\Omega) \times L^2(\Omega) \to \mathbb{R}$ in Eq. (1) is weakly lower semi-continuous and twice continuously Fréchet-differentiable. One particular example of this class of model problems of non-smooth semi-linear elliptic optimal control problems, where $\ell(y) = \max(0, y)$, can be found in [1]. There the authors show, among other things, that the resulting non-smooth control-to-state operator is directionally differentiable. They also precisely characterize its Bouligand subdifferentials, derive first-order optimality conditions using the Bouligand subdifferentials and use the directional derivative of the control-to-state mapping to establish strong stationarity conditions. Following the approach in [1] and applying standard arguments for monotone operators, it can be shown that for any given control $u \in L^2(\Omega)$ the PDE of the optimization problem (1) is well posed

for
$$i = 1, ..., s$$
 do
 $z_i = \psi_i(y, (\sigma_j z_j)_{j < i})$
 $\sigma_i = \operatorname{sign}(z_i)$
 $\hat{\ell}(y, \sigma z) = \psi_{s+1}(y, (\sigma_i z_i)_{1 \le i \le s})$ with $\sigma z = (\sigma_1 z_1, ..., \sigma_s z_s)$

Table 1: Structured Evaluation of $\ell(y)$

and has a unique solution y. Further analysis reveals that the optimal control problem admits a solution under the given assumptions.

For the optimization we have to take into account, that it is usually not possible to realize arbitrary large controls $u \in L^2(\Omega)$. Therefore control constraints in the form of

$$u \in U_{ad} \subseteq L^2(\Omega)$$

with the bounded and convex set of admissible controls

$$U_{ad} = \{ u \in L^2(\Omega) : u_a(x) \leq u(x) \leq u_b(x) \text{ a.e. } x \in \Omega \}$$

can be introduced into the model problem. However, this is not directly dealt with in this paper.

Reformulating the PDE Constraint

Now, we introduce an essential reformulation of the PDE constraint based on the idea described in [3, 5]. For this purpose, we define the Nemytskij-operator

$$\Phi: L^2(\Omega) \mapsto L^2(\Omega), \qquad [\Phi(y)](x) = \ell(v(x)) \quad \text{for almost all } x \in \Omega$$

Thus the Nemytskij-Operator is defined by the non-linear part of the PDE. Inspired by the finite dimensional approach of Griewank and Walther, we assume that the non-smooth operator ℓ can be described as a composition of elemental functions that are either continuously Fréchet differentiable or the absolute value operator. Subsequently, consecutive continuously Fréchet differentiable elemental functions can be conceptually combined to obtain a representation, where all evaluations of the absolute value function can be clearly identified and exploited, see Tab. 1. In the finite dimensional case, one has $z_i \in \mathbb{R}$ and therefore $\sigma_i \in \{-1, 0, 1\}$. For the infinite dimensional setting considered here, one has $z_i \in L^2(\Omega)$ and the functions σ_i are also Nemytskij operators defined by

$$\sigma_i : L^2(\Omega) \mapsto L^2(\Omega), \qquad [\sigma_i(v)](x) = \operatorname{sign}(z_i(x)) \cdot v(x) \quad \text{for almost all } x \in \Omega$$

as a function of z_i . This choice ensures that $\sigma_i(z_i) = \operatorname{abs}(z_i) \in L^2(\Omega)$ holds. From now on, we will use the notation $\hat{\ell}(y, \sigma z) = \ell(y)$ for $\sigma z = (\sigma_1 z_1, \dots, \sigma_s z_s)$ to refer explicitly to this particular representation of the non-smooth part $\ell(y)$ based on the auxiliary variables z_i and σ_i , $1 \le i \le s$. It follows from the representation in Tab. 1 that ℓ is locally Lipschitz continuous. Hence, ℓ and therefore also the equivalent $\hat{\ell}(y, \sigma z)$ are also continuous due to the assumed smoothness of ψ_i , $i = 1, \dots, s$, [7, Theo. 3.15] and [12, Cha. 1]. Furthermore, and this is important to note, the new function $\hat{\ell}(.,.)$ is smooth, i.e., Fréchet differentiable, in its two arguments due to the chosen formulation. This fact will be exploited later to define the smooth branch problems. Using the well-known reformulations

$$\min(v, u) = (v + u - abs(v - u))/2 \text{ and} \max(v, u) = (v + u + abs(v - u))/2,$$
(2)

a large class of nonsmooth functions is covered by this function model.

Example 2.2. Consider the non-smooth operator $\ell(y) = \max(5y, y|y|)$. Exploiting the identities (2), we can reformulate ℓ as a function in terms of the absolute value function and smooth elemental functions in the following way:

$$\ell(y) = \max(5y, \ y|y|) = \frac{1}{2} \Big(5y + y|y| + |5y - y|y|| \Big) .$$

The corresponding structured evaluation is shown in Tab. 2.

$$\begin{aligned} z_1 &= \psi_1(y) &= y \\ \sigma_1 &= \text{sign}(z_1) \\ z_2 &= \psi_2(y, \sigma_1 z_1) = 5y - y\sigma_1 z_1 \\ \sigma_2 &= \text{sign}(z_2) \\ \hat{\ell}(y, \sigma z) &= \psi_3(y, \sigma z) &= \frac{1}{2} \Big(5y + y\sigma_1 z_1 + \sigma_2 z_2 \Big) \end{aligned}$$

Table 2: Structured evaluation for $\ell(y) = \max(5y, |y|)$

Inserting the formulation $\hat{\ell}(y, \sigma z)$ with the auxiliary functions σ_i and z_i of ℓ into the original optimal control problem (1), one obtains for the functions $(y, z, u) \in H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$ the smooth optimization problem

$$\begin{array}{l} \min_{y,z,u} \quad \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2 \\ \text{s.t} \quad -\Delta y + \hat{\ell}(y, \sigma z) - u = 0 \\ \psi_i(y, (\sigma_j z_j)_{j < i}) - z_i &= 0 \\ \sigma_i z_i &\geqslant 0 \\ \sigma_i : \Omega \to \{-1, 1\} \end{array} \right\} \quad \forall \ i = 1, \dots, s \ . \tag{3}$$

Assume that u^* and the corresponding $y^* \equiv y^*(u^*)$ are solutions of the original optimization problem (1). Defining the auxiliary functions z_i^* and σ_i^* by

$$z_i^* = \psi_i(y, (\sigma_j^* z_j^*)_{j < i}), \qquad \sigma_i^* = \operatorname{sign}(z_i^*) \qquad \forall \quad i = 1, \dots, s$$

it follows that (y^*, z^*, u^*) is a solution of the optimization problem (3) if $\sigma_i = \sigma_i^*$ holds. Here, the additional equality and inequality constraints for the definitions of the additional functions z_i^* and $\sigma_i^*, 1 \leq i \leq s$, ensure that $\sigma_i^*(z_i^*) = \operatorname{abs}(z_i^*) \in L^2(\Omega)$ holds for $1 \leq i \leq s$. This observation motivates the optimization algorithm proposed in this paper, i.e., a solution of a sequences of smooth subproblems of the form Eq. (3) to solve the original non-smooth optimization problem (1). To determine the sequence of branch problems to be solved, we examine the necessary optimality conditions for Eq. (3). Using standard KKT theory for smooth PDE-constrained optimization problems [6], i.e., introducing corresponding Lagrange multipliers λ_{PDE} , $\lambda = (\lambda_1, \dots, \lambda_s)$, and $\mu = (\mu_1, \dots, \mu_s)$, one obtains for the Lagrangian

$$\mathcal{L}(y, z, u, \lambda_{PDE}, \lambda, \mu) = \mathcal{J}(y, u) + (\nabla \lambda_{PDE}, \nabla y)_{L^{2}(\Omega)} + (\lambda_{PDE}, \hat{\ell}(y, \sigma z) - u)_{L^{2}(\Omega)} + \sum_{i=1}^{s} (\lambda_{i}, \psi_{i}(y, (\sigma_{j} z_{j})_{j < i}) - z_{i})_{L^{2}(\Omega)} - \sum_{i=1}^{s} (\mu_{i}, \sigma_{i} z_{i})_{L^{2}(\Omega)}$$

at the optimal point the first order necessary conditions

$$0 = D_{y}\mathcal{L}(\tilde{y}) \qquad = \frac{\partial \mathcal{J}}{\partial y}\tilde{y} + \left(\nabla\lambda_{PDE},\nabla\tilde{y}\right)_{L^{2}(\Omega)} + \left(\lambda_{PDE},\frac{\partial \hat{\ell}}{\partial y}\tilde{y}\right)_{L^{2}(\Omega)} \\ + \sum_{i=1}^{s} \left(\lambda_{i},\frac{\partial \psi_{i}(y,(\sigma_{j}z_{j})_{j< i})}{\partial y}\tilde{y}\right)_{L^{2}(\Omega)} \qquad \forall \tilde{y}$$
(4)

$$0 = D_u \mathcal{L}(\tilde{u}) \qquad = \frac{\partial \mathcal{J}}{\partial u} \tilde{u} - \left(\lambda_{PDE}, \tilde{u}\right)_{L^2(\Omega)} \qquad \forall \tilde{u} \qquad (5)$$

$$0 = D_{\lambda_{PDE}} \mathcal{L}(\tilde{\lambda}_{PDE}) = \left(\nabla \tilde{\lambda}_{PDE}, \nabla y\right)_{L^{2}(\Omega)} + \left(\tilde{\lambda}_{PDE}, \hat{\ell} - u\right)_{L^{2}(\Omega)} \qquad \forall \tilde{\lambda}_{PDE}$$
(6)

$$0 = D_{\lambda_i} \mathcal{L}(\tilde{\lambda}_i) \qquad = \left(\tilde{\lambda}_i, \psi_i(y, (\sigma_j z_j)_{j < i}) - z_i\right)_{L^2(\Omega)} \qquad \forall \tilde{\lambda}_i, i = 1, \dots, s$$
(7)

$$0 = D_{z_k} \mathcal{L}(\tilde{z}_k) = \left(\lambda_{PDE}, \sigma_k \frac{\partial \ell(y, \sigma_z)}{\partial z_k} \tilde{z}_k\right)_{L^2(\Omega)} - \left(\lambda_k, \tilde{z}_k\right)_{L^2(\Omega)} \\ + \sum_{i=k+1}^s \left(\lambda_i, \sigma_k \frac{\partial \psi_i(y, (\sigma_j z_j)_{j < i})}{\partial z_k} \tilde{z}_k\right)_{L^2(\Omega)} \\ - (\mu_k, \sigma_k \tilde{z}_k)_{L^2(\Omega)} \qquad \forall \tilde{z}_k, k = 1, \dots, s \quad (8)$$

$$0 = (\mu_i, \sigma_i z_i)_{L^2(\Omega)} \qquad i = 1, \dots, s$$

$$0 \le \mu_i \qquad \qquad i = 1, \dots, s , \qquad (9)$$

where the arguments of \mathcal{L} are omitted for brevity. Note that in these equations one obtains extra factors $\bar{\sigma}_k$ due to the chain rule. Rearranging the terms in the integrals, the condition (8) yields for k = 1, ..., s

$$0 = \sigma_k \frac{\partial \hat{\ell}(y, \sigma z)}{\partial z_k} \lambda_{PDE} - \lambda_k + \sum_{i=k+1}^s \sigma_k \frac{\partial \psi_i(y, (\sigma_j z_j)_{j < i})}{\partial z_k} \lambda_i - \sigma_k \mu_k \; .$$

In this case the right hand sight represents the zero function in the corresponding Hilbert space. Applying σ_k and exploiting the non-negativity of μ_k according to Eq. (9), one obtains

$$0 \leq \mu_{k} |\sigma_{k}| = |\sigma_{k}| \frac{\partial \hat{\ell}(y,\sigma_{z})}{\partial z_{k}} \lambda_{PDE} - \sigma_{k} \lambda_{k} + \sum_{i=k+1}^{s} |\sigma_{k}| \frac{\partial \psi_{i}(y,(\sigma_{j}z_{j})_{j
$$\equiv r(\sigma_{k}, y, z, \lambda) \qquad \text{a.e. in } \Omega .$$
(10)$$

We will use this inequality later to define the sequence of subproblems to be solved.

3 Defining and Solving the Branch Problems

Now, everything is prepared to introduce the main idea of the new optimization algorithm. For fixed functions $\bar{\sigma}_i \in L^2(\Omega)$, $\bar{\sigma}_i : \Omega \to \{-1,1\}$ for $1 \leq i \leq s$, we define for $(y, z, u) \in H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$ the branch problem

$$\min_{y,z,u} \mathcal{J}(y,u) \tag{11}$$

s.t.
$$-\Delta y + \hat{\ell}(y, \bar{\sigma}z) - u = 0$$
 (12)

$$\psi_i(y, (\bar{\sigma}_j z_j)_{j < i}) - z_i = 0 \quad \forall \ i = 1, \dots, s$$
(13)

$$\bar{\sigma}_i z_i \ge 0 \quad \forall \ i = 1, \dots, s \ . \tag{14}$$

All functions occurring in this branch problem are smooth in the variables y, u and z because the function $\hat{\ell}(.,.)$ is smooth in its arguments as mentioned already in the last section. Therefore, standard smooth optimization methods can be used to solve the branch problem (11)–(14). Naturally, the question arises how to chose the functions $\bar{\sigma}_i$, $1 \le i \le s$, such that the solutions of the branch problems approach the solution of the original non-smooth problem (1). A corresponding strategy will be derived in this section.

The Lagrangian with Bi-quadratic Penalty

As mentioned already above, so far the solution of the non-smooth optimization problem using a reduced formulation is not possible due to the lack of the chain rule. For this reason, we propose here a penalty-based approach to solve the optimization problem (11)-(14), where the constraints (12) and (13) are handled explicitly. Approaches based on a reduced formulation will be subject of future research.

From a formal point of view, we treat the inequality constraints (14) with a penalty approach such that the target function (11) is modified to

$$\min_{y,z,u} \quad \mathcal{J}(y,u) + \mu \int_{\Omega} \sum_{i=1}^{s} \left(\max(-\bar{\sigma}_{i}z_{i},0) \right)^{4} d\Omega$$
(15)

with a penalty factor $\mu > 0$. Here, we chose the exponent 4 to ensure that the target function is twice continuously differentiable despite the max function that is used for the formulation of the

penalty function. This modified target function is then coupled with the equality constraints by means of Lagrange multipliers yielding the Lagrangian

$$\mathcal{L}^{p}(y, z, u, \lambda_{PDE}, \lambda_{1}, ..., \lambda_{s}) = \mathcal{J}(y, u) + (\nabla \lambda_{PDE}, \nabla y)_{L^{2}(\Omega)} + (\lambda_{PDE}, \hat{\ell}(y, \bar{\sigma}z) - u)_{L^{2}(\Omega)} + \sum_{i=1}^{s} (\lambda_{i}, \psi_{i}(y, (\bar{\sigma}_{j}z_{j})_{j⁽¹⁶⁾$$

A similar penalty approach was studied in [11], where the logarithm was used as barrier function. Here, we use the max-function since we have to evaluate the penalty function also at 0.

Example 3.1. We consider again $\ell(y) = \max(5y, y|y|) = \frac{1}{2}(5y + y|y| + |5y - y|y||)$. For the reformulated optimization problem given by

$$\begin{split} \min_{\substack{(y,z,u)\in H_0^1\times H_0^1\times L^2}} \ \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2 \\ \text{s.t.} \quad -\Delta y + \ \frac{1}{2} \Big(5y + y\bar{\sigma}_1 z_1 + \bar{\sigma}_2 z_2 \Big) - u = 0 \quad \text{in } \Omega \\ y - z_1 = 0 \\ 5y - y\bar{\sigma}_1 z_1 - z_2 = 0 \\ \bar{\sigma}_1 z_1 \geqslant 0 \\ \bar{\sigma}_2 z_2 \geqslant 0 \end{split}$$

one obtains the Lagrangian

$$\begin{split} \mathcal{L}^{p}(y, z, u, \lambda_{PDE}, \lambda_{1}, \lambda_{2}) \\ &= \mathcal{J}(y, u) + \left(\nabla \lambda_{PDE}, \nabla y\right)_{L^{2}(\Omega)} + \left(\lambda_{PDE}, \frac{1}{2} \left(5y + y\bar{\sigma}_{1}z_{1} + \bar{\sigma}_{2}z_{2}\right) - u\right)_{L^{2}(\Omega)} \\ &+ \left(\lambda_{1}, y - z_{1}\right)_{L^{2}(\Omega)} + \left(\lambda_{2}, 5y - y\bar{\sigma}_{1}z_{1} - z_{2}\right)_{L^{2}(\Omega)} + \mu \int_{\Omega} \sum_{i=1}^{2} \left(\max(-\bar{\sigma}_{i}z_{i}, 0)\right)^{4} d\Omega \,. \end{split}$$

Deriving Necessary Optimality Conditions

For a branch problem, the first-order necessary optimality conditions can now be derived from the Lagrangian (16) by using once more standard KKT theory for smooth PDE-constrained optimization problems. This yields as necessary first order conditions the equations

$$0 = D_{y}\mathcal{L}^{p}(\tilde{y}) \qquad = \frac{\partial \mathcal{J}}{\partial y}\tilde{y} + \left(\Delta\lambda_{PDE}, \Delta\tilde{y}\right)_{L^{2}(\Omega)} + \left(\lambda_{PDE}, \frac{\partial \ell}{\partial y}\tilde{y}\right)_{L^{2}(\Omega)} \\ + \sum_{i=1}^{s} \left(\lambda_{i}, \frac{\partial \psi_{i}(y,(\tilde{\sigma}_{j}z_{j})_{j< i})}{\partial y}\tilde{y}\right)_{L^{2}(\Omega)} \qquad \forall \tilde{y} \qquad (17)$$

$$0 = D_{u} \mathcal{L}^{p}(\tilde{u}) \qquad = \frac{\partial \mathcal{J}}{\partial u} \tilde{u} - \left(\lambda_{PDE}, \tilde{u}\right)_{L^{2}(\Omega)} \qquad \qquad \forall \tilde{u} \qquad (18)$$

$$0 = D_{\lambda_{PDE}} \mathcal{L}^{p}(\tilde{\lambda}_{PDE}) = \left(\Delta \tilde{\lambda}_{PDE}, \Delta y\right)_{L^{2}(\Omega)} + \left(\tilde{\lambda}_{PDE}, \hat{\ell}\right)_{L^{2}(\Omega)} - \left(\tilde{\lambda}_{PDE}, u\right)_{L^{2}(\Omega)} \quad \forall \tilde{\lambda}_{PDE}$$
(19)

$$0 = D_{\lambda_i} \mathcal{L}^p(\tilde{\lambda_i}) \qquad = \left(\tilde{\lambda}_i, \psi_i(y, (\bar{\sigma}_j z_j)_{j < i}) - z_i\right)_{L^2(\Omega)} \qquad \qquad \forall \tilde{\lambda}_i, 1 \le i \le s \quad (20)$$

$$0 = D_{z_{k}} \mathcal{L}^{p}(\tilde{z}_{k}) = \left(\lambda_{PDE}, \bar{\sigma}_{k} \frac{\partial \ell(y, \bar{\sigma}z)}{\partial z_{k}} \tilde{z}_{k}\right)_{L^{2}(\Omega)} - \left(\lambda_{k}, \tilde{z}_{k}\right)_{L^{2}(\Omega)} + \sum_{i=k+1}^{s} \left(\lambda_{i}, \bar{\sigma}_{k} \frac{\partial \psi_{i}(y, (\bar{\sigma}_{j}z_{i})_{j < i})}{\partial z_{k}} \tilde{z}_{k}\right)_{L^{2}(\Omega)} + \mu \int_{\Omega} -4\sigma_{k} \max(-\sigma_{k}z_{k}, 0)^{3} \tilde{z}_{k} d\Omega \qquad \forall \tilde{z}_{k}, 1 \leq k \leq s$$

$$(21)$$

As one can easily see, the optimality conditions (4)-(7) coincide with the optimality conditions (17)-(20). Hence, if one computes a solution of the slightly modified branch problem with the target function (15) and the constraints (12)-(13), the necessary first order conditions (4)-(7)



Table 3: The different optimization problems.

of the original optimisation problem are already satisfied. Hence, the only condition to verify is Eq. (10). Since the expressions on the right-hand side are completely independent of the Lagrange multiplier μ of the original optimisation problem, one can compute this quantity also for the solution of the modified branch problem. If it is non-negative, the computed solution (y^*, z^*, u^*) of the modified branch problem fulfills the necessary first order conditions of the original optimisation problem for the chosen functions $\bar{\sigma}_i \in L^2(\Omega)$ and the optimisation algorithm can be stopped. Otherwise, it is a very natural strategy to choose the index k for which the right-hand side of the condition (10) is minimal, to modify the corresponding $\bar{\sigma}_k$ appropriately and to solve the then newly defined branch problem by the same strategy. Due to the structure of Eq. (10), the Lagrange multiplier λ_k identifies the regions where the sign of $\bar{\sigma}_k$ has to be changed to obtain a reduction in the function value. Obviously, other strategies to choose the index k as alternatives to the greedy approach described here might be applied as well.

Tab. 3 illustrates the nature of the relationships between the different problem formulations that are derived and discussed in this paper.

4 The Resulting Optimization Algorithm

Motivated by the observations of the last section, we propose the following method to solve optimal control problems with non-smooth PDEs of the class considered here as constraints:

Algorithm 1

```
Input: Initial values: \bar{\sigma}^0 = (\bar{\sigma}_1^0, ..., \bar{\sigma}_s^0), y^0, z^0 = (z_1^0, ..., z_s^0), u^0

Parameter: \alpha, \mu, i = 0

for i = 0, 1, ... do

Solve branch problem (15) with constraints (12)–(13) to obtain y^i, z^i, u^i, \lambda_{PDE}^i, \lambda^i

if Eq. (10) holds for k = 1, ..., s then

y^i, z^i, u^i stationary for original optimal control problem, stop

else

\kappa = \operatorname{argmax}\{k \in \{1, ..., s\} : -r(\bar{\sigma}_k^i, y, z, \lambda)\}, \text{ where } r(.) \text{ is given by Eq. (10)}.

Use \lambda_{\kappa} to define \bar{\sigma}_{\kappa}^{i+1}

Set \bar{\sigma}_k^{i+1} = \bar{\sigma}_k^i for k = 1, ..., s, k \neq \kappa

end if

i+=i

end for
```

Since the proposed algorithm is essentially motivated by the special handling of the absolute value function, i.e., the abs-linearization, we call the resulting optimization algorithm SALi for Successive Abs-Linearization. Note that the formulation of the algorithm is done in the function space. Therefore, up to this point one can use the own method of choice to solve the smooth modified branch problems. For the numerical results shown in the next section, we used a Finite-

Element-Approach based on FEniCS to discretise the PDEs and to describe the other constraints in combination with a Newton method for the solution of the smooth modified branch problems.

Finite Dimensional Formulation

In the last paragraph, the algorithm was presented and explained in the continuous function space setting. Now, the natural question is how to put this into practice and, especially, how to solve the individual branch problems. For the numerical treatment of the optimal control problem (15) with the constraints given by Eqs. (12) and (13), the Lagrange equation (16) will be discretized. Therefore we apply a standard finite element method with piecewise linear and continuous ansatz functions for the functions y and z_i , i = 1, ..., s, and piecewise constant ansatz functions for the control u. The resulting problem is solved by the Galerkin method within the open source simulation tool FEniCS [9]. For the initial state, control and parameters $\bar{\sigma}_i$, the nonlinear variational Lagrange problem is solved by Newton's method using the derivatives calculated within FEniCS. The computed solution is examined according to the switching rule and the branch problem is modified by updating the corresponding σ_i . Here again the update strategy is based on Eq. (10). Since the calculation of the function r(.) is relatively complicated and expensive, we derive a heuristic described below which, as we will see in the numerical results, provides the desired results. By exploiting the essence of Eq. (10), a beneficial and comparatively easy way to implement an update strategy for the parameters $\bar{\sigma}_i$ can be created. Reformulation of Eq. (10) and application of σ_k provides

$$0 \leqslant \left(\lambda_{PDE}, |\sigma_k| \frac{\partial \hat{\ell}(y, \sigma_z)}{\partial z_k} \tilde{z}_k\right) - \left(\lambda_k \sigma_k, \tilde{z}_k\right) + \sum_{i=k+1}^s \left(\lambda_i, |\sigma_k| \frac{\partial \psi_i(y, (\sigma_j z_j)_{j < i})}{\partial z_k} \tilde{z}_k\right) \, \forall \tilde{z}_k, \forall k = 1, \dots, s.$$

This condition is violated if and only if there exists an index $k \in \{1, ..., s\}$ such that $\sigma_k = sign(\lambda_k)$ with

$$0 > \left(\lambda_{PDE}, |\sigma_k| \frac{\partial \hat{\ell}(y, \sigma_z)}{\partial z_k} \tilde{z}_k\right) - \left(\lambda_k \sigma_k, \tilde{z}_k\right) + \sum_{i=k+1}^{s} \left(\lambda_i, |\sigma_k| \frac{\partial \psi_i(y, (\sigma_j z_i)_{j < i})}{\partial z_k} \tilde{z}_k\right).$$

Since $|\sigma_k| \equiv 1$, this is equivalent to

$$0 > \left(\lambda_{PDE}, \frac{\partial \hat{\ell}(y, \sigma z)}{\partial z_{k}} \tilde{z}_{k}\right) - \left(|\lambda_{k}|, \tilde{z}_{k}\right) + \sum_{i=k+1}^{s} \left(\lambda_{i}, \frac{\partial \psi_{i}(y, (\sigma_{j} z_{j})_{j < i})}{\partial z_{k}} \tilde{z}_{k}\right).$$
(22)

Again, as already discussed in Sec. 3 it is a natural strategy to choose the index k for which the right hand side in Eq. (22) is minimal. Since this is significantly influenced by the Lagrange multiplier λ_k , we use this as an indicator to switch from the current branch problem to the next one by switching the signs of σ_k in the regions where the corresponding $|\lambda_k|$ is largest. For this purpose, the Lagrange multipliers λ_i corresponding to the solution of the current branch problem are projected to the adequate function space and their max-norm is computed in order to determine the Lagrange multiplier λ_k with maximum influence on Eq. (22). If this maximum value (almost) vanishes, the stationary point is already reached and the algorithm stops. Otherwise the sign of the corresponding discretized σ_k is switched at those mesh points where $|\lambda_k|$ is large and exceeds a certain threshold. Despite the fact that this heuristic works well in practice, we will continue to develop our existing approach further and adapt it for the calculation of Eq. (10) and a related systematic switching strategy of the branch problems.

If no switching occurs, the algorithm stops. Otherwise the branch problem is updated accordingly and a new solution is computed by once again solving the non-linear variational Lagrange problem by applying Newton's method. This way a successive reduction in the objective function value is observed. This can also be seen in Fig. 2.

If one considers the discretized and hence finite dimensional problem, the convergence of the algorithm follows immediately. This is due to the fact that the original problem was decomposed into finitely many discretized branch problems and the function value decreases with each iteration step. Therefore a minimal solution is reached after finitely many steps.

5 Numerical Results

For the numerical tests we considered two dimensional examples defined below in Case 1 to Case 3. In each case Ω was chosen to be the unit square and we take as an initial guess $y \equiv 0, u \equiv 0, z_1 \equiv 0, z_2 \equiv 0$. Furthermore, σ_1 and σ_2 are chosen such that they fit the ones defined by the desired state y_d . We terminate the iteration if either the L^2 -Norm of the Lagrange multipliers λ_i becomes less than 10^{-9} and therefore no further switching between branch problems is done, or if the difference between the Lagrange function value which includes the bi-quadratic penalty terms and the original objective functional becomes less then 10^{-12} . The latter implicitly ensures that the sign condition $\sigma_i z_i \ge 0$ is correctly adhered to.

Case 1

$$\begin{split} \min_{(y,u)} & \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2 \\ \text{s.t.} & -\Delta y + \max(0, y) - u = 0 \quad \text{in } \Omega = (0, 1)^2 \text{ ,} \\ \text{with } y_d(x_1, x_2) &= \begin{cases} ((x_1 - \frac{1}{2})^4 + \frac{1}{2}(x_1 - \frac{1}{2})^3) \sin(\pi x_2), & \text{if } x \leqslant \frac{1}{2} \\ 0, & \text{otherwise} \end{cases} \end{split}$$

Case 2

$$\begin{split} \min_{(y,u)} & \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2 \\ \text{s.t.} & -\Delta y + \max(5y, y|y|) - u = 0 \quad \text{in } \Omega \text{,} \end{split}$$

with $y_d(x_1, x_2) = \frac{\sin\left(10\pi((x_1 - \frac{1}{2})^2 + (x_2 - \frac{1}{2})^2)\right)}{\sqrt{\frac{1}{100} + (x_1 - \frac{1}{2})^2 + (x_2 - \frac{1}{2})^2}} - 1 \text{.}$

Case 3

$$\begin{split} \min_{(y,u)} & \frac{1}{2} \|y - y_d\|_{L^2}^2 + \frac{\alpha}{2} \|u\|_{L^2}^2 \\ \text{s.t.} & -\varepsilon \Delta y + \max(5y, y|y|) - u = 0 \quad \text{in } \Omega \text{ ,} \\ \text{with } y_d(x_1, x_2) &= \min\left(\max\left(|x_1 - \frac{1}{2}|, |x_2 - \frac{1}{2}|\right) - \frac{1}{4}, 0\right) \text{ and } \varepsilon \ge 0, \text{ const} \end{split}$$

The numerical results for these three cases, considering different values of the mesh size denoted by h, the penalty parameter α for the control in the objective functional, and the penalty parameter μ in the bi-quadratic penalty term, are presented in Tab. 4 -7.

It can be observed that in almost all cases only a few Newton iterations are needed to solve the problem and to compute the minimal solution.

A commonly used method for solving such non-smooth problems are semi-smooth Newton-like methods. Therefore, we also provide a comparison with results obtained with a semi-smooth Newton approach.

Case 1 represents an example taken from [1]. The parameters were adopted accordingly and the mesh size was reconstructed in the best possible way. Tab. 4 shows a comparison between the non-regularized approach presented here and the proposed semi-smooth Newton's method in [1]. It can be observed that in the more involved example, according to [1], the approach presented here requires only one single Newton step and no switches between branch problems to compute the optimal solution. The semi-smooth Newton method on the other hand requires an average of three to five steps for the considered problem. Tab. 1 shows also the quality of the resulting approximation which is given the relative error $||y_h - y||_{L^2} / ||y||_{L^2}$.

The fact, that SALi does not require any switches between branch problems is mainly due to the fact, that the reformulation described in Tab. 1 makes it possible to exploit as much information as possible given by the optimization problem and in particular by the given desired state y_d . The initial choice of the σ_i motivated by the desired state already provides the perfect guess of the

h	α	μ	Obj. Value	$\frac{\ y_h - y\ _{L^2}}{\ y\ _{L^2}}$	# Newton SALi	# Newton [1]
3.009e-02	1e-4	50	1.174e-12	5.765e-04	1	4
1.537e-02	1e-4	50	8.102e-14	1.514e-04	1	5
7.728e-03	1e-4	50	5.119e-15	3.790e-05	1	3
3.885e-03	1e-4	50	3.306e-16	9.664e-06	1	3
3.009e-02	1e-4	100	1.174e-12	5.764e-04	1	4
1.537e-02	1e-4	100	8.102e-14	1.514e-04	1	5
7.728e-03	1e-4	100	5.120e-15	3.790e-05	1	3
3.885e-03	1e-4	100	3.306e-16	9.664e-06	1	3
7.728e-03	1e-4	500	5.121e-15	3.790e-05	1	3
7.728e-03	1e-2	100	1.345e-14	8.106e-05	1	2
7.728e-03	1e-3	100	1.037e-14	6.609e-05	1	2
7.728e-03	1e-5	100	1.236e-15	1.237e-05	1	5
7.728e-03	1e-6	100	1.778e-16	3.056e-06	1	no conv.

Table 4: Numerical results in Case 1.

h	α	μ	Objective	$\frac{ y-y_d }{ y_d }$	# Swaps	# Newton
1.537e-02	1e-4	100	1.633	7.996e-01	10	63
1.159e-02	1e-4	100	1.640	8.000e-01	11	65
7.071e-03	1e-4	100	1.645	8.005e-01	21	72
1.159e-02	1e-4	500	1.640	8.002e-01	15	89
7.071e-03	1e-4	500	1.646	8.009e-01	13	90
1.159e-02	1e-6	100	0.361	2.920e-01	3	23
7.071e-03	1e-6	100	0.363	2.925e-01	4	28

Table 5: Numerical results for smooth but non reachable y_d (Case 2).

 σ_i . Since the desired state which is reachable by the given state equation no switches between branch problems are required and the optimal solution can be computed by solving the initial branch problem which is already the final one.

The numerical results for Case 2 are given in Tab. 5. In this demanding case where a genuine nonlinear and non-smooth operator in the PDE and an unreachable target function y_d occur, comparatively more switches between branch problems and also more Newton iterations are needed to compute the minimal solution.

Fig. 1 shows the initial and the last iteration step in σ_1 , σ_2 as well as the resulting states y, z with an over line plot for the z and σ components showing how the prescribed signs are observed. The target function y_d is shown in the top left corner. Fig. 2 shows how the successive exploitation of the corresponding dual variables leads to the next branch problem and thus to successive reduction in the function value.

The method presented here also allows the treatment of optimization problems of the considered problem class with non-smooth target functions y_d as given in Case 3. Such non-smooth target functions are not achievable due to the PDE constraint with the Laplace operator as differential operator. Nevertheless, in the example considered in Case 3, with non damped Laplacian, i.e., $\varepsilon \equiv 1$, no switches and only two Newton steps are required to calculate the minimum solution. The numerical results are given in Tab. 6.

However, if the Laplace operator is attenuated by a factor $\varepsilon < 1$, also less smooth solutions for y are achievable. Fig. 3 shows the non-smooth target function y_d as well as the solution y and u in Case 3 when setting $\varepsilon \equiv 1e - 2$. Tab. 7 shows the numerical results for different values for ε in Case 3.



Figure 1: Case 2. (a) Initial Branch problem with resulting solution for y, z_1 and z_2 . (b) Final iteration step with final Branch problem and resulting solution for y, z_1 and z_2 .



Figure 2: History of the objective function value with respect to the branch problem switches in Case 2 corresponding to the parameters given in he first row in Tab. 5.

h	α	μ	Objective	$ y - y_d $	# Swaps	# Newton
1.537e-02	1e-4	100	3.884e-04	2.132e-02	0	2
1.159e-02	1e-4	100	3.878e-04	2.129e-02	0	2
7.071e-03	1e-4	100	3.884e-04	2.131e-02	0	2
1.159e-02	1e-4	500	3.878e-04	2.129e-02	0	2
7.071e-03	1e-4	500	3.884e-04	2.131e-02	0	2
7.071e-03	1e-6	100	2.273e-05	3.673e-03	0	2

Table 6: Numerical results in Case 3 for $\varepsilon \equiv 1$.



Figure 3: Considered target function y_d and resulting solution for the sate y and control u in Case 3 with $\varepsilon \equiv 1e - 2$.

h	ε	α	μ	Objective	$ y - y_d $	# Swaps	# Newton
1.159e-03	1e-1	1e-4	100	2.453e-05	3.691e-03	1	4
7.071e-03	1e-1	1e-4	100	2.476e-05	3.600e-03	1	4
1.537e-02	1e-2	1e-4	500	1.202e-06	7.027e-04	0	2
1.159e-03	1e-2	1e-4	500	1.145e-06	6.422e-04	0	2
7.071e-03	1e-2	1e-4	500	1.175e-06	6.689e-04	0	2
1.537e-02	1e-4	1e-4	100	1.348e-07	4.100e-05	0	2
1.159e-03	1e-4	1e-4	100	1.341e-07	3.685e-05	0	2
7.071e-03	1e-4	1e-4	100	1.340e-07	3.311e-05	0	2
7.071e-03	1e-6	1e-4	100	1.302e-07	5.820e-06	0	2

Table 7: Numerical results in Case 3 with damped Laplacian.

6 Conclusion and Outlook

We presented a new approach based on successive abs linearization for the solution of optimization problems constrained by non-smooth PDEs. This approach enables for the considered class of genuinely non-smooth problems the optimization without any substitute assumptions and regularizations for the non-smoothness. The key idea is to appropriately decompose the non-smooth problem into smooth branch problems, which can be solved by classical smooth optimization problems. Optimality conditions for the considered formulations were derived and discussed. Solving the current branch problem, exploiting standard optimality conditions for the smooth case as well as using an indicator strategy to determine the next branch problem, ensures successive reduction in the objective function value and leads to the minimal solution. By treating the inequality condition with a bi-quadratic penalty approach the sign condition could easily be incorporated into the algorithmic framework. Finally, several non-smooth PDE-constrained problems that fit into the considered setting were discussed. However, a comprehensive convergence analysis for the continuous case is still lacking and remains subject of future research.

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