Variational discretization and semi-smooth Newton methods; implementation, convergence and globalization in pde constrained optimization with control constraints

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Abstract: When combining the numerical concept of variational discretization introduced in [5, 6] and semi-smooth Newton methods for the numerical solution of pde constrained optimization with control constraints [3, 11] special emphasis has to be taken on the implementation, convergence and globalization of the numerical algorithm. In the present work we address all these issues. In particular we prove fast local convergence of the algorithm and propose two different globalization strategies which are applicable in many practically relevant mathematical settings. We illustrate our analytical and algorithmical findings by numerical experiments.

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1 Introduction and mathematical setting

We are interested in the numerical treatment of the following control problem

\[
\begin{aligned}
\min_{(y,u) \in Y \times U_{\text{ad}}} & \ J(y,u) := \frac{1}{2} \|y - z\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_U^2 \\
\text{s.t.} & \ -\Delta y = Bu \quad \text{in} \ \Omega, \\
& \ y = 0 \quad \text{on} \ \partial\Omega.
\end{aligned}
\]

(1.1)

Here, \( \Omega \subset \mathbb{R}^d \) \((d \geq 1)\) denotes an open, bounded sufficiently smooth (polyhedral) domain. Given some Hilbert space \( U \) and some closed, convex admissible set \( U_{\text{ad}} \subset U \) for the controls and a linear, continuous control operator \( B : U \to H^{-1}(\Omega) \), the states lie in \( Y := H_0^1(\Omega) \). Let us note that also additional state constraints could be included into our problem setting, as done in [1] and [2], and also more general (linear) elliptic or parabolic state equations. However, all structural issues discussed in the present work are induced by the control constraints, hence to keep the exposition as simple as possible state constraints are not considered here. Typical configurations of \( P \) are
Examples.

(i) $U := \mathbb{R}^m$, $Y = H^1_0(\Omega)$, $B : \mathbb{R}^m \to H^{-1}(\Omega)$, $Bu := \sum_{j=1}^m u_j F_j$, $F_j \in H^{-1}(\Omega)$, $U_{ad} := \{v \in \mathbb{R}^m; a_j \leq v_j \leq b_j\}$, $a, b \in \mathbb{R}^m$, $a < b$.

(ii) $U := L^2(\Omega)$, $Y = H^1_0(\Omega)$, $B = \iota : L^2(\Omega) \to H^{-1}(\Omega)$, $\iota$ being the canonical injection, $U_{ad} := \{v \in L^2(\Omega); a \leq v \leq b\}$, $a, b \in L^\infty(\Omega)$, $a < b$.

Remark 1.1. One may as well consider elliptic equations with Neumann boundary control,

$$\begin{align*}
-\Delta y + y &= 0 \quad \text{in } \Omega, \\
\partial_\eta y &= u \quad \text{on } \partial \Omega,
\end{align*}$$

thus setting $U := L^2(\Gamma)$, $Y = H^1(\Omega)$, $U_{ad} := \{v \in L^2(\Gamma); a \leq v \leq b\}$, $a, b \in L^\infty(\Gamma)$, $a < b$.

Problem $\mathcal{P}$ admits a unique solution $(y, u) \in Y \times U_{ad}$, and can equivalently be rewritten as the optimization problem

$$\min_{u \in U_{ad}} \hat{J}(u) \quad (1.2)$$

for the reduced functional $\hat{J}(u) := J(y(u), u) \equiv J(SBu, u)$ over the set $U_{ad}$, where $S : Y^* \to Y$ denotes the (continuous) solution operator associated with $-\Delta$. We further know that the first order necessary (and here also sufficient) optimality conditions take the form

$$\langle \hat{J}'(u), v - u \rangle_{U^*, U} \geq 0 \text{ for all } v \in U_{ad} \quad (1.3)$$

where $\hat{J}'(u) = \alpha u + B^* S^*(SBu - z) \equiv \alpha u + B^* p$, with $p := S^*(SBu - z)$ denoting the adjoint variable. The function $p$ in our setting satisfies

$$\begin{align*}
-\Delta p &= y - z \quad \text{in } \Omega, \\
p &= 0 \quad \text{on } \partial \Omega. 
\end{align*} \quad (1.4)$$

For the numerical treatment of problem (1.1) it is convenient to rewrite (1.3) for $\sigma > 0$ arbitrary in form of the following non–smooth operator equation;

$$u = P_{U_{ad}} \left( u - \sigma \nabla \hat{J}(u) \right)^{\sigma=1/\alpha} = P_{U_{ad}} \left( -\frac{1}{\alpha} R^{-1} B^* p \right),$$

with the Riesz isomorphism $R : U \to U^*$ and the gradient $\nabla \hat{J}(u) = R^{-1} \hat{J}'(u)$.

2 Finite element discretization

To discretize ($\mathcal{P}$) we concentrate on Finite Element approaches and make the following assumptions.

Assumption 2.1.

$\Omega \subset \mathbb{R}^d$ denotes a polyhedral domain, $\bar{\Omega} = \bigcup_{j=1}^n \bar{T}_j$ with admissible quasi-uniform sequences of partitions $\{T_j\}_{j=1}^n$ of $\Omega$, i.e. with $h_{nt} := \max_j \text{diam } T_j$ and $\sigma_{nt} := \min_j \{\sup \text{diam } K; K \subseteq T_j\}$ there holds $c \leq \frac{h_{nt}}{\sigma_{nt}} \leq C$ uniformly in $nt$ with positive constants $0 < c \leq C < \infty$ independent of $nt$. We abbreviate $T_h := \{T_j\}_{j=1}^n$. 

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For \( k \in \mathbb{N} \) we set

\[
W_h := \{ v \in C^0(\Omega) \mid v|_{T_j} \in P_k(T_j) \text{ for all } 1 \leq j \leq nt \} =: \langle \phi_1, \ldots, \phi_{ng} \rangle, \text{ and } Y_h := \{ v \in W_h, v|_{\partial \Omega} = 0 \} =: \langle \phi_1, \ldots, \phi_n \rangle \subseteq Y;
\]

with some \( 0 < n < ng \). The resulting Ansatz for \( y_h \) then is of the form \( y_h = \sum_{i=1}^{n} y_i \phi_i \). Now we approximate problem \((\mathcal{P})\) by

\[
(P_h) \quad \begin{cases}
\min_{(y_h,u) \in Y_h \times U_{ad}} J(y_h,u) := \frac{1}{2} \| y_h - z \|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \| u \|_{U}^2 \\
\text{s.t.} \\
a(y_h,v_h) = (Bu,v_h)_{Y^*,Y} \quad \text{for all } v_h \in Y_h,
\end{cases}
\]

where \( a(y,v) := \int_{\Omega} \nabla y \nabla v \, dx \) denotes the bilinear form associated with \(-\Delta\). Problem \((P_h)\) admits a unique solution \((y_h,u) \in Y_h \times U_{ad}\) and, as above, can equivalently be rewritten as the optimization problem

\[
\min_{u \in U_{ad}} \tilde{J}_h(u)
\]

for the discrete reduced functional \( \tilde{J}_h(u) := J(y_h(u),u) \equiv J(S_h Bu,u) \) over the set \( U_{ad}\), where \( S_h : Y^* \to Y_h \subset Y \) denotes the solution operator associated with the finite element discretization of \(-\Delta\). The first order necessary (and here also sufficient) optimality conditions take the form

\[
(\tilde{J}_h'(u_h),v - u_h)_{U^*,U} \geq 0 \quad \text{for all } v \in U_{ad}
\]

(2.3)

where \( \tilde{J}_h'(v) = \alpha v + B^* S_h^*(S_h Bu - z) \equiv \alpha u + B^* p_h \), with \( p_h := S_h^*(S_h Bu - z) \) denoting the adjoint variable. The function \( p_h \) in our setting satisfies

\[
a(v_h,p_h) = (y_h - z,v_h)_{Y^*,Y} \quad \text{for all } v_h \in Y_h.
\]

(2.4)

Analogously to (1.3), for \( \sigma > 0 \) arbitrary, we have

\[
u_h = P_{U_{ad}} \left( u_h - \sigma \nabla \tilde{J}_h(u_h) \right) \left. \right|_{\sigma=1/\alpha} \equiv P_{U_{ad}} \left( -\frac{1}{\alpha} R^{-1} B^* p_h \right) .
\]

(2.5)

**Remark 2.2.** Problem (2.1) is still infinite-dimensional in that the control space is not discretized. This is reflected through the appearance of the projector \( P_{U_{ad}} \) in (2.5). The numerical challenge now consists in designing numerical solution algorithms for problem (2.1) which are implementable, and which reflect the infinite-dimensional structure of the discrete problem (2.1) [5, 6].

Next let us investigate the error \( \| u - u_h \|_U \) between the solutions \( u \) of (1.2) and \( u_h \) of (2.2), compare [7].

**Theorem 2.3.** Let \( u \) denote the unique solution of (1.2), and \( u_h \) the unique solution of (2.2). Then there holds

\[
\alpha \| u - u_h \|^2_U + \frac{1}{2} \| y(u) - y_h \|^2 \leq (B^* (p(u) - \tilde{p}_h(u)),u_h - u)_{U^*,U} + \frac{1}{2} \| y(u) - y_h(u) \|^2_{L^2(\Omega)},
\]

(2.6)

where \( \tilde{p}_h(u) := S_h^*(SBu - z) \), \( y_h(u) := S_h Bu \), and \( y(u) := SBu \).
Proof. Since \((2.2)\) is an optimization problem defined on all of \(U_{ad}\), the unique solution \(u\) of \((1.2)\) is an admissible test function in \((2.3)\). Let us emphasize, that this is different for approaches, where the control space is discretized explicitly. In this case we may only expect that \(u_h\) is an admissible test function for the continuous problem (if ever). So let us test \((1.3)\) with \(u_h\) and \((2.3)\) with \(u\), and then add the resulting variational inequalities. This leads to

\[
\langle \alpha(u - u_h) + B^*S^*(SBu - z) - B^*S_h^*(ShBu_h - z), u_h - u \rangle_{U^*, U} \geq 0.
\]

This inequality is equivalent to

\[
\alpha\|u - u_h\|^2_U \leq \langle B^*(p(u) - \tilde{p}_h(u)) + B^*(\tilde{p}_h(u) - p_h(u_h)), u_h - u \rangle_{U^*, U}.
\]

Let us investigate the second addend on the right hand side of this inequality. By definition of the adjoint variables there holds

\[
\langle B^*(\tilde{p}_h(u) - p_h(u_h), u_h - u)_{U^*, U} = \langle \tilde{p}_h(u) - p_h(u_h), B(uh - u)\rangle_{Y, Y^*} =
\]

\[
= a(y_h - y(u), \tilde{p}_h(u) - p_h(u_h)) = \int (y_h(u) - y(u))(y(u) - y_h(u))dx =
\]

\[
= -\|y - y_h\|^2_{L^2(\Omega)} + \int (y - y_h)(y - y_h)dx \leq -\frac{1}{2}\|y - y_h\|^2_{L^2(\Omega)} + \frac{1}{2}\|y - y_h\|^2_{L^2(\Omega)}
\]

so that the claim of the theorem follows. \(\blacksquare\)

What can we learn from Theorem \((2.4)\)? It tells us that an error estimate for \(\|u - u_h\|_U\) is at hand, if

- an error estimate for \(\|R^{-1}B^*(p(u) - \tilde{p}_h(u))\|_U\) is available, and
- an error estimate for \(\|y(u) - y_h(u)\|_{L^2(\Omega)}\) is available.

Remark 2.4. The error \(\|u - u_h\|_U\) between the solution \(u\) of problem \((1.2)\) and \(u_h\) of \((2.2)\) is completely determined by the approximation properties of the discrete solution operators \(S_h\) and \(S_h^*\).

3 Semi-smooth Newton algorithm

In the following we restrict our considerations to the practically relevant case of the second example given in Section 1, i.e. we set \(U = L^2(\Omega)\), \(Y = H^1_0(\Omega)\), \(U_{ad} = \{v \in L^2(\Omega); a \leq v \leq b\}\) with \(a, b \in L^\infty(\Omega)\), \(b - a > \sigma > 0\) and \(\sigma \in \mathbb{R}\). Also the control operator is the injection \(i : L^2(\Omega) \to Y^*\), hence the adjoint \(B^* = i^*\) is the injection from \(Y\) into \(L^2(\Omega)\). Below, the operators \(B, B^*\) and \(R\) are omitted for notational convenience. The variationally discretized problem associated to \((P)\) then reads

\[
(P_h)
\]

\[
\min_{(y_h, v_h) \in Y \times L^2(\Omega)} J(y_h, u) := \frac{1}{2}\|y - z\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}
\]

s.t.

\[
a(y_h, v_h) = \langle u, v_h \rangle_{L^2(\Omega)} \quad \text{for all} \; v_h \in Y_h
\]

and

\[
a \leq u \leq b, \text{ a.e. in } \Omega.
\]
To apply the semi-smooth Newton algorithm proposed in the following, the bounds are required to be elements of the finite element space $Y_h$. Let therefore $a_h, b_h \in Y_h$ be obtained from $a, b$ by interpolation or projection and let us consider the problem

$$(\mathbb{P}_{hh}) \quad \begin{cases} \min_{(y_h, u_h) \in Y \times L^2(\Omega)} J(y, u) := \frac{1}{2} \| y - z \|^2_{L^2(\Omega)} + \frac{\alpha}{2} \| u \|^2_{L^2(\Omega)} \\ \text{s.t.} \quad a(y_h, v_h) = \langle u, v \rangle_{L^2(\Omega)} \quad \text{for all } v_h \in Y_h \\ \text{and} \quad a_h \leq u \leq b_h, \text{ a.e. in } \Omega, \end{cases}$$

It is clear that for $h > 0$ small enough the admissible set $a_h \leq u \leq b_h$ is non-empty, if $a_h, b_h \to a, b$ uniformly, say which can be guaranteed for sufficiently smooth bounds $a, b$ and $a_h = I_h a$, $b_h = I_h b$, with $I_h$ denoting the Lagrange interpolation operator or the $L^2$-projection. In this case problem $(\mathbb{P}_{hh})$ admits a unique solution $(u_{hh}, y_{hh})$. Let us assume, that this solution exists.

**Lemma 3.1 (Perturbed Bounds).** The solutions $(y_{hh}, u_{hh})$ and $(y_h, u_h)$ of $(\mathbb{P}_{hh})$ and $(\mathbb{P})$ satisfy the estimate

$$\| u_{hh} - u_h \|_{L^2(\Omega)} \leq \left( 1 + \frac{1}{\alpha} \| S_h \|^2 \right) (\| a - a_h \|_{L^2(\Omega)} + \| b - b_h \|_{L^2(\Omega)}).$$

**Proof.** Let

$$u_h^P(\omega) = P_{[a_h(\omega), b_h(\omega)]} \left( -\frac{1}{\alpha} [S_h^*(S_h u_h - z)](\omega) \right) .$$

Then by (2.5) there holds

$$\| u_h^P - u_h \|_{L^2(\Omega)} \leq \| a_h - a \|_{L^2(\Omega)} + \| b_h - b \|_{L^2(\Omega)} .$$

(3.1)

Since $u_h^P$ is admissible for $\mathbb{P}_{hh}$ we have

$$\langle u_h + \frac{1}{\alpha} S_h^*(S_h u_h - z), u_h^P - u_h \rangle_{L^2(\Omega)} \geq 0$$

while the definition of $u_h^P$ gives

$$\langle u_h^P + \frac{1}{\alpha} S_h^*(S_h u_h - z), u_h - u_h^P \rangle_{L^2(\Omega)} \geq 0$$

since $u_{hh}$ lies between $a_h$ and $b_h$. Adding these inequalities leads to

$$\| u_h^P - u_h \|^2_{L^2(\Omega)} \leq \frac{1}{\alpha} \langle S_h^* S_h (u_h - u_{hh}), u_h - u_h^P \rangle_{L^2(\Omega)}$$

$$= \frac{1}{\alpha} \langle S_h^* S_h (u_h - u_h^P), u_h - u_h^P \rangle_{L^2(\Omega)} + \frac{1}{\alpha} \langle S_h^* S_h (u_h^P - u_{hh}), u_h - u_h^P \rangle_{L^2(\Omega)}$$

and finally we have

$$\| u_h^P - u_h \|^2_{L^2(\Omega)} + \frac{1}{\alpha} \langle S_h (u_h^P - u_{hh}), u_h - u_h^P \rangle_{L^2(\Omega)} \leq \frac{1}{\alpha} \langle S_h^* S_h (u_h - u_h^P), u_h - u_h^P \rangle_{L^2(\Omega)}$$

$$\leq \frac{1}{\alpha} \| S_h \|^2 \| u_h - u_h^P \|_{L^2(\Omega)} \| u_h - u_h^P \|_{L^2(\Omega)}$$

which combined with (3.1) implies the lemma.
Now let
\[ G(v) := v - P_{[a,b]} \left( -\frac{1}{\alpha} p(y(v)) \right), \quad \text{and} \quad G_h(v) := v - P_{[a_h,b_h]} \left( -\frac{1}{\alpha} p_h(y_h(v)) \right), \quad (3.2) \]
where for given \( v \in L^2(\Omega) \) the functions \( p, p_h \) are defined through (1.4) and (2.4), respectively. It follows from the characterization of orthogonal projectors in real Hilbert spaces that the unique solutions \( u, u_h \) to (1.1) and (2.1) are characterized by the equations
\[ G(u), \ G_h(u_h) = 0 \text{ in } L^2(\Omega). \quad (3.3) \]
These equations will be shown to be amenable to semi–smooth Newton methods as proposed in [3] and [11]. We begin with formulating

**Algorithm 3.2.** (Semi–smooth Newton algorithm for (3.3))

Start with \( v \in L^2(\Omega) \) given. Do until convergence

Choose \( M \in \partial G_h(v) \).

Solve \( M \delta v = -G_h(v), \ v := v + \delta v. \)

If we choose Jacobians \( M \in \partial G_h(v) \) with \( \|M^{-1}\| \) uniformly bounded throughout the iteration, and at the solution \( u_h \) the function \( G_h \) is \( \partial G_h \)-semismooth of order \( \mu \), this algorithm is locally superconvergent of order \( 1 + \mu \). Although Algorithm 3.2 works on the infinite dimensional space \( L^2(\Omega) \), it is possible to implement it numerically, as is shown subsequently.

### 3.1 Semismoothness

To apply the Newton algorithm, we need to confirm that the discretized operator \( G_h \) is indeed semismooth. To establish this fact we rewrite \( G_h \) in the form
\[ G_h(u) = u - (b - a) P_{[0,1]} \left( (b - a)^{-1} \left( -\frac{1}{\alpha} (S_h^*(S_h u - z)) - a \right) \right) + a \]
and apply ([11], Theorem 5.2), with \( P_{[0,1]} : \mathbb{R} \to \mathbb{R} \) taking the role of \( \psi \). Here and in the following, for notational convenience we assume \( a, b \in Y_h \), which is no restriction due to Lemma 3.1. The smoothing–operator \( F : L^2 \to L^q \) from [11] in our case reads
\[ F(u) = (b - a)^{-1} \left( -\frac{1}{\alpha} (S_h^*(S_h u - z)) - a \right). \]

We note that
- since we require \( a, b \in L^\infty(\Omega) \), \( b - a > \sigma > 0 \) with \( \sigma \in \mathbb{R} \), both \( (b - a) \) and \( (b - a)^{-1} \) are in \( L^\infty(\Omega) \) and the pointwise multiplication by either \( (b - a) \) or \( (b - a)^{-1} \) is a continuous endomorphism in \( L^p(\Omega) \) for any \( p \).
- the operator \( F \) is differentiable with constant derivative for any \( q \geq 1 \). In fact, for sufficiently smooth domains \( \Omega \), the operators \( S_h \) and \( S_h^* \) map \( L^2(\Omega) \) continuously into \( H^2(\Omega) \), which is continuously embedded in \( L^q(\Omega) \) for any \( q \in [1, \infty] \).
- \( P_{[0,1]} : \mathbb{R} \to \mathbb{R} \) is \( \partial P_{[0,1]} \)-semismooth of order 1, with
\[
\partial P_{[0,1]}(x) = \begin{cases} 
0 & \text{if } x \notin [0,1] \\
1 & \text{if } x \in (0,1) \\
[0,1] & \text{if } x = 0 \text{ or } x = 1 
\end{cases}.
\quad (3.4)
\]
• for piecewise linear elements the semismooth complementarity condition (5.3) in ([11], theorem 5.2) holds automatically with \( \gamma = 1 \).

Thus we are in the position to apply ([11], theorem 5.2) with \( \alpha = 1 \) and \( q_0 > r = 2 \) and \( \gamma = 1 \) and obtain

**Theorem 3.3.** The function \( G_h \) defined in ([3],2) is \( \partial G_h \)-semismooth of order \( \mu < \frac{1}{3} \). There holds

\[
\partial G_h(v)w = w + \frac{1}{\alpha} \partial P_{[a,b]} \left( - \frac{1}{\alpha} p_h(y_h(v)) \right) \cdot (S_h^* S_h w),
\]

where the application of the differential \( \partial P_{[a,b]} \) and the multiplication by \( S_h^* S_h w \) are pointwise operations a.e. in \( \Omega \).

**Remark 3.4.** In [4] the mesh independence of the superlinear convergence is stated. Recent results from [12] indicate semismoothness of \( G \) of order \( \frac{1}{4} \) as well as mesh independent \( q \)-superlinear convergence of the Newton algorithm of order \( \frac{3}{2} \), if for example the modulus of the slope of \( -\frac{1}{\alpha} p(y(\bar{u})) \) is bounded away from zero on the border of the active set, and if the mesh parameter \( h \) is reduced appropriately. This is the key to our second globalization strategy proposed in Section 3.4.

### 3.2 Newton-Algorithm

The generalized differential \( \partial P_{[a,b]} \) can be defined analogously to (3.4) and the set-valued function \( \partial P_{[a,b]} \left( - \frac{1}{\alpha} p_h(y_h(v)) \right) \) contains the characteristic function \( \chi_{\mathcal{I}(v)} \) of the inactive set

\[
\mathcal{I}(v) = \{ \omega \in \Omega \mid \left( - \frac{1}{\alpha} p_h(y_h(v)) \right)(\omega) \in (a(\omega), b(\omega)) \}.
\]

By \( \chi^v \) we will denote synonymously the characteristic function \( \chi_{\mathcal{I}(v)} \) as well as the self-adjoint endomorphism in \( L^2(\Omega) \) given by the pointwise multiplication with \( \chi_{\mathcal{I}(v)} \). The Newton-step in Algorithm 3.2 now takes the form

\[
\left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \right) \delta v = -v + P_{[a,b]} \left( - \frac{1}{\alpha} p_h(y_h(v)) \right).
\]

(3.5)

To obtain an impression of the structure of the next iterate \( v^+ = v + \delta v \) we rewrite (3.5) as

\[
v^+ = P_{[a,b]} \left( - \frac{1}{\alpha} p_h(y_h(v)) \right) - \frac{1}{\alpha} \chi^v S_h^* S_h \delta v.
\]

Since the range of \( S_h^* \) is \( Y_h \), the first addend is continuous and piecewise polynomial (of degree \( k \)) on a refinement \( K_h \) of \( T_h \). The partition \( K_h \) is obtained from \( T_h \) by inserting nodes and edges along the boundary between the inactive set \( \mathcal{I}(v) \) and the according active set, and in general contains simplices of higher order than \( T_h \). The inserted edges are level sets of \( \chi^v \).

The second addend, involving the cut-off function \( \chi^v \), is also piecewise polynomial of degree \( k \) on \( K_h \) but may jump along the edges not contained in \( T_h \).

Finally \( v^+ \) lies in the following finite dimensional subspace of \( L^2(\Omega) \)

\[
Y^+_h = \{ \chi^v \varphi_1 + (1 - \chi^v) \varphi_2 \mid \varphi_1, \varphi_2 \in Y_h \} = \text{span} (\{ \phi_j \chi^v \}_{j=1}^n, \{ \phi_j (1 - \chi^v) \}_{j=1}^n).
\]

The iterates generated by the Newton-algorithm can be represented exactly with about constant effort, since the number of inserted nodes varies only mildly from step to step, once
the algorithm begins to converge. Furthermore the number of inserted nodes is bounded, see [5],[6].

Since the Newton-increment \( \delta v \) may have jumps along the borders of both the new and the old active and inactive sets, it is advantageous to compute \( v^+ \) directly, because \( v^+ \) lies in \( Y^+_h \). To achieve an equation for \( v^+ \) we add \( G_h'(v)v \) on both sides of (3.5) to obtain

\[
\left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \right) v^+ = P_{[a,b]} \left( -\frac{1}{\alpha} p_h(y_h(v)) \right) + \frac{1}{\alpha} \chi^v S_h^* S_h v, \tag{3.6}
\]

and reformulate Algorithm 3.2 as

**Algorithm 3.5** (Newton Algorithm).

\[ v \in U \text{ given. Do until convergence} \]

Solve (3.6) for \( v^+ \), \( v := v^+ \).

### 3.3 Computing the Newton-Step 3.6

Since \( v^+ \) defined by (3.6) is known on the active set \( \mathcal{A}(v) := \Omega \setminus \mathcal{I}(V) \) it remains to compute \( v^+ \) on the inactive set. So we rewrite (3.6) in terms of the unknown \( \chi^v v^+ \) by splitting \( v^+ \) as

\[
v^+ = (1 - \chi^v) v^+ + \chi^v v^+
\]

and obtain

\[
\left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \right) \chi^v v^+ = P_{[a,b]} \left( -\frac{1}{\alpha} p_h(y_h(v)) \right) + \frac{1}{\alpha} \chi^v S_h^* S_h v - \left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \right) (1 - \chi^v) v^+.
\]

As \( (1 - \chi^v) v^+ \) is already known, we can restrict the latter equation to the inactive set \( \mathcal{I}(v) \)

\[
\left( \chi^v + \frac{1}{\alpha} \chi^v S_h^* S_h \chi^v \right) v^+ = \frac{1}{\alpha} \chi^v S_h^* z - \frac{1}{\alpha} \chi^v S_h^* S_h (1 - \chi^v) v^+. \tag{3.7}
\]

On the left-hand side of (3.7) we have now a continuous, selfadjoint Operator on \( L^2(\mathcal{I}^v) \), which is positive definite, because it is the restriction of the positive definite Operator \( \left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \chi^v \right) \) to \( L^2(\mathcal{I}^v) \).

Hence we are in the position to apply a CG-algorithm to solve (3.7). Moreover under the assumption of the first iterate lying in

\[
Y^+_h|_{\mathcal{I}^v} = \{ \chi^v \varphi \mid \varphi \in Y_h \},
\]

as does the solution \( \chi^v v^+ \), the algorithm does not leave this space because of

\[
\left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \chi^v \right) Y^+_h|_{\mathcal{I}^v} \subset Y^+_h|_{\mathcal{I}^v}
\]

and all CG-iterates lie in \( Y^+_h|_{\mathcal{I}^v} \). These considerations lead to the following

**Algorithm 3.6** (Solving (3.6)).

Compute the active and inactive sets \( \mathcal{A}^v \) and \( \mathcal{I}^v \).

\[ \forall q \in \mathcal{A}^v \text{ set} \]

\[
v^+(q) = P_{[a,b]} \left( -\frac{1}{\alpha} p_h(y_h(v))(q) \right).
\]
Solve
\[(I + \frac{1}{\alpha} \chi^v S_h^* S_h) \chi^v v^+ = \frac{1}{\alpha} \chi^v S_h^* z - \frac{1}{\alpha} \chi^v S_h^* S_h (1 - \chi^v) v^+\]
for \(\chi^v v^+\) by CG-iteration. By choosing a starting point in \(Y_h^+ \mid_{V^v}\) one ensures that all iterates lie inside \(Y_h^+ \mid_{V^v}\).

\[v^+ = (1 - \chi^v) v^+ + \chi^v v^+\]

We note that the use of this procedure in Algorithm 3.5 coincides with the active set strategy proposed in [3].

### 3.4 Globalization

Globalization of Algorithm 3.5 may require a damping step of the form

\[v^+_\lambda = v + \lambda(v^+ - v)\]

with some \(\lambda > 0\). According to the considerations above, we have

\[v^+_\lambda = (1 - \lambda)v + \lambda \left( P_{[a,b]} \left( -\frac{1}{\alpha} p_h(y_h(v)) \right) - \frac{1}{\alpha} \chi^v S_h^* S_h \delta v \right) .\]

Unless \(\lambda = 1\) the effort of representing \(v^+_\lambda\) will in general grow with every iteration of the algorithm, due to the jumps introduced in each step. This problem can be bypassed by focussing on the adjoint state \(p_h(v)\) instead of the control \(v\). In fact the function \(\chi^v\) and thus also Equation (3.6) do depend on \(v\) only indirectly via the adjoint \(p = p_h(v) = S_h^*(S_h v - z)\)

\[\left( I + \frac{1}{\alpha} \chi^v S_h^* S_h \right) v^+ = P_{[a,b]} \left( -\frac{1}{\alpha} p \right) + \frac{1}{\alpha} \chi^v \left( S_h^* z \right) . \]  \hspace{1cm} (3.8)

Now in each iteration the next full-step iterate \(v^+\) is computed from (3.8). If damping is necessary, one computes \(p^+_\lambda = p_h(v^+_\lambda)\) instead of \(v^+_\lambda\). In our (linear) setting the adjoint state \(p^+_\lambda\) simply is a convex combination of \(p = p_h(v)\) and \(p^+ = p_h(v^+)\)

\[p^+_\lambda = \lambda p^+ + (1 - \lambda)p ,\]

and unlike \(v^+_\lambda\) the adjoint state \(p^+_\lambda\) lies in the finite element space \(Y_h\). Thus only a set of additional nodes according to the jumps of the most recent full-step iterate \(v^+\) have to be managed, exactly as in the undamped case.

**Algorithm 3.7** (Dampened Newton-Algorithm). \(v \in U\) given.

Do until convergence

1. Solve Equation (3.8) for \(v^+\).
2. Compute \(p^+ = p_h(y_h(v^+))\).
3. Choose the damping-parameter \(\lambda\). (for example by Armijo line search)
4. Set \(p := p^+_\lambda = \lambda p^+ + (1 - \lambda)p\).

Algorithm 3.5 is identical to Algorithm 3.7 without damping (\(\lambda = 1\)).

**Remark 3.8.** The above algorithm is equivalent to a dampened Newton algorithm applied to the equation

\[p_h = S_h^* S_h P_{[a,b]} \left( -\frac{1}{\alpha} p_h \right) - S_h^* z , \quad u := P_{[a,b]} \left( -\frac{1}{\alpha} p_h \right) .\]
Another approach, leading to a globalization of Algorithm 3.5, is to use some globalized, fully discrete scheme and then perform Algorithm 3.5 as a post-processing step, compare also [9]. Suppose \( v_h \) is a discrete approximation to the optimal control \( u \), such that
\[
\| v_h - u \|_{L^2(\Omega)} = \mathcal{O}(h),
\]
and let \( u_{hh} \) be its variationally discretized counterpart solving (P_{hh}). Now, if the q-superlinear convergence of order \( \frac{3}{2} \) of the Newton algorithm is mesh independent (see Remark 3.4), then there exists a radius \( \delta \) and a mesh parameter \( h_0 > 0 \), such that inside the ball \( B_\delta(u_{hh}) \) and for \( h \leq h_0 \) the Newton iteration for \( G_h \) converges q-superlinearly of order \( \frac{3}{2} \) towards \( u_{hh} \).

Let \( \tilde{u}_{hh} \) be the second iterate of Algorithm 3.5 initialized with \( v_h \). Then, for sufficiently small \( h \), we have \( v_h \in B_\delta(\bar{u}_h) \) and thus
\[
\| \tilde{u}_{hh} - u \|_{L^2(\Omega)} \leq \| \bar{u}_h - u_{hh} \|_{L^2(\Omega)} + \| u_{hh} - u \|_{L^2(\Omega)} \leq \| v_h - u_{hh} \|_{L^2(\Omega)}^{\frac{3}{2}} + \mathcal{O}(h^2) = \mathcal{O}(h^2).
\]
This motivates Algorithm 3.9 (Post Processing).

Solve the fully discretized optimization problem.

Perform 2 steps of Algorithm 3.6.

### 3.5 Global Convergence of the undamped Newton Algorithm

It is not difficult to see, that the fixed-point equation for problem (P_{hh})
\[
u_{hh} = P_{[a,b]} \left( -\frac{1}{\alpha} S_h^* (S_h u_{hh} - z) \right)
\]
can be solved by simple fixed-point iteration that converges globally for \( \alpha > \| S_h \|_{L^2(\Omega),L^2(\Omega)} \), see [5, 6]. A similar global convergence result holds for the undamped Newton algorithm 3.5.

**Lemma 3.10.** The Newton algorithm 3.5 converges globally if \( \alpha > \frac{4}{3} \| S \|^2 \).

**Proof.** See [13].

### 4 Numerical examples

We end this paper by illustrating our theoretical findings by numerical examples. The first two examples are solved by Algorithm 3.5 i.e. Algorithm 3.7 without damping, making use of the global convergence property from Lemma 3.10. The third one involves a small parameter \( \alpha = 10^{-7} \) and is hence treated using the globalization strategy 3.7 with Armijo line search. Finally the globalization 3.9 is applied at multiple parameters \( \alpha \) and mesh parameters \( h \).

As stopping criterion we require \( \| P_{[a,b]}(-\frac{1}{\alpha} P^+_h) - \tilde{u}_h \|_{L^2(\Omega)} < 10^{-11} \) in Algorithm 3.7 using the a posteriori bound for admissible \( v \in U_{ad} \)
\[
\| v - \tilde{u}_h \|_{L^2(\Omega)} \leq \frac{1}{\alpha} \| \zeta \|_{L^2(\Omega)}, \quad \zeta(\omega) = \begin{cases} 
\alpha v + p_h(v) & \text{if } v(\omega) = a \\
\alpha v + p_h(v) & \text{if } v(\omega) = b \\
\alpha v + p_h(v) & \text{if } a < v(\omega) < b
\end{cases},
\]
presented in [8] and [10].
Example 4.1 (Dirichlet). We consider problem $(\mathbb{P})$ in (1.1) with controls $u \in L^2(\Omega)$ on the unit square $\Omega = (0,1)^2$ with $a \equiv 0.3$ and $b \equiv 1$. Further we set
\[ z = -4\pi^2\alpha \sin(\pi x) \sin(\pi y) + (S \circ i)r, \]where $r = \min \left(1, \max \left(0, 0.3 \sin(\pi x) \sin(\pi y)\right)\right)$. The choice of parameters implies a unique solution $\bar{u} = r$ to the continuous problem $(\mathbb{P})$.

Throughout this section, solutions to the state equation are approximated by continuous, piecewise linear finite elements on a quasiuniform triangulation $T_h$ with maximal edge length $h > 0$. The meshes are generated through regular refinement starting from the coarsest mesh.

As discussed in Section 2, problem $(\mathbb{P}_{hh})$ admits a unique solution $\bar{u}_h$ and we have
\[ \|\bar{u}_h - \bar{u}\|_{L^2(\Omega)} = O(h^2) \]
as $h \to 0$. There also holds nearly quadratic convergence in $L^\infty(\Omega)$
\[ \|\bar{u}_h - \bar{u}\|_{L^\infty(\Omega)} = O(\log(h) h^2) \]
for domains $\Omega \subset \mathbb{R}^2$, see [5]. Both convergence rates are observed in Table 1 that shows the $L^2$- and the $L^\infty$-errors together with the corresponding experimental orders of convergence
\[ EOC_i = \frac{\ln \text{ERR}(h_{i-1}) - \ln \text{ERR}(h_i)}{\ln(h_{i-1}) - \ln(h_i)} \]
for Example 4.1. Lemma 3.10 ensures global convergence of the undamped Algorithm 3.5 only for $\alpha > 1/(3\pi^4) \simeq 0.0034$, but it is still observed for $\alpha = 0.001$.

The algorithm is initialized with $v_0 \equiv 0.3$. The resulting number of Newton steps as well as the value of $\zeta/\alpha$ for the computed solution are also given in Table 1.

Figure 1 shows the Newton iterates, active and inactive sets are very well distinguishable, the jumps along their frontier can be observed.

Next we demonstrate another Example, our theory may also be applied to.

| mesh param. $h$ | $\text{ERR}$ | $\text{ERR}_\infty$ | $EOC$ | $EOC_\infty$ | Iterations | Quality |
|-----------------|-------------|------------------|--------|----------------|------------|---------|
| $\sqrt{2}/16$   | 2.5865e-03  | 1.2370e-02       | 1.95   | 1.79           | 4          | 2.16e-15|
| $\sqrt{2}/32$   | 6.5043e-04  | 3.2484e-03       | 1.99   | 1.93           | 4          | 2.08e-15|
| $\sqrt{2}/64$   | 1.6090e-04  | 8.1167e-04       | 2.02   | 2.00           | 4          | 2.03e-15|
| $\sqrt{2}/128$  | 4.0844e-05  | 2.1056e-04       | 1.98   | 1.95           | 4          | 1.99e-15|
| $\sqrt{2}/256$  | 1.0025e-05  | 5.3806e-05       | 2.03   | 1.97           | 4          | 1.69e-15|
| $\sqrt{2}/512$  | 2.5318e-06  | 1.3486e-05       | 1.99   | 2.00           | 4          | 1.95e-15|

Table 1: $L^2$- and $L^\infty$-error development for Example 4.1 (Dirichlet)
Table 2: Development of the error in Example 4.2 (Neumann)

| mesh param. $h$ | $ERR$     | $ERR_{\infty}$ | $EOC$ | $EOC_{\infty}$ | Iterations | Quality   |
|-----------------|-----------|-----------------|-------|-----------------|------------|-----------|
| $\sqrt{2}/16$   | 3.9866e-03| 1.1218e-02      | 1.94  | 1.74            | 3          | 1.81e-12  |
| $\sqrt{2}/32$   | 1.0025e-03| 3.2332e-03      | 1.99  | 1.79            | 3          | 2.31e-12  |
| $\sqrt{2}/64$   | 2.5188e-04| 8.4398e-04      | 1.99  | 1.94            | 3          | 9.74e-13  |
| $\sqrt{2}/128$  | 6.2936e-05| 2.1856e-04      | 2.00  | 1.95            | 3          | 9.37e-13  |
| $\sqrt{2}/256$  | 1.5740e-05| 5.5223e-05      | 2.00  | 1.99            | 3          | 8.91e-13  |
| $\sqrt{2}/512$  | 3.9346e-06| 1.3928e-05      | 2.00  | 2.00            | 3          | 8.86e-13  |

**Example 4.2** (Neumann). We next consider an elliptic problem with Neumann boundary conditions

$$-\Delta y + y = u \quad \text{in } \Omega,$$

$$\partial_n y = 0 \quad \text{on } \partial \Omega,$$

on $\Omega = (0, 1)^2$, with a similar discrete setting as in the previous example. It then is clear, how $(P)$ and $(P_{hh})$ have to be understood. We set $\alpha = 1$ and choose

$$z = -2(2\pi^2 + 1)\alpha \cos(\pi x) \cos(\pi y) + (S \circ i)r,$$

with $r = \min\left(1, \max\left(-1, 2 \cos(\pi x) \cos(\pi y)\right)\right)$ and bounds $a \equiv -1$ and $b \equiv 1$. The optimal control to the continuous problem is $\bar{u} = r$.

For $\alpha = 1$ the undamped iteration still converges globally, although the solution operator has norm $\|S\| = 1$ as an endomorphism in $L^2(\Omega)$. The predicted convergence properties and the stopping criterion are the same as above; Algorithm 3.7 is initialized by $v_0 \equiv -1$. The first four steps of the iteration are displayed in Figure 2 and the behaviour of the approximation error between the exact and the semidiscrete solution, as well as the number of iterations and the final value of $\zeta/\alpha$, is shown in Table 2.

The Algorithm has also been implemented successfully for parabolic discontinuous Galerkin discretized problems as well as elliptic problems with Lavrentiev-regularized state constraints.

To demonstrate Algorithm 3.7 with damping we again consider Example 4.1 this time with $\alpha = 10^{-7}$. We choose

$$MF(p) = \left\| p - S_h^* S_h P_{[a,b]} \left( -\frac{1}{\alpha} p \right) + S_h^* \nu \right\|^2_{L^2(\Omega)},$$

as merit function governing the step size of the algorithm. Again we use the same stopping criterion as in the previous examples.

Figure 2: The first steps of the Newton-algorithm for Example 4.2 (Neumann) with $\alpha = 1$. 

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Table 3: Development of the error in Example 4.1 (Dirichlet) for $\alpha = 10^{-7}$.

Table 3 shows errors and the number of iterations for different mesh parameters $h$ at a smoothing parameter $\alpha = 10^{-7}$. To compare the number of iterations we choose a common initial guess $u_0 \equiv 1$. The number of iterations appears to be independent of $h$.

Finally, to demonstrate the efficiency of Algorithm 3.9, the EOC in the $L^2(\Omega)$-norm is plotted in Table 4. The disturbances that can be observed for smaller parameter $\alpha$ indicate the decay of the environment of q-superlinear convergence with decreasing $\alpha$.

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