Globalization of Nonsmooth Newton Methods for Optimal Control Problems

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Abstract We present a new approach for the globalization of the primal-dual active set or equivalently the nonsmooth Newton method applied to an optimal control problem. The basic result is the equivalence of this method to a nonsmooth Newton method applied to the nonlinear Schur complement of the optimality system. Our approach does not require the construction of an additional merrit function or additional descent direction. The nonsmooth Newton directions are naturally appropriate descent directions for a smooth dual energy and guarantee global convergence if standard damping methods are applied.

1 Introduction

We consider the optimal control problem of minimizing the functional

$$\mathscr{J}(y,u) = \frac{1}{2}\|y-y_d\|_0^2 + \frac{\alpha}{2}\|u\|_0^2$$

subject to the constraints

$$u \leq \psi \qquad \text{and} \qquad -\Delta y = u$$

where the state y and the control u are from suitable function spaces on the domain Ω and $\|\cdot\|_0$ denotes the $L^2(\Omega)$-norm.

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It turned out that semismooth or nonsmooth Newton methods and interior point methods are amongst the most efficient techniques to deal with this kind of problem. Interior point methods ([2, 10] ...) regularize the problem by a sequence of barrier functions to overcome the nonsmoothness inherited by the inequality constraints.

Nonsmooth Newton methods introduced in [8, 7, 9] solve such problems directly by certain linearizations of nonsmooth operators. These methods have the advantage that no regularization parameter has to be controlled. They differ in the nonsmooth operator used to incorporate the inequality constraints and in the concept of differentiability and semismoothness used to get linearizations and convergence results. There are finite dimensional ([1, 6, 5] ...) as well as infinite dimensional ([11, 6] ...) approaches. The convergence results are in general only local and globalization is tackled by the construction of merrit function and descent directions for these functions if the Newton directions fail.

The approach used in [6] is shown to be equivalent to the primal-dual active set method and a global convergence result is obtailed. However, this does only hold under restrictive assumptions on α and in case of exact solution of the linear subproblems. In [5] the nonsmooth Newton idea is applied to a discrete dual minimization problem. Thus the nonsmooth Newton directions are natural descent directions an global convergence is achived by damping bases on the dual energy. This paper shows that the methods in [6] and [5] basically coincide. Hence [5] offers a natural way to globalize the method of [6].

The paper is organized as follows. In Section 2 various reformulations of the problem are presented. Sections 3 and 4 recall the methods of [6] and [5] respectively. Finaly the equivalence of both methods is shown in Section 5.

2 An Optimal Control Problem

Using Green's formula and appropriate Sobolev spaces the above problem can be formulated in weak form as

$$(\mathscr{M}) \begin{cases} \text{Find } (y,u) \in H_0^1(\Omega) \times L^2(\Omega) \text{ such that} \\ \qquad\qquad \mathscr{J}(y,u) \le \mathscr{J}(w,v) \\ \text{s.t.} \quad u \in \mathscr{K}, \quad (\nabla y, \nabla v) = (u,v) \quad \forall v \in H_0^1(\Omega) \end{cases}$$

with the convex set $\mathscr{K} = \{v \in L^2(\Omega) : v \le \psi \text{ a.e in } \Omega\}$.

From now on we consider a corresponding discrete problem. Since we will not discuss the discretization itself but the solution of the arising algebraic problem this problem is formulated in terms of vectors and matrices instead of discrete function spaces. Furthermore, to simplify notation we use $y \in \mathbb{R}^m$ and $u, \psi \in \mathbb{R}^n$ as well for the discrete approximations of the state, the control and the obstacle respectively. The discrete analog of $(\mathscr{M})$ then reads:

$$
\text{(M)}\quad \begin{cases} \text{Find } (y,u) \in \mathbb{R}^m \times \mathbb{R}^n \text{ such that} \\ \qquad\qquad J(y,u) \le J(w,v) \\ \text{s.t.} \qquad u \in K, \qquad Ly = Iu \end{cases}
$$

with the discrete convex set $K = \{v \in \mathbb{R}^n : v \le \psi\}$ and the discrete convex energy

$$
J(y,u) = \frac{1}{2}\langle D_1 y, y\rangle + \frac{\alpha}{2}\langle D_2 u, u\rangle - \langle b, y\rangle
$$

$b \in \mathbb{R}^m$ is a discrete approximations of the linear functional $(y_d, \cdot)$ incorporating the desired state y_d. The vectors y and u may have different dimensions since they will in general come from different discrete spaces. In the following we assume that D_1 and D_2 are symmetric and positive definite and L is assumed to be invertible. These assumptions are matched e.g. if $(\mathscr{M})$ is discretized by piecewise linear finite elements. Notice that D_1, D_2 and I are discrete analogs of the identity operator. For a finite element discretization they represent discrete L^2 inner products coupling functions from possibly different finite element spaces. Hence the matrices might differ in general.

Analogously to the continuous case the optimality system is given by

$$
\text{(S)}\quad \begin{cases} \text{Find } (y,u,w) \in \mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^m \text{ such that} \\ \begin{pmatrix} D_1 & 0 & L^T \\ 0 & \alpha D_2 + \partial\chi_K & -I^T \\ L & -I & 0 \end{pmatrix} \begin{pmatrix} y \\ u \\ w \end{pmatrix} \ni \begin{pmatrix} b \\ 0 \\ 0 \end{pmatrix}. \end{cases}
$$

The elimination of the state $y(u) = L^{-1}Iu$ leads to a reduced problem

$$
u \in K : \qquad \tilde{J}(u) \le \tilde{J}(v) \qquad \forall v \in K
$$

with the energy $\tilde{J}(u) := J(L^{-1}Iu, u)$. Its optimality system is given by

$$
\text{(PD)}\quad \begin{cases} \text{Find } (u,\lambda) \in \mathbb{R}^n \times \mathbb{R}^n \text{ such that} \\ \qquad Au + \lambda = f \\ \qquad u \le \psi,\ \lambda \ge 0, \lambda(u-\psi) = 0 \end{cases}
$$

with $A = (L^{-1}I)^T D_1 (L^{-1}I) + \alpha D_2$ and $f = (L^{-1}I)^T b$.

3 Primal-Dual Active Set Method

The primal-dual active set method for the discrete problem is based on the primal-dual formulation (PD). For given $u^0, \lambda^0 \in L^2(\Omega)$ it reads:

Algorithm 3.1

1. *Set* $\mathscr{A}_k = \{i : \lambda_i^k + c(u_i^k - \psi_i) > 0\}$ *and* $\mathscr{I}_k = \{1,\dots,n\} \setminus \mathscr{A}_k$
2. *Solve*

$$Au^{k+1} + \lambda^{k+1} = f,$$

$$u_i^{k+1} = \psi_i \text{ for } i \in \mathscr{A}_k, \quad \lambda_i^{k+1} = 0 \text{ for } i \in \mathscr{I}_k.$$

In [6] it is shown that the method can be interpreted as semismooth Newton method and that the following convergence results hold.

Theorem 1 (cf. [6]). *The sequence* (u^k, λ^k) *generated by algorithm 3.1 converges superlinearly to the solution* (u^*, λ^*) *of* (PD) *if* $\|(u^0, \lambda^0) - (u, \lambda)\|$ *is sufficiently small. Furthermore, it converges for arbitrary* (u^0, λ^0) *if A is the sum of an M-matrix and a sufficiently small perturbation matrix. For the case of a discretized control problem the latter is the case if* α *is small enough.*

Unfortunately global convergence is in general not preserved if α is to small or if the linear systems are solved inexactly. A similar result holds also in the infinite dimensional case (cf. [6]).

4 Schur Complement Nonsmooth Newton

Another approach for the solution of the discrete algebraic problem introduced in [5] is based on the elimination of the primal unknowns in (S) by

$$\begin{pmatrix} y(w) \\ u(w) \end{pmatrix} := \begin{pmatrix} D_1 & 0 \\ 0 & \alpha D_2 + \partial \chi_K \end{pmatrix}^{-1} \begin{pmatrix} b - L^T w \\ I^T w \end{pmatrix}. \tag{1}$$

Similar to linear saddle point problems (S) can be equivalently formulated as unconstrained minimization problem

$$(\mathrm{M}^*) \begin{cases} \text{Find } w \in \mathbb{R}^n \text{ such that} \\ \qquad h(w) \le h(v) \qquad \forall v \in \mathbb{R}^n. \end{cases}$$

with the energy

$$h(w) = -\mathscr{L}(y(w), u(w), w) \tag{2}$$

where $\mathscr{L} : \mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^m$ is the Lagrange functional associated with the saddle point problem (S) given by

$$\mathscr{L}(y,u,w) = \frac{1}{2}\langle D_1 y, y\rangle + \frac{\alpha}{2}\langle D_2 u, u\rangle + \chi_K(u) - \langle b, y\rangle + \langle Ly - Iu, w\rangle. \tag{3}$$

Proposition 1 (cf. [5]). *The energy h defined by* (2) *is strictly convex, coercive, and continuously differentiable. Its gradient is given by the Lipschitz continuous operator*

$$\nabla h(w) = -(Ly(w) - Iu(w)).$$

This operator is also denoted the nonlinear Schur complement operator of (S).

Using these properties descent algorithms of the form

$$w^{k+1} = w^k + \rho^k d^k \tag{4}$$

with appropriate descent directions d^k and step sizes ρ^k can be applied to solve (M*). Choosing $d^k = -\nabla h(w^k)$ leads to the gradient method which is equivalent to a nonlinear Uzawa method ([3], [4]) applied to (S). Since ∇h is Lipschitz continuous a nonsmooth Newton approach is used to obtain linearizations S_k of ∇h at w^k leading to the (damped) nonsmooth Newton method:

Algorithm 4.1

1. *Solve* $d^k = -S_k^{-1}\nabla h(w^k)$
2. *Set* $w^{k+1} = w^k + \rho^k d^k$

The linearizations S_k of the Schur complement ∇h at w^k are given by

$$S_k = LD_1^{-1}L^T + I\widehat{D}_2(w^k)I^T$$

where $\widehat{D}_2(w^k)$ is the linearization of $(\alpha D_2 + \partial\chi_K)^{-1}$ constructed by

$$\widehat{D}_2(w^k) = T_{\overline{\mathscr{A}}_k}\left(I - T_{\overline{\mathscr{A}}_k} + T_{\overline{\mathscr{A}}_k}\alpha D_2 T_{\overline{\mathscr{A}}_k}\right)^{-1} T_{\overline{\mathscr{A}}_k}$$

using the projection

$$(T_{\overline{\mathscr{A}}_k})_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } i \notin \overline{\mathscr{A}}_k \\ 0 & \text{else} \end{cases}$$

associated with the active set

$$\overline{\mathscr{A}}_k = \{i : u(w_k)_i = \psi_i\}.$$

Its easy to see that these directions are descent directions i.e. $\langle d^k, \nabla h(w^k)\rangle < 0$ if $\nabla h(w^k) \neq 0$. The selected step sizes should guarantee sufficient descent. This can be achieved by selecting them using the Armijo rule or bisection such that they are *efficient*, i.e. they satisfy

$$\exists C > 0\,\forall k: \qquad h(w^k + \rho^k d^k) \leq h(w^k) - C\left(\frac{\langle \nabla h(w^k), d^k\rangle}{\|d^k\|}\right)^2. \tag{5}$$

Having the descent property the following convergence result can be obtained.

Theorem 2 (cf. [5]). *Assume that the stepsizes ρ^k are efficient. Then the sequence generated by algorithm 4.1 converges to the solution w^* of* (M*) *for arbitrary initial iterates w^0.*

This convergence result is in general preserved if inexact evaluation of S_k^{-1} is considered.

Algorithm 4.2

1. *Solve* $\tilde{d}^k = -S_k^{-1}\nabla h(w^k) + \varepsilon^k$
2. *Set* $w^{k+1} = w^k + \rho^k \tilde{d}^k$

Theorem 3 (cf. [5]). *Assume that the step sizes* ρ^k *are efficient, that the vectors* $\tilde{d}^k$ *are descent directions, and that* $\|\varepsilon^k\|/\|\tilde{d}^k\| \to 0$ *Then the sequence generated by algorithm 4.2 converges to the solution* w^* *of* (M^*) *for arbitrary initial iterates* w^0.

It is easy to see that these convergence results also hold if the S_k are replaced by preconditioners $\overline{S}_k$ defined analogously using the smaller active sets

$$\overline{\overline{\mathscr{A}}}_k = \left\{i : (\alpha D_2 u(w_k))_i \neq (I^T w_k)_i\right\} \subset \overline{\mathscr{A}}_k.$$

Remark 1. Each damping startegy requires the evaluation of either h or ∇h possibly multiple times. These evaluations incorporate the solution of the nonlinear convex problem in (1). However, solving this problem is in general very cheap since D_2 represents the L^2 inner produkt or the identity and not a differential operator. Thus a nonlinear Gauß-Seidel method will converge to machine accuracy in a few steps.

5 Globalization of Primal-Dual Active Set Method

Now we analyze the relation between the presented methods. In the following let (u^k, λ^k) the sequence generated by algorithm 3.1. Defining the sequences

$$y^k = L^{-1} I u^k, \qquad w^k = L^{-T} b - L^{-T} D_1 L^{-1} I u^k$$

the multiplier is given by

$$\lambda^{k+1} = I^T w^{k+1} - \alpha D_2 u^{k+1} \tag{6}$$

and the linear system in algorithm 3.1 is equivalent to

$$\begin{pmatrix} D_1 & 0 & L^T \\ 0 & T_{\mathscr{I}_k} + T_{\mathscr{A}_k}\alpha D_2 & T_{\mathscr{A}_k}(-I^T) \\ L & -I & 0 \end{pmatrix} \begin{pmatrix} y^{k+1} \\ u^{k+1} \\ w^{k+1} \end{pmatrix} = \begin{pmatrix} b \\ T_{\mathscr{I}_k}\psi \\ 0 \end{pmatrix}. \tag{7}$$

A simple computation shows that the constant c in the definition of the active set drops out after the first iteration. More precisely using (6) we have

Lemma 1. *Let* $k > 0$ *then* $\mathscr{A}_k$ *can be equivalently defined by*

$$\mathscr{A}_k = \left\{ i : (I^T w^k - \alpha D_2 u^k)_i + c_i(u_i^k - \psi_i) > 0 \right\}$$

for any $c_i > 0$.

Proof. Since $k > 0$ each index i is either in $\mathscr{A}_{k-1}$ or in $\mathscr{I}_{k-1}$. Hence $(u_i^k - \psi_i)$ or $(I^T w^k - \alpha D_2 u^k)_i = \lambda_i^k$ must be zero. Therefore the sum is positive iff one of these expressions is positive. Having $c, c_i > 0$ it is clear that

$$c(u_i^k - \psi_i) > 0 \Leftrightarrow (u_i^k - \psi_i) > 0 \Leftrightarrow c_i(u_i^k - \psi_i) > 0.$$

The definition of $\mathscr{A}_k$ is closely related to the Euclidean projection which differs from the projection with respect to D_2 if it is not diagonal. However, we need this projection in the following since it is the proper discrete analog of the continuous L^2-projection. Therefore we assume

(A) D_2 is a diagonal matrix.

This is not very restrictive since (A) holds if u is discretized by finite differences, by piecewise constant finite elements, or by piecewise linear finite elements using mass lumping for D_2.

Using (A) and lemma 1 with $c_i = (\alpha D_2)_{ii}$ we get

Lemma 2. *Let* $k > 0$ *then*

$$\mathscr{A}_k = \left\{ i : (\alpha D_2 u(w_k))_i \neq (I^T w_k)_i \right\}.$$

By this representation $u(w^k)$ can be expressed by a linear equation depending on the active set $\mathscr{A}_k$. Thus from (7) we get

$$\begin{pmatrix} D_1 & 0 & L^T \\ 0 & T_{\mathscr{I}_k} + T_{\mathscr{A}_k} \alpha D_2 T_{\mathscr{A}_k} & -T_{\mathscr{A}_k} I^T \\ L & -I T_{\mathscr{A}_k} & 0 \end{pmatrix} \begin{pmatrix} y^{k+1} - y(w^k) \\ u^{k+1} - u(w^k) \\ w^{k+1} - w^k \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \nabla h(w^k) \end{pmatrix}. \tag{8}$$

Here we used the fact that $u^{k+1} - u(w^k) = T_{\mathscr{A}_k}(u^{k+1} - u(w^k))$. By this representation we instantly get the main result:

Theorem 4. *Assume that assumption (A) holds. For* $k > 0$ *algorithm 3.1 is equivalent to the iteration*

$$w^{k+1} = w^k \underbrace{- \overline{S}_k^{-1} \nabla h(w^k)}_{d^k} \tag{9}$$

with the symmetric, positive definite preconditioner

$$\overline{S}_k = L D_1^{-1} L^T + I T_{\overline{\mathscr{A}}_k} \left(I - T_{\overline{\mathscr{A}}_k} + T_{\overline{\mathscr{A}}_k} \alpha D_2 T_{\overline{\mathscr{A}}_k} \right)^{-1} T_{\overline{\mathscr{A}}_k} I^T$$

in the sense that (y^k, u^k) *is computed from* w^k *using* (7)*. Thus global convergence of this descent method can be achieved by introducing appropriate damping parameters* ρ^k *in* (9) *even in the case of inexact evaluation in the sense of theorem 3.*

Proof. (9) follows from (8) by elimination of the state and control variables. The convergence results are direct consequences of theorem 2 and theorem 3.

Remark 2. Theorem 4 shows that the primal-dual active set method and the (undamped) Schur complement nonsmooth Newton method applied to control problems basically coincide. The interpretation as descent method provides a natural way to globalize the method using damping even in the case of inexact solution of the linear systems. Notice that no artificial merrit function and descent directions have to be contructed if this approach is used.

Remark 3. The above result does not carry over to the continuous problem. Since the natural embedding $\mathscr{I} : H_0^1(\Omega) \to H_0^1(\Omega)'$ is not invertible the elimination of the state used in (1) is in general only possible in a suitable subspace. In this subspace algorithm 4.2 can also be defined in the infinite dimensional case. However, the convergence theory given in [5] is no longer applicable.

This might suggest that the convergence gets slower for larger discrete problems. The numerical results presented in [5] seem contradict this conjecture even in the case that damping is applied. Extension of the ideas to the infinite dimensional case is the topic of current research.

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