A PROSPECTIVE LOOK AT SQP METHODS FOR SEMILINEAR PARABOLIC CONTROL PROBLEMS

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1 Introduction

In this paper we present different optimization methods which can be used to solve optimal control problems with nonlinear parabolic differential equations. In particular, we want to show how more sophisticated methods can be implemented for these problems.

We consider the following optimization problem in infinite dimensions as the framework in which we present various algorithms:

$$\min f(x) \text{ s.t. } h(x) = 0 \tag{1.1}$$
$$f : X \to I\!R,\ h : X \to Z,$$

where X is a real Hilbert space and Z is a Banach space. Quite some progress has been made in the past few years in the analysis of quasi-Newton methods for infinite-dimensional problems. This includes recently also SQP methods and later we want to focus on some of these new results.

In Section 2 we introduce a decoupling of variables which is typical for control problems because the unknowns separate into state and control. We start our tour of optimization algorithms with brief comments on the gradient method, Newton's method and the BFGS method as a representative of the family of quasi-Newton methods [6]. In all the previous methods we view the state as a dependent variable so that the minimization is only with respect to the control. While this viewpoint is the correct one with regard to storage it has its disadvantages because each gradient evaluation for some control requires the computation of the corresponding state. In our application this means the solution of a nonlinear boundary value problem.

SQP (Sequential Quadratic Programming) methods, see e.g. [15], have turned out to be one of the most successful methods in nonlinear optimization. Here the nonlinear equality constraint is linearized at each iteration and a quadratic approximation of the Lagrangian is minimized. Since the calculation of second derivatives is very expensive quasi-Newton updates for the Hessian of the Lagrangian are commonly used. This, however, causes some difficulty since the positive definiteness of this Hessian can only be guaranteed on a subspace. Another drawback is the large dimension of the space of discretized variables which includes both states and controls. These two disadvantages of the full SQP method lead us to consider reduced SQP methods. They have the advantage that the requirement on positive definiteness is in line with the second order sufficiency condition and that the update is carried out in the control space.

In the third section we consider a semilinear parabolic differential equation

$$\begin{array}{rcll} y_t(t,x) & = & (\Delta y)(t,x) + c(t,x,y(t,x)) & t \in (0,T), \quad x \in \Omega \\ y(0,x) & = & y_0(x) & x \in \Omega \\ \frac{\partial y}{\partial n}(t,\xi) & = & g(\xi)u(t) & t \in (0,T), \quad \xi \in \Gamma \end{array} \tag{1.2}$$

and minimize

$$\int_0^T \int_\Omega l(t,x,y(t,x))\, dx\, dt + \int_0^T k(t,u(t))\, dt. \tag{1.3}$$

We are led by the objective to introduce the reader to modern methods in optimization and to show for an optimal control problem with a nonlinear partial differential equation how these methods can be implemented. It is not our goal in this paper to justify rigorously all the assumptions. This is by all means no trivial task and currently under research as well as the actual numerical computation. One can formulate the nonlinear partial differential equation as an integral equation in a Banach space, see e.g. [17], compute derivatives and adjoints which we interpret as classical solutions with data sufficiently smooth. It is conceivable that one remains during the iteration in spaces with smooth controls and states, if one starts in these spaces. The problem with this approach is that the convergence theory and conditions of second order sufficiency usually require a Hilbert space framework so that one cannot use any of the Banach spaces in [16].

The use of SQP methods in their reduced version with a quasi-Newton update presents a new approach to an efficient solution of (1.2) and (1.3). In this paper we formulate reduced SQP methods in a framework of separable variables which is well suited for optimal control problems. This setting suggests to use a representation of the nullspace of h' which is nonstandard in the reduced SQP context. We interpret each step in the iteration of the reduced SQP method for the control problem and give the corresponding initial-boundary value problems which need to be solved.

The last section reviews some of the convergence results for the different algorithms. The various statements which describe local convergence properties give the reader some insight why one tends to prefer certain methods over others. This section includes recent results on the convergence of reduced SQP methods in infinite dimensions [11].

2 General Optimization Methods

In this section we discuss various optimization algorithms which include those that are commonly used for control problems and others which are not so well known in the control community.

We treat optimal control problems as infinite-dimensional optimization problems with equality constraints as defined in (1.1). The point $\hat{x}$ denotes the solution of the problem and capital letters with an asterisk are used for the adjoints of linear bounded operators and for dual spaces. Furthermore, Hilbert spaces will be identified with their duals. Let f and h be twice Fréchet-differentiable and let the Lagrangian of the problem be defined in the following way

$$L(x,l) = f(x) - l(h(x)) \quad , \quad x \in X \, , \, l \in Z^*.$$

Since some of the algorithms use linearized constraints we make a few comments about the linearization of h. Assume that each element of the nullspace of $h'(x)$ is the image of

a linear bounded operator $T = T(x)$:

$$\begin{aligned} \mathcal{N}(h'(x)) &= \{p \in X : h'(x)p = 0\} = \{T(x)w : w \in W\} = \mathcal{R}(T(x)), \\ & x \in X,\ T(x) \in \mathcal{L}(W, X),\ W \text{ real Hilbert space.} \end{aligned}$$

In the finite-dimensional case $T(x)$ is any matrix providing a basis for the nullspace of the gradients of the constraints and also for our infinite-dimensional application this representation of the kernel is easily verified.

In control problems one usually distinguishes between the control variables and the state variables. Therefore, we assume that $X = Y \times U$ is a product space with Hilbert spaces Y and U, $x = (y, u)$ and $Z = Y$. We have

$$h'(y,u)(\bar{y},\bar{u}) = h_1(y,u)\bar{y} + h_2(y,u)\bar{u}\,,$$

where $h_1(y,u) \in \mathcal{L}(Y)$ and $h_2(y,u) \in \mathcal{L}(U,Y)$ are the partial derivatives with respect to y and u. Provided h_1 is bijective, each element of the nullspace can be expressed as follows:

$$(\bar{y},\bar{u}) \in \mathcal{N}(h'(y,u)) \quad \Leftrightarrow \quad (\bar{y},\bar{u}) = (-h_1(y,u)^{-1}h_2(y,u)\bar{u}, \bar{u}).$$

This allows the following natural choice for the operator T which is typical for problems with separable variables

$$T(y,u) = (-h_1(y,u)^{-1}h_2(y,u), I) \in \mathcal{L}(U, Y \times U) \text{ and } W = U. \tag{2.1}$$

The separability of variables can also be used directly to reduce the dimension of the problem. However, one has to assume that for each $u \in U$ there exists a unique $y = S(u) \in Y$ such that $h(y,u) = h(S(u),u) = 0$, where, in general, S is a nonlinear operator. Then the original problem can be treated as an unconstrained problem in the variable u:

$$\min_{u \in U} f(S(u),u) = \varphi(u) \quad , \quad \varphi : U \to \mathbb{R}.$$

One iteration of the gradient method is defined in the following way

$$u^+ = u - \alpha\varphi'(u)\,,$$

where $\alpha \in \mathbb{R}$ is chosen from some stepsize rule. In the following the current and the next iterate are denoted by u and u^+, respectively.

In order to compute φ' which is just the reduced gradient of the original constrained problem note that by the implicit function theorem $S'(u)$ is given by

$$S'(u) = -h_1(S(u),u)^{-1}h_2(S(u),u)$$

and with (2.1) for $\nu \in U$

$$\begin{aligned} \varphi'(u)\nu &= f_1(S(u),u)S'(u)\nu + f_2(S(u),u)\nu \\ &= f'(S(u),u)(T(S(u),u)\nu). \end{aligned} \tag{2.2}$$

Therefore

$$\varphi'(u) = T(S(u),u)^* f'(S(u),u)\,. \tag{2.3}$$

Hence, one iteration of a gradient method is of the following form

Algorithm 1 (Gradient Method)

$$u^+ = u - \alpha T(S(u),u)^* f'(S(u),u).$$

All gradient type methods are known for a rather robust behavior initially but in the final phase they tend to converge at a very slow rate. In this situation one likes to switch to faster methods like Newton's method. An iteration is given by

Algorithm 2 (Newton's Method)

$$\begin{aligned} \varphi''(u)\Delta u &= -T(S(u),u)^* f'(S(u),u) \\ u^+ &= u + \Delta u. \end{aligned}$$

The major problem with Newton's method for optimal control problems is the computation of the step, which involves exact second order information of the objective function. Obviously, the differentiation of (2.3) is a very difficult task numerically and theoretically. In order to avoid an expensive calculation of φ'' one can use a quasi-Newton method instead. Here the second derivative of φ is approximated by operators $B \in \mathcal{L}(U)$ which are updated after each calculation of the step. Hence an iteration has the following form in general

$$u^+ = u - B^{-1}\varphi'(u).$$

One iteration for the BFGS algorithm looks as follows, if we take into account the structure of separable variables

Algorithm 3 (BFGS Method)

$$\begin{aligned} B\Delta u &= -T(S(u),u)^* f'(S(u),u) \\ u^+ &= u + \Delta u \\ \eta &= T(S(u^+),u^+)^* f'(S(u^+),u^+) - T(S(u),u)^* f'(S(u),u) \\ B_+ &= B + \frac{\eta \otimes \eta}{<\eta, \Delta u>} - \frac{(B\Delta u) \otimes (B\Delta u)}{<\Delta u, B\Delta u>} \in \mathcal{L}(U), \end{aligned}$$

where $u \otimes v$ denotes the outer product in U.

Another approach to equality constrained optimization consists of a quadratic approximation of the Lagrangian and, at the same time, a linearization of the constraint. In this framework we are required to solve only a linear equation for the constraint per iteration as opposed to the solution of a nonlinear equation (computation of $S(u)$) for the methods considered previously. Methods of this type are called SQP (Sequential Quadratic Programming) methods . It can be shown under weak assumptions that the SQP-step can be decomposed into a restoration step and a minimization step which leads to the following representation of a full SQP-step

$$\begin{aligned} (y^+,u^+) - (y,u) = & -T(y,u)[T(y,u)^* M T(y,u)]^{-1} T(y,u)^* [f'(y,u) - MR(y,u)h(y,u)] \\ & -R(y,u)h(y,u). \end{aligned}$$

Here $M \in \mathcal{L}(X)$ is an approximation to the Hessian of the Lagrangian and $R(y,u) \in \mathcal{L}(Y,X)$ is an arbitrary right-inverse of $h'(y,u)$, i.e. $h'(y,u)R(y,u)v = v$ for all $v \in Y$. Obviously,

$$R(y,u) = (h_1(y,u)^{-1}, 0) \tag{2.4}$$

is a right-inverse of h', where the second component is the null-operator in $\mathcal{L}(Y,U)$.

Using the definitions (2.4) and (2.1) for R and T, the SQP-step can be written in the following way:

$$\begin{aligned}(y^+,u^+) - (y,u) &= T(y,u)\Delta u - R(y,u)h(y,u) \\ &= (-h_1(y,u)^{-1}h_2(y,u)\Delta u - h_1(y,u)^{-1}h(y,u), \Delta u) \\ &= (-h_1(y,u)^{-1}(h_2(y,u)\Delta u + h(y,u)), \Delta u)\ ,\end{aligned}$$

where Δu is the solution of

$$T(y,u)^*MT(y,u)\Delta u = -T(y,u)^*[f'(y,u) - MR(y,u)h(y,u)].$$

This leads to the following iteration of a full SQP method

Algorithm 4 (Full SQP Method)

$$\begin{aligned}T(y,u)^*MT(y,u)\Delta u &= -T(y,u)^*[f'(y,u) - MR(y,u)h(y,u)] \\ h_1(y,u)\Delta y &= -h_2(y,u)\Delta u - h(y,u) \\ u^+ &= u + \Delta u \\ y^+ &= y + \Delta y \\ M_+ &= M + Update \in \mathcal{L}(X).\end{aligned}$$

Issues of full SQP methods for finite-dimensional problems are discussed in [15]. We have not specified an update for M because we will see later that this method is not suitable for control problems with a 'large' state space. Also, standard secant updates are excluded unless one makes the strong assumption that the Hessian of the Lagrangian is positive definite on the entire space.

An alternative to the restrictive assumption of requiring $L''_{(y,u)}(\hat{y},\hat{u},\hat{l})$ positive definite is the application of a reduced SQP method. In this case the last part of the minimization step in the SQP-Newton-step is dropped and the remaining reduced Hessian $T(y,u)^*L''_{(y,u)}T(y,u)$ is approximated by an operator $B \in \mathcal{L}(U)$. This yields the reduced SQP-step

$$(y^+,u^+) - (y,u) = -T(y,u)B^{-1}T(y,u)^*f'(y,u) - R(y,u)h(y,u). \tag{2.5}$$

This approach can be motivated from the case of linear constraints where all iterates generated by an SQP method are feasible, except possibly the starting point. Hence $h(y,u)$ vanishes after the first iteration. Therefore the full SQP-step is identical with the reduced SQP-step, if $B = T(y,u)^*MT(y,u)$.

For finite-dimensional problems there is special emphasis on a particular choice for R and T in (2.5) namely R is the Moore-Penrose pseudoinverse of h' and T is an orthonormal basis, taken from a smooth QR-decomposition , see [4], [12] and [3]. The

general reduced SQP method (2.5) was investigated by [8] and with modifications by [9]. Moreover, it is well known for the finite-dimensional case that the cancellation of the term $T(y,u)^*MR(y,u)h(y,u)$ in the SQP-step results in a loss of the q-superlinear convergence. In general only a two-step q-superlinear rate can be achieved for reduced methods which is only a slight disadvantage.

Apart from the fact that it is reasonable to approximate only the positive definite portion of the Hessian, the resulting savings in storage is another characteristic advantage of reduced over full SQP methods. The importance of this property becomes even more evident in infinite-dimensional applications. In the full SQP method we have to update the operator M which is defined on the whole space $X = Y \times U$. If the dimension of the discretized state space Y is considerably higher than that of the control space U, the savings in storage can be enormous when a reduced method is used. In the next section this will be demonstrated for a parabolic boundary control problem.

On the other hand, we should mention that a reduced secant method in the formulation below needs two gradient evaluations at each iteration. For the semilinear parabolic control problem studied in the next section this means the solution of four linear initial-boundary value problems. We could avoid the second gradient evaluation by using (y^+, u^+) in the definition of η, however, we are not able to retain superlinear convergence in this case. The additional gradient evaluation at the intermediate point $(y,u)+T(y,u)\Delta u$ can be seen in the following iteration of a reduced SQP method

Algorithm 5 (Reduced SQP Method)

$$
\begin{aligned}
B\Delta u &= -T(y,u)^* f'(y,u) \\
h_1(y,u)\Delta y &= -h_2(y,u)\Delta u - h(y,u) \\
u^+ &= u + \Delta u \\
y^+ &= y + \Delta y \\
\eta &= T((y,u)+T(y,u)\Delta u)^* f'((y,u)+T(y,u)\Delta u) - T(y,u)^* f'(y,u) \\
B_+ &= B + \frac{\eta \otimes \eta}{<\eta, \Delta u>} - \frac{(B\Delta u)\otimes(B\Delta u)}{<\Delta u, B\Delta u>}.
\end{aligned}
$$

At this point it should also be noted that with the separability approach we circumvent a problem which occurs often when reduced methods are studied in a finite-dimensional context. From the above definition of the right-inverse and the operator T we can immediately deduce that R and T have the same smoothness properties as h'. Therefore, under standard smoothness assumptions for f and h we do not encounter the difficulty with the Lipschitz-continuity of $T(y,u)$ which appears when T is chosen as orthonormal basis obtained from a QR-decomposition of the Jacobian of the constraints , see [5].

Let us summarize the arguments which give the motivation for the application of reduced SQP methods to parabolic boundary control problems. First they are reasonable since in general only the reduced Hessian is positive definite at the solution. This allows the use of secant update formulas maintaining positive definiteness. Furthermore, a fast convergence rate can be achieved and the reduction to the control space results in a significant decrease in storage. Moreover, the natural nullspace representation of h' leads to Lipschitz-continuity of $T(y,u)$. Finally, the linearization of the constraint results in the solution of a linear equation as opposed to a nonlinear one in Algorithms 1–3.

3 Optimization Methods for Optimal Control Problems

In this section we want to consider the problem of controlling the semilinear parabolic differential equation through the boundary

$$\begin{array}{rcll} y_t(t,x) &=& (\Delta y)(t,x) + c(t,x,y(t,x)) & t \in (0,T), \quad x \in \Omega \\ y(0,x) &=& y_0(x) & x \in \Omega \\ \frac{\partial y}{\partial n}(t,\xi) &=& g(\xi)u(t) & t \in (0,T), \quad \xi \in \Gamma \end{array} \tag{3.1}$$

where Ω is a bounded domain in $\mathbb{R}^n$ with sufficiently smooth boundary Γ. The nonlinear function $c : [0,T] \times \bar{\Omega} \times \mathbb{R} \to \mathbb{R}$ is smooth and $g \in C(\Gamma)$ is fixed. The objective is to find u such that

$$\int_0^T \int_\Omega l(t,x,y(t,x))\, dx\, dt + \int_0^T k(t,u(t))\, dt \tag{3.2}$$

is minimized. The nonlinear functions l and k are also assumed to be smooth. We denote by k_u, l_y, c_y the derivatives with respect to the second and third variable, respectively.

In the preceding paragraph we presented various methods to solve optimal control problems. The goal of this section is to demonstrate the advantage of a reduced SQP method in particular for the parabolic boundary control problem (3.1), (3.2). Since this method requires a number of technical details we concentrate on the derivation of the method and not on the setup of the spaces, existence of optimal controls and solutions of the semilinear parabolic differential equation and Fréchet- differentiability. As mentioned in the introduction the latter is not a simple verification, e.g. by using a semigroup approach, but requires more work which is under investigation by the authors.

Let $U = U[0,T]$ denote the function space for the controls and $Y = Y([0,T] \times \Omega)$ the function space for the states. In the setup of the previous section the variables are $(y,u) \in Y \times U$. We consider the linearized constraint and compute its representation of the nullspace. The equation

$$h'(y,u)(\bar{y},\bar{u}) = 0$$

is satisfied, if $\bar{y}$ solves the linear partial differential equation for given $\bar{u}$

$$\begin{array}{rcll} \bar{y}_t(t,x) &=& (\Delta \bar{y})(t,x) + c_y(t,x,y(t,x))\bar{y}(t,x) & t \in (0,T), \quad x \in \Omega \\ \bar{y}(0,x) &=& 0 & x \in \Omega \\ \frac{\partial \bar{y}}{\partial n}(t,\xi) &=& g(\xi)\bar{u}(t) & t \in (0,T), \quad \xi \in \Gamma. \end{array} \tag{3.3}$$

Even in discretized form this does not suggest a parametrization of the nullspace through an orthonormal basis, obtained from a QR-decomposition, which is used in most reduced SQP methods for finite-dimensional problems. An obvious representation of all $(\bar{y},\bar{u})$ which satisfy (3.3) is through $\bar{u}$. Hence we set

$$T(y,u)\bar{u} = \begin{pmatrix} \bar{y} \\ \bar{u} \end{pmatrix}$$

where $\bar{y} \in Y$ solves (3.3). This parametrization is very natural and smooth dependence on the data yields Lipschitz-continuity or Fréchet-differentiability of T. We use this definition of T to compute the gradient $T(y^+,u^+)^* f'(y^+,u^+)$, where we choose (y^+,u^+) instead of (y,u) for a more consistent formulation of the algorithms. This element is given by

$$\gamma^+(t) = (T(y^+,u^+)^* f'(y^+,u^+))(t) = \int_\Gamma g(\xi) d^+(t,\xi)\, d\xi + k_u(t,u^+(t)) \qquad (3.4)$$

where d^+ is the solution of the adjoint equation (see e.g. [17])

$$\begin{array}{lcll} -d_t^+(t,x) & = & (\Delta d^+)(t,x) + c_y(t,x,y^+(t,x))d^+(t,x) & \\ & & + l_y(t,x,y^+(t,x)) & t \in (0,T),\ x \in \Omega \\ d^+(T,x) & = & 0 & x \in \Omega \\ \frac{\partial d^+}{\partial n}(t,\xi) & = & 0 & t \in (0,T),\ \xi \in \Gamma. \end{array} \qquad (3.5)$$

In the gradient method one needs to compute the gradient (2.3) of the objective function φ which can be achieved by (3.4).

Gradient Method

Given	control u and gradient γ
Step 1	Set $u^+ = u - \alpha\gamma$
Step 2	Compute the solution y^+ of the nonlinear b.v.p. (3.1) with control input u^+
Step 3	Compute the solution d^+ of the linear b.v.p. (3.5)
Step 4	Compute the gradient $\gamma^+(\cdot)$ from (3.4)

The step-size parameter α is selected according to some step size rule. We see that this method requires per iteration the solution of one linear and one nonlinear initial-boundary value problem. However, in general this method converges rather slowly so that we turn our attention to Newton's method. We consider again the computation of the gradient. It itself takes the solution of a linear initial-boundary value problem whose data depend on the solution of the nonlinear problem (3.1). Hence it is obvious that the analytical calculation of the derivative of the gradient is a rather tedious task. One should remember that this is already quite nasty for optimal control problems with ordinary differential equations and even more so for problems with partial differential equations.

In order to improve this situation we turn our attention to quasi-Newton methods. Here we approximate the Hessian of the objective function in a proper way.

BFGS Method

Given	control u, gradient γ and an operator $B \in \mathcal{L}(U)$
Step 1	Solve $B\Delta u = -\gamma$
Step 2	Set $u^+ = u + \Delta u$
Step 3	Compute the solution y^+ of the nonlinear b.v.p. (3.1) with control input u^+
Step 4	Compute the solution d^+ of the linear b.v.p. (3.5)
Step 5	Compute the gradient $\gamma^+(\cdot)$ from (3.4)
Step 6	Set $\eta = \gamma^+ - \gamma$
Step 7	Set $B_+ = B + \frac{\eta \otimes \eta}{<\eta,\Delta u>} - \frac{(B\Delta u)\otimes(B\Delta u)}{<\Delta u, B\Delta u>}$

If we compare the number of boundary value problems which we need to solve during one iteration of the BFGS method with those of the gradient method we see that they are

the same. The big advantage of the BFGS method is that it exhibits locally a superlinear rate of convergence under certain assumptions. The only additional cost is the solution of the linear equation in Step 1 and the storage of B. Both aspects can be solved rather efficiently, see e.g. [6].

At this point we want to focus on SQP methods. These methods have the common feature that they linearize the nonlinear function which defines the equality constraint. Hence we expect for these methods to omit the solution of a nonlinear initial-boundary value problem. If we consider Algorithm 4 (full SQP method) from the previous section, then we notice that we have to store and update an operator $M \in \mathcal{L}(Y \times U)$. If one discretizes the time-dependent space U by a d_t-dimensional space and the space- and time-dependent $Y = Y([0,T] \times \Omega)$ by a $d_t n d_x$-dimensional space where n denotes the space dimension and d_x the discretization in one space component, then the matrix to be stored for a full SQP update is of the size $\mathbb{R}^{d_t(1+nd_x)\times d_t(1+nd_x)}$. This shows that for parabolic differential equations of the type under consideration the full method is not recommendable. It is the main advantage of the reduced SQP method (Algorithm 5) that it allows to use the structure of the nullspace of $h'(y,u)$ by parametrizing the state.

The last missing ingredient for the reduced SQP-step (2.5) is the calculation of the restoration step. If we choose $R(y,u)$ according to (2.4), then

$$R(y,u)h(y,u) = \begin{pmatrix} y - w \\ 0 \end{pmatrix}$$

where $w \in Y$ solves

$$\begin{array}{lcll} w_t(t,x) & = & (\Delta w)(t,x) + c_y(t,x,y(t,x))w(t,x) & \\ & & + c(t,x,y(t,x)) - c_y(t,x,y(t,x))y(t,x) & t \in (0,T), \quad x \in \Omega \\ w(0,x) & = & y_0(x) & x \in \Omega \\ \frac{\partial w}{\partial n}(t,\xi) & = & g(\xi)u(t) & t \in (0,T), \quad \xi \in \Gamma. \end{array} \tag{3.6}$$

Note that the element $R(y,u)h(y,u)$ is not needed explicitly in Algorithm 5. However, it can be used to determine the new state y^+ in a convenient way. Therefore, recall that the new iterate in the reduced SQP method is given by (2.5):

$$\begin{pmatrix} y^+ \\ u^+ \end{pmatrix} = \begin{pmatrix} y \\ u \end{pmatrix} + T(y,u)\Delta u - R(y,u)h(y,u) = \begin{pmatrix} \bar{y} + w \\ u + \Delta u \end{pmatrix}$$

where $\bar{y}$ solves (3.3) with control input $\bar{u} = \Delta u$ and w solves (3.6). A combination of these two formulas shows that y^+ then solves the following linear initial-boundary value problem

$$\begin{array}{lcll} y_t^+(t,x) & = & (\Delta y^+)(t,x) + c_y(t,x,y(t,x))y^+(t,x) & \\ & & + c(t,x,y(t,x)) - c_y(t,x,y(t,x))y(t,x) & t \in (0,T), \quad x \in \Omega \\ y^+(0,x) & = & y_0(x) & x \in \Omega \\ \frac{\partial y^+}{\partial n}(t,\xi) & = & g(\xi)u^+(t) & t \in (0,T), \quad \xi \in \Gamma. \end{array} \tag{3.7}$$

The step to compute a new correction for the update B requires an additional effort because for reasons mentioned in the previous section we cannot use y^+ directly for this

computation. The element

$$\begin{pmatrix} y \\ u \end{pmatrix} + T(y,u)\Delta u = \begin{pmatrix} y \\ u \end{pmatrix} + \begin{pmatrix} \bar{y} \\ \Delta u \end{pmatrix} = \begin{pmatrix} y+\bar{y} \\ u^+ \end{pmatrix}$$

can be computed by a solution of

$$\begin{array}{lcll} \bar{y}_t(t,x) & = & (\Delta\bar{y})(t,x) + c_y(t,x,y(t,x))\bar{y}(t,x) & t \in (0,T), \quad x \in \Omega \\ \bar{y}(0,x) & = & 0 & x \in \Omega \\ \frac{\partial \bar{y}}{\partial n}(t,\xi) & = & g(\xi)\Delta u(t) & t \in (0,T), \quad \xi \in \Gamma. \end{array} \tag{3.8}$$

Then we form

$$\tilde{y} = y + \bar{y}$$

to formulate

$$\begin{array}{lcll} -\tilde{d}_t(t,x) & = & (\Delta\tilde{d})(t,x) + c_y(t,x,\tilde{y}(t,x))\tilde{d}(t,x) & \\ & & + l_y(t,x,\tilde{y}(t,x)) & t \in (0,T), \quad x \in \Omega \\ \tilde{d}(T,x) & = & 0 & x \in \Omega \\ \frac{\partial \tilde{d}}{\partial n}(t,\xi) & = & 0 & t \in (0,T), \quad \xi \in \Gamma. \end{array} \tag{3.9}$$

Then we compute the function $\tilde{\gamma}$ which is used in the calculation of the update

$$\tilde{\gamma}(t) = \int_\Gamma g(\xi)\tilde{d}(t,\xi)\, d\xi + k_u(t,u^+(t)) \tag{3.10}$$

(see also (3.4) and (3.5)).

In detail, the reduced SQP method for the semilinear boundary control problem (3.1),(3.2) requires the following steps

Reduced SQP Method

Given	control u, state y, gradient γ and an operator $B \in \mathcal{L}(U)$
Step 1	Solve $B\Delta u = -\gamma$
Step 2	Set $u^+ = u + \Delta u$
Step 3	Compute the solution y^+ of the linear b.v.p. (3.7)
Step 4	Compute the solution d^+ of the linear b.v.p. (3.5)
Step 5	Compute the gradient $\gamma^+(\cdot)$ from (3.4)
Step 6	Compute the solution $\bar{y}$ of the linear b.v.p. (3.8)
Step 7	Set $\tilde{y} = y + \bar{y}$
Step 8	Compute the solution $\tilde{d}$ of the linear b.v.p. (3.9)
Step 9	Compute $\tilde{\gamma}(\cdot)$ from (3.10)
Step 10	Set $\eta = \tilde{\gamma} - \gamma$
Step 11	Set $B_+ = B + \frac{\eta \otimes \eta}{<\eta,\Delta u>} - \frac{(B\Delta u)\otimes(B\Delta u)}{<\Delta u, B\Delta u>}$

Note that the solution for (3.8) and (3.7) involves the same linear parabolic equation with different inhomogeneous terms. The adjoint equations (3.5) and (3.9) are not the same, because the coefficients in the differential equation differ.

4 Convergence Results

Here we give a review of the convergence behavior of the methods discussed in the previous paragraphs. Throughout this section we make use of the following definition: Let V_1, V_2 normed linear spaces, $D \subset V_1$ an open set and $\hat{v} \in D$. A mapping $F : D \to V_2$ satisfies a Lipschitz-condition at $\hat{v}$ in D, $F \in Lip(D)$, if there exists a constant $M > 0$ such that

$$\|F(v) - F(\hat{v})\|_{V_2} \leq M\|v - \hat{v}\|_{V_1} \quad \text{for all } v \in D.$$

Recall that $X = Y \times U$ where Y and U are real Hilbert spaces. Since the convergence results for Algorithms 1–3 are well known we state them only very briefly.

Gradient Method

Let φ be twice continuously Fréchet-differentiable and assume a convexity condition. Then the standard result yields that the gradient method with an appropriate stepsize converges to the solution, cf. [13] . Moreover, if $u_k \neq \hat{u}$ for all k, the convergence is q-linear:

$$\|u_{k+1} - \hat{u}\| \leq q\|u_k - \hat{u}\| \text{ for some } q \in (0,1).$$

This convergence can be fairly slow, in particular, when u_k is close to $\hat{u}$.

Newton's Method

The reward for the high price paid in computing the second derivative of φ at each step, is the q-quadratic convergence rate of Newton's method. The following result can be found in [13], for example.

Theorem 4.1 *Let φ be twice Fréchet-differentiable and $\varphi'' \in Lip(D)$ for a neighborhood D of $\hat{u}$. Furthermore, assume that $\varphi''(\hat{u})$ is bijective.*
If $\|u_0 - \hat{u}\|$ is sufficiently small, then the sequence $\{u_k\}$ from Newton's method converges to $\hat{u}$ at a q-quadratic rate.

BFGS Method

At least in the finite-dimensional case the standard BFGS-method for unconstrained minimization (see e.g. [6]) and the full SQP-BFGS method are known for their q-superlinear convergence (see e.g. [7]) under appropriate assumptions. However, as mentioned before the SQP method suffers from the drawback that in general the Hessian of the Lagrangian is not positive definite on the entire space. Unfortunately, the use of the reduced version to overcome this difficulty is at the expense of the one-step superlinear convergence rate: the best we can expect from a reduced SQP method is superlinear convergence in two steps, see e.g. [1], [18].

Griewank [10] shows local q-linear convergence of the sequence $\{u_k\}$ from Algorithm 3 . Moreover, he proves q-superlinear convergence, if in addition the initial discrepancy $B_0 - \varphi''(\hat{u})$ is compact. The following theorem is a special case of the results in [10].

Theorem 4.2 *Let the assumptions of Theorem 4.1 hold and assume in addition that $\varphi''(\hat{u})$ is positive definite. Let the sequence $\{u_k\}$ be generated by Algorithm 3 with $B_0 \in \mathcal{L}(U)$ selfadjoint and positive definite.*

Then there exist positive scalars δ and ϵ such that if $\|u_0 - \hat{u}\| < \epsilon$ and $\|B_0 - \varphi''(\hat{u})\| < \delta$, then $\{u_k\}$ converges q-linearly to $\hat{u}$. Moreover, if $B_0 - \varphi''(\hat{u})$ is compact, then the rate of convergence is q-superlinear.

Reduced SQP Method

Since we are primarily interested in the application of reduced SQP methods to optimal control problems, we present the convergence behavior of these methods in a more detailed way. Therefore, we apply the general theory from [11] to the separability approach. For sake of simplicity we often use x for the variable instead of (y, u). Recall that f and h denote the objective and the constraint of the original problem (1.1).

Suppose there is a neighborhood $D := \{x : \|x - \hat{x}\| < \rho\}$ of the solution $\hat{x} = (\hat{y}, \hat{u})$ such that the following assumption holds which is standard in the context of constrained minimization:

(A): f and h are twice Fréchet-differentiable on D and $f'', h'' \in Lip(D)$:
$\|f''(x) - f''(\hat{x})\|$, $\|h''(x) - h''(\hat{x})\| \leq M\|x - \hat{x}\|$, $x \in D$, $M > 0$.

The definitions (2.4) and (2.1) of R and T and the assumptions in Section 2 lead with (A) to the Fréchet- differentiability of $T : D \to \mathcal{L}(U, Y \times U)$ and $R : D \to \mathcal{L}(Y, Y \times U)$ with $T', R' \in Lip(D)$.

For abbreviation we set

$$\hat{H} = T(\hat{x})^* L_x''(\hat{x}, \hat{l}) T(\hat{x}).$$

We consider for a moment a reduced SQP method with a general BFGS-update. Therefore, we replace the updating procedure in Algorithm 5 by the formula

$$B_{k+1} = B_k + \frac{\eta_k \otimes \eta_k}{< \eta_k, w_k >} - \frac{(B_k w_k) \otimes (B_k w_k)}{< w_k, B_k w_k >}, \tag{4.1}$$

where $\eta_k, w_k \in U, B_k \in \mathcal{L}(U)$ and η_k, w_k are not specified any further. In this way it is possible to establish convergence results for reduced SQP-BFGS methods where the sequences $\{\eta_k\}$ and $\{w_k\}$ are chosen from the variety of possible choices proposed in the literature [12]. We will see that the following condition for these sequences is essential to prove convergence:

$$< \eta_k, w_k > > 0 \quad \text{and} \quad \|\eta_k - \hat{H} w_k\| \leq K \max\{\|x_k - \hat{x}\|, \|x_{k+1} - \hat{x}\|\} \|w_k\| \tag{4.2}$$

for a constant $K > 0$ and all $k \geq 0$.

It is shown by [11] that locally a two-step q-linear rate can be achieved for a reduced SQP-BFGS method, if the approximation error $\|B_k - \hat{H}\|$ is sufficiently small at each iteration. If (4.2) is satisfied, the latter condition can be guaranteed from a bounded deterioration property for the sequence $\{B_k\}$. In particular, if (A) and the classical second order sufficient optimality condition for problem (1.1) hold, i.e. there exists $m > 0$ such that

$$< v, L_x''(\hat{x}, \hat{l}) v > \geq m\|v\|^2 \text{ for all } v \in \mathcal{N}(h'(\hat{x})), \tag{4.3}$$

then the property (4.2) can easily be verified for

$$\begin{aligned} w_k &= -B_k^{-1}T(x_k)^*f'(x_k) \qquad \text{and} \\ \eta_k &= T(x_k+T(x_k)w_k)^*f'(x_k+T(x_k)w_k) - T(x_k)^*f'(x_k). \end{aligned} \tag{4.4}$$

These are the choices taken in Algorithm 5 and in Steps 9–11 of the reduced SQP algorithm for the semilinear parabolic boundary control problem from Section 3. Consequently, if (A) and (4.3) are valid, we obtain local q-linear convergence in two steps for the sequence $\{(y_k, u_k)\}$ from Algorithm 5, provided the update is skipped in the case $\Delta u = 0$. We point out again that the same convergence rate can be achieved for any other choice of the input of the update formula, as long as (4.2) is satisfied. This can be important, if a standard choice of η_k or w_k cannot be calculated exactly and some approximation has to be used, a situation that is likely to occur if the computation of η_k involves the solution of boundary value problems.

We now address the superlinear convergence behavior. It is shown in [11] that the Powell-condition [14] is sufficient for two-step q-superlinear convergence of reduced SQP methods also in Hilbert space, i.e. the limit

$$\lim_{k\to\infty} \frac{\|(B_k - \hat{H})B_k^{-1}T(x_k)^*f'(x_k)\|}{\|x_{k+1}-x_k\|} = 0 \tag{4.5}$$

implies that

$$\lim_{k\to\infty} \frac{\|x_{k+1}-\hat{x}\|}{\|x_{k-1}-\hat{x}\|} = 0\,,$$

if the sequence $\{x_k\}$ converges to $\hat{x}$.

To prove the consistency condition (4.5) we make use of the following general result on the BFGS-update which is valid in an arbitrary real Hilbert space U. Hence, it is applicable to constrained and unconstrained optimization and independent of any particular method. It is an immediate consequence of a more general theorem proven by Griewank [10] in his study of secant methods to solve nonlinear operator equations in Hilbert space.

Theorem 4.3 *Let $\{B_k\}$ be generated by the BFGS-update formula (4.1) where $B_0 \in \mathcal{L}(U)$ is bijective, selfadjoint, positive definite and $\lambda_*(B_0) > 0$. Furthermore, assume that $\{\eta_k\}$ and $\{w_k\}$ satisfy*

$$< \eta_k, w_k > > 0 \quad \textit{and} \quad \|\eta_k - \hat{D}w_k\| \le \alpha_k\|w_k\|\,,\ k \ge 0\,,$$

for some positive definite, selfadjoint and bijective operator $\hat{D} \in \mathcal{L}(U)$ and a sequence $\{\alpha_k\}$ with the property $\sum_{k=0}^{\infty}\alpha_k < \infty$.
If $B_0 - \hat{D}$ is compact, then

$$\lim_{k\to\infty} \frac{\|(B_k-\hat{D})w_k\|}{\|w_k\|} = 0.$$

Here $\lambda_*(B) = \inf\{\|B - C\| : \mathcal{L}(U) \ni C \text{ compact}\}$ denotes the essential norm of B. The restrictive assumption $\lambda_*(B_0) > 0$ can be replaced by requiring that U is infinite-dimensional and for the finite-dimensional case the above result was proven in [2].

Theorem 4.3 indicates the crucial role of compactness and the importance of property (4.2) in the infinite-dimensional convergence analysis of quasi-Newton methods. To our knowledge a convergence result for the full SQP method (Algorithm 4) has not yet been established in infinite-dimensional spaces. Theorem 4.3 can serve as a tool to prove superlinear convergence also for this method, if the BFGS-formula is used in an appropriate way.

To finish the discussion on convergence rates, we apply Theorem 4.3 to show local two-step q-superlinear convergence of the reduced SQP method from Algorithm 5. The proof, see [11], uses the linear convergence result just mentioned and the extended Powell-condition (4.5).

Theorem 4.4 *Assume (A) and (4.3).*
Let the sequence $\{(y_k, u_k)\}, (y_k, u_k) \neq (\hat{y}, \hat{u})$, *be generated by Algorithm 5 with* $B_0 \in \mathcal{L}(U)$ *selfadjoint and positive definite.*
Then there exist positive scalars δ *and* ϵ *such that if* $\|(y_0, u_0) - (\hat{y}, \hat{u})\| < \epsilon$ *and* $\|B_0 - \hat{H}\| < \delta$, *then* $\{(y_k, u_k)\}$ *converges to* $(\hat{y}, \hat{u})$ *at a two-step q-linear rate. Moreover, if* $B_0 - \hat{H}$ *is compact, then the rate of convergence is two-step q-superlinear:*

$$\lim_{k \to \infty} \frac{\|(y_{k+1}, u_{k+1}) - (\hat{y}, \hat{u})\|}{\|(y_{k-1}, u_{k-1}) - (\hat{y}, \hat{u})\|} = 0.$$

Theorem 4.4 shows that the compactness of the starting discrepancy is significant for fast convergence of reduced SQP methods. This condition always appears when a quasi-Newton method is applied to an infinite-dimensional problem. The same can be said of the smoothness properties of f and h required in (A): a comparison of the assumptions in the convergence theorems of this section shows that they are very similar for all the methods discussed in this paper. The verification of these assumptions in the application of a reduced SQP method to semilinear parabolic boundary control problems will be the subject of our future work. Another point in this context will be the setup of the spaces. In view of the approach taken to prove second order sufficiency conditions it seems likely that an adaption of the convergence theory to the specific needs of control problems is necessary for a successful treatment of the open questions.

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