Hamburger Beiträge
zur Angewandten Mathematik

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Nr. 2010-05
April 2010

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Received 09 April 2010

Key words elliptic optimal control problem, state & control constraints, error analysis.
MSC (2000) 49J20, 49K20, 35B37

Solutions to optimization problems with pde constraints inherit special properties; the associated state solves the pde which in the optimization problem takes the role of a equality constraint, and this state together with the associated control solves an optimization problem, i.e. together with multipliers satisfies first and second order necessary optimality conditions. In this note we review the state of the art in designing discrete concepts for optimization problems with pde constraints with emphasis on structure conservation of solutions on the discrete level, and on error analysis for the discrete variables involved. As model problem for the state we consider an elliptic pde which is well understood from the analytical point of view. This allows to focus on structural aspects in discretization. We discuss the approaches *First discretize, then optimize* and *First optimize, then discretize*, and consider in detail two variants of the *First discretize, then optimize* approach, namely variational discretization, a discrete concept which avoids explicit discretization of the controls, and piecewise constant control approximations. We consider general constraints on the control, and also consider pointwise bounds on the state. We outline the basic ideas for providing optimal error analysis and accomplish our analytical findings with numerical examples which confirm our analytical results.

1 Introduction

In PDE-constrained optimization, we have usually a pde as state equation and constraints on control and/or state. Let us write the pde for the state $y \in Y$ with the control $u \in U$ in the form $e(y,u) = 0$ in Z. Assuming smoothness, we are then lead to optimization problems of the form

$$\min_{(y,u) \in Y \times U} J(y,u) \text{ s.t. } e(y,u) = 0, \quad c(y) \in \mathcal{K}, \quad u \in U_{ad}, \tag{1}$$

∗ The material presented in this chapter in parts is based on joint work with Klaus Deckelnick (Universität Magdeburg), Andreas Günther (Freie Universität Berlin), Ulrich Matthes (Universität Hamburg) and Morten Vierling (Universität Hamburg).

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where $e : Y \times U \to Z$ and $c : Y \to R$ are continuously Fréchet differentiable, $\mathcal{K} \subset R$ is a closed convex cone representing the state constraints, and $U_{ad} \subset U$ is a closed convex set representing the control constraints. We are interested in illuminating discrete approaches to problem (1), where we place particular emphasis on structure preservation on the discrete level, and also on analysing the contributions to the total error of the discretization errors in the variables and multipliers involved.

To approach an optimal control problem of the form (1) numerically one may either discretize this problem by substituting all appearing function spaces by finite dimensional spaces, and all appearing operators by suitable approximate counterparts which allow their numerical evaluation on a computer, say. Denoting by h the discretization parameter, one ends up with the problem

$$\min_{(y_h,u_h)\in Y_h\times U_h} J_h(y_h,u_h) \text{ s.t } e_h(y_h,u_h)=0 \text{ and } c_h(y_h)\in\mathcal{K}_h,\ u_h\in U_{ad}^h, \tag{2}$$

where $J_h : Y_h \times U_h \to \mathbb{R}$, $e_h : Y_h \times U_h \to Z$, and $c_h : Y_h \to R$ with $\mathcal{K}_h \subset R_h$. For the finite dimensional subspaces one may require $Y_h \subset Y, U_h \subset U$, say, and $\mathcal{K}_h \subseteq R_h$ a closed and convex cone, $U_{ad}^h \subseteq U_h$ closed and convex. This approach in general is referred to as first discretize, then optimize.

On the other hand one may switch to the Karush-Kuhn-Tucker system associated to (1)

$$e(\bar y,\bar u)=0,\quad c(\bar y)\in\mathcal{K}, \tag{3}$$

$$\bar\lambda\in\mathcal{K}^\circ,\quad \langle\bar\lambda, c(\bar y)\rangle_{R^*,R}=0, \tag{4}$$

$$L_y(\bar y,\bar u,\bar p)+c'(\bar y)^*\bar\lambda=0, \tag{5}$$

$$\bar u\in U_{ad},\quad \langle L_u(\bar y,\bar u,\bar p),u-\bar u\rangle_{U^*,U}\ge 0\quad \forall\, u\in U_{ad}. \tag{6}$$

and substitute all appearing function spaces and operators accordingly, where $L(y,u,p) := J(y,u) - \langle p, e(y,u)\rangle_{Z^*,Z}$ denotes the Lagrangian associated to (1). This leads to solving

$$e_h(y_h,u_h)=0,\quad c_h(y_h)\in\mathcal{K}_h, \tag{7}$$

$$\lambda_h\in{\mathcal{K}_h}^\circ,\quad \langle\lambda_h, c_h(y_h)\rangle R^*,R=0, \tag{8}$$

$$L_{h_y}(y_h,u_h,p_h)+c_h'(y_h)^*\lambda_h=0, \tag{9}$$

$$\bar u_h\in U_{ad}^h,\quad \langle L_{h_u}(y_h,u_h,p_h),u-u_h\rangle_{U^*,U}\ge 0\quad \forall\, u\in U_{ad}^h \tag{10}$$

for $\bar y_h, \bar u_h, \bar p_h, \bar\lambda_h$. This approach in general is referred to as first optimize, then discretize, since it builds the discretization upon the first order necessary optimality conditions.

Instead of applying discrete concepts to problem (1) or (3)-(6) directly we may first apply an SQP approach on the continuous level and then apply first discretize, then optimize to the related linear quadratic constrained subproblems, or first optimize, then discretize to the SQP systems appearing in each iteration of the Newton method on the infinite dimensional level. This motivates us to illustrate the discrete approach for a linear model pde which is well understood w.r.t. analysis and discretization concepts and to focus the presentation on structural aspects inherent to optimal control problems with pde constraints. However, error analysis for optimization problems with nonlinear state equations in the presence of constraints on controls and/or state is not straightforward and requires special techniques such as extensions of

Newton-Kantorovich-type theorems, and second order sufficient optimaltiy conditions. This complex of questions also will be discussed briefly.

The outline of this note is as follows. In Section 2, we consider an elliptic model optimal control problem containing all relevant features which need to be resolved by a numerical approach. We use the finite element element method for the discretization of the state equation and propose two different approximation approaches of the *First discretize, then optimize* to the optimal control problem, including numerical analysis. In Section 3, we discuss improvements of the approximation properties of discrete states and controls if the constraints on the state and/or the control obey special structures. Let us finally note that the structural aspects discussed in the present note also carry over to optimal control problems with parabolic pdes in a straightforward manner.

2 A model problem

To explain the main results that can be expected in numerical approximation, let us discuss a simple model problem with pointwise bounds on control and state. We consider the Neumann problem

$$(\mathbb{S}) \quad \left\{ \begin{array}{l} \min_{(y,u)\in Y\times U_{ad}} J(y,u) := \frac{1}{2}\int_\Omega |y-y_0|^2 + \frac{\alpha}{2}\|u\|_U^2 \\ \text{s.t.} \\ \left.\begin{array}{rcll} Ay &=& Bu & \text{in } \Omega, \\ \partial_\eta y &=& 0 & \text{on } \Gamma, \end{array}\right\} :\Longleftrightarrow y = \mathcal{G}(Bu) \\ \text{and} \\ y \in Y_{\text{ad}} := \{y\in Y, y(x)\le b(x) \text{ a.e. in } \Omega\}. \end{array} \right. \tag{11}$$

Here, $Y := H^1(\Omega)$, A denotes a uniformly elliptic operator, for example $Ay = -\Delta y + y$, and $\Omega \subset \mathbb{R}^d$ $(d = 2,3)$ denotes an open, bounded sufficiently smooth (or polyhedral) domain. Furthermore, we suppose that $\alpha > 0$ and that $y_0 \in L^2(\Omega)$, and $b \in W^{2,\infty}(\Omega)$ are given. $(U,(\cdot,\cdot)_U)$ denotes a Hilbert space and $B : U \to L^2(\Omega) \subset H^1(\Omega)^*$ the linear, continuous control operator. By $R : U^* \to U$ we denote the inverse of the Riesz isomorphism. Furthermore, we associate to A the continuous, coercive bilinear form $a(\cdot,\cdot)$.

Example 2.1 There are several examples for the choice of B and U.

(i) Distributed control: $U = L^2(\Omega)$, $B = Id : L^2(\Omega) \to Y'$.

(ii) Boundary control: $U = L^2(\partial\Omega)$, $Bu(\cdot) = \int u\gamma_0(\cdot)\,dx : L^2(\Omega) \to Y'$, where γ_0 is the boundary trace operator in Y.

(iii) Linear combinations of input fields: $U = \mathbb{R}^n$, $Bu = \sum_{i=1}^n u_i f_i$, $f_i \in Y'$.

If not stated otherwise we from here onwards consider the situation (i) of the previous example. In view of $\alpha > 0$, it is standard to prove that problem (11) admits a unique solution $(y,u) \in Y_{ad} \times U_{ad}$. In pde constrained optimization, the pde for given data frequently is uniquely solvable. In equation (11) this is also the case, so that for every control $u \in U_{ad}$ we have a unique state $y = \mathcal{G}(Bu) \in H^1(\Omega) \cap C^0(\bar\Omega)$. We need $y \in C^0(\bar\Omega)$ to satisfy the Slater condition required below. Problem (11) therefore is equivalent to the so called reduced optimization problem

$$\min_{v\in U_{ad}} \hat J(v) := J(\mathcal{G}(Bv), v) \text{ s.t. } \mathcal{G}(Bv) \in Y_{ad}. \tag{12}$$

The key to the proper numerical treatment of problems (11) and (12) can be found in the first order necessary optimality conditions associated to these control problems. To formulate them properly we require the following constraint qualification, often referred to as *Slater condition*. It requires the existence of a state in the interior of the set Y_{ad} considered as a subset of $C^0(\bar{\Omega})$ and ensures the existence of a Lagrange multiplier in the associated dual space. Moreover, it is useful for deriving error estimates.

Assumption 2.2 $\exists \tilde{u} \in U_{ad} \quad \mathcal{G}(B\tilde{u})(x) < b(x)$ for all $x \in \bar{\Omega}$.

Following Casas [7, Theorem 5.2] for the problem under consideration we now have the following theorem, which specifies the KKT system (3)-(6) for the setting of problem (11).

Theorem 2.3 *Let $u \in U_{ad}$ denote the unique solution to* (11)*. Then there exist a Lagrange multiplier $\mu \in \mathcal{M}(\bar{\Omega})$ and an adjoint state $p \in L^2(\Omega)$ such that, with $y = \mathcal{G}(Bu)$, there holds*

$$\int_\Omega pAv = \int_\Omega (y-y_0)v + \int_{\bar{\Omega}} v d\mu \qquad \forall v \in H^2(\Omega) \text{ with } \partial_\eta v = 0 \text{ on } \partial\Omega, \tag{13}$$

$$(RB^*p + \alpha u, v-u)_U \geq 0 \qquad \forall v \in U_{ad}, \tag{14}$$

$$\mu \geq 0,\ y(x) \leq b(x) \text{ in } \Omega \text{ and } \int_{\bar{\Omega}} (b-y) d\mu = 0. \tag{15}$$

Here, $(\mathcal{M}(\bar{\Omega}), \|\cdot\|_{\mathcal{M}(\bar{\Omega})})$ denotes the space of Radon measures which is defined as the dual space of $C^0(\bar{\Omega})$. Since $\hat{J}'(v) = B^*p + \alpha(\cdot, u)_U$, a short calculation shows that the variational (14) is equivalent to

$$u = P_{U_{ad}}(u - \sigma R\hat{J}'(u))\ (\sigma > 0),$$

where $P_{U_{ad}}$ denotes the orthogonal projection in U onto U_{ad}. This nonsmooth operator equation constitutes a relation between the optimal control u and its associated adjoint state p. In the present situation, when we consider the special case without control constraints, i.e. $U_{ad} \equiv L^2(\Omega)$, this relation boils down to

$$\alpha u + p = 0 \text{ in } L^2(\Omega),$$

$\sigma > 0$. This relation already gives a hint to the discretization of the state y and the control u in problem (11), if one wishes to conserve the structure of this algebraic relation also on the discrete level.

2.1 Finite element discretization

For the convenience of the reader we recall the finite element setting. To begin with, let $\mathcal{T}_h$ be a triangulation of Ω with maximum mesh size $h := \max_{T \in \mathcal{T}_h} \text{diam}(T)$ and vertices $x_1, \ldots, x_m$. We suppose that $\bar{\Omega}$ is the union of the elements of $\mathcal{T}_h$ so that element edges lying on the boundary are possibly curved. In addition, we assume that the triangulation is quasi-uniform in the sense that there exists a constant $\kappa > 0$ (independent of h) such that each $T \in \mathcal{T}_h$ is contained in a ball of radius $\kappa^{-1}h$ and contains a ball of radius κh... Let us define the space of linear finite elements,

$$X_h := \{v_h \in C^0(\bar{\Omega}) \mid v_h \text{ is a linear polynomial on each } T \in \mathcal{T}_h\}$$

with the appropriate modification for boundary elements. In what follows it is convenient to introduce a discrete approximation of the operator $\mathcal{G}$. For a given function $v \in L^2(\Omega)$, we denote by $z_h = \mathcal{G}_h(v) \in X_h$ the solution of the discrete Neumann problem

$$a(z_h, v_h) \quad = \quad \int_\Omega v v_h \quad \text{for all } v_h \in X_h.$$

2.1.1 Variational discretization

From the point of view of numerical analysis, variational discretization allows the easiest analysis of the discretization error and in general yields approximation errors of higher order than the other approaches discussed below. Problem (11) is now approximated by the following sequence of so called *variational discrete* control problems [26] depending on the mesh parameter h:

$$\begin{aligned} &\min_{u \in U_{ad}} \hat{J}_h(u) := \frac{1}{2}\int_\Omega |y_h - y_0|^2 + \frac{\alpha}{2}\|u\|_U^2 \\ &\text{subject to } \ y_h = \mathcal{G}_h(Bu) \text{ and } y_h(x_j) \le b(x_j) \text{ for } j = 1, \dots, m. \end{aligned} \tag{16}$$

Notice that the integer m is not fixed and tends to infinity as $h \to 0$, so that the number of state constraints in this optimal control problem increases with decreasing mesh size of underlying finite element approximation of the state space. This discretization approach can be understood as a generalization of the *First discretize, then optimize* approach in that it avoids discretization of the control space U. It leads to a convex infinite-dimensional optimization problem of similar structure as problem (11), but with only finitely many equality and inequality constraints for the state, which form a convex admissible set. So we are again in the setting of (1) with Y replaced by the finite element space X_h (compare also the analysis of Casas presented in [8]). Since $\mathcal{G}_h(B\tilde{u}) \to \mathcal{G}(B\tilde{u})$ in $L^\infty(\Omega)$, a Slater condition for (16) automatically is satisfied, if h is small enough. We thus have

Lemma 2.4 *Problem (16) has a unique solution $u_h \in U_{ad}$. There exist $\mu_1, \dots, \mu_m \in \mathbb{R}$ and $p_h \in X_h$ such that with $y_h = \mathcal{G}_h(Bu_h)$ and $\mu_h = \sum_{j=1}^m \mu_j \delta_{x_j}$ we have*

$$a(v_h, p_h) = \int_\Omega (y_h - y_0)v_h + \int_{\bar{\Omega}} v_h d\mu_h \qquad \forall v_h \in X_h, \tag{17}$$

$$(RB^* p_h + \alpha u_h, v - u_h)_U \ge 0 \qquad \forall v \in U_{ad}, \tag{18}$$

$$\mu_j \ge 0,\ y_h(x_j) \le b(x_j), j = 1, \dots, m, \text{ and } \int_{\bar{\Omega}} \big(I_h b - y_h\big) d\mu_h = 0. \tag{19}$$

Here, δ_x denotes the Dirac measure concentrated at x and I_h is the usual Lagrange interpolation operator. We have $\hat{J}_h'(v) = B^* p_h + \alpha(\cdot, u_h)_U$, so that the considerations after Theorem 2.3 also apply in the present setting, but with p replaced by the discrete function p_h. Consequently, there holds

$$u_h = P_{U_{ad}}(u_h - \sigma R \hat{J}_h'(u_h)) \quad (\sigma > 0).$$

For $\sigma = \frac{1}{\alpha}$ we obtain

$$u = P_{U_{ad}}\left(-\frac{1}{\alpha} RB^* p\right) \text{ and } u_h = P_{U_{ad}}\left(-\frac{1}{\alpha} RB^* p_h\right). \tag{20}$$

It follows from this relation that the variational discrete optimal control u_h can be understood as a discrete object which is automatically discretized through (20). Its structure depends on the discrete adjoint p_h and the properties of the orthogonal projection $P_{U_{ad}}$, the Riesz isomorphism R, and the control operator B. Let us clarify the situation for the case $U = L^2(\Omega), B = Id_{L^2 \to (H^1)^*}$, and $U_{ad} = \{v \in U; a_l \leq v \leq a_r\}$ with constant bounds $a_l < a_r$. Due to the presence of P_{Uad}, in variational discretization the function $u_h = P_{U_{ad}}(-\frac{1}{\alpha}p_h) \in U_{ad}$ will in general not belong to X_h. However, in many practical situations it can be calculated on the computer, see for instance [26, 30, 31]. In the case of a purely state constrained problem, we have $P_{U_{ad}} \equiv Id$, so that $u_h = -\frac{1}{\alpha}p_h \in X_h$ by (20). This means that the optimal variational discrete optimal control u_h automatically is a discrete function. Therefore, the space $U = L^2(\Omega)$ in (16) may be replaced by X_h to obtain the same discrete solution u_h, which results in a finite–dimensional discrete optimization problem instead. However, we emphasize that the infinite–dimensional formulation of (16) is very useful in numerical analysis [28, Chap. 3].

2.1.2 Piecewise constant controls

In this section, we consider the special case $U = L^2(\Omega)$, so that B denotes the injection of $L^2(\Omega)$ into $H^1(\Omega)^*$ with box constraints $a_l \leq u \leq a_r$ on the control. Controls are approximated by element-wise constant functions. For details we refer to [17]. We define the space of piecewise constant functions

$$Y_h := \{v_h \in L^2(\Omega) \,|\, v_h \text{ is constant on each } T \in \mathcal{T}_h\}.$$

and denote by $Q_h : L^2(\Omega) \to Y_h$ the orthogonal projection onto Y_h so that

$$(Q_h v)(x) := \frac{1}{T}\int_T v, \quad x \in T, T \in \mathcal{T}_h,$$

In order to approximate (11) we introduce a discrete counterpart of U_{ad},

$$U_{ad}^h := \{v_h \in Y_h \,|\, a_l \leq v_h \leq a_u \text{ in } \Omega\}. \tag{21}$$

Problem (11) is now approximated by the following sequence of control problems depending on the mesh parameter h:

$$\begin{aligned} &\min_{u \in U_{ad}^h} J_h(u) := \frac{1}{2}\int_\Omega |y_h - y_0|^2 + \frac{\alpha}{2}\int_\Omega |u|^2 \\ &\text{subject to } \; y_h = \mathcal{G}_h(u) \text{ and } y_h(x_j) \leq b(x_j) \text{ for } j = 1, \ldots, m. \end{aligned} \tag{22}$$

Problem (22), as problem (16), represents a convex finite-dimensional optimization problem of similar structure as problem (11), but with only finitely many equality and inequality constraints for state and control, which form a convex admissible set. Note that $U_{ad}^h \subset U_{ad}$ and that $Q_h v \in U_{ad}^h$ for $v \in U_{ad}$. Since $\mathcal{G}_h(Q_h\tilde{u}) \to \mathcal{G}(\tilde{u})$ in $L^\infty(\Omega)$, again a Slater condition is satisfied for problem (22) below so that the following optimality conditions can be argued as those given in (2.4) for problem (16).

Lemma 2.5 *Problem (22) has a unique solution $u_h \in U_{ad}^h$. There exist $\mu_1, \dots, \mu_m \in \mathbb{R}$ and $p_h \in X_h$ such that with $y_h = \mathcal{G}_h(u_h)$ and $\mu_h = \sum_{j=1}^m \mu_j \delta_{x_j}$ we have*

$$a(v_h, p_h) = \int_\Omega (y_h - y_0)v_h + \int_{\bar\Omega} v_h d\mu_h \qquad \forall v_h \in X_h, \tag{23}$$

$$\int_\Omega (p_h + \alpha u_h)(v_h - u_h) \geq 0 \qquad \forall v_h \in U_{ad}^h, \tag{24}$$

$$\mu_j \geq 0,\, y_h(x_j) \leq b(x_j), j = 1, \dots, m \text{ and } \int_{\bar\Omega} (I_h b - y_h) d\mu_h = 0. \tag{25}$$

Here, δ_x denotes the Dirac measure concentrated at x and I_h is the usual Lagrange interpolation operator.

Similar considerations hold for control approximations by continuous, piecewise polynomial functions. Discrete approaches to problem (11) relying on control approximations directly lead to fully discrete optimization problems like (22). These approaches lead to large-scale finite-dimensional optimization problems, since the discretization of the pde in general introduces a large number of degrees of freedom. Numerical implementation then is easy, which certainly is an important advantage of control approximations over variational discretization, whose numerical implementation is more involved. The use of classical NLP solvers for the numerical solution of the underlying discretized problems only is feasible, if the solver allows to exploit the underlying problem structure e.g. by providing user interfaces for first- and second-order derivatives.

On the other hand, the numerical implementation of variational discretization is not straightforward. The great advantage of variational discretization however is its property of optimal approximation accuracy, which is completely determined by that of the related state and adjoint state. Fig. 3.3 compares active sets obtained by variational discretization and piecewise linear control approximations in the presence of box constraints. One clearly observes that the active sets are resolved much more accurate when using variational discretization. In particular, the boundary of the active set is in general different from finite element edges.

The error analysis for problem (11) relies on the regularity of the involved variables, which is reflected by the optimality system presented in (13)-(15). If only control constraints are present, neither the multiplier μ in (13) nor the complementarity condition (15) appear. Then the variational inequality (14) restricts the regularity of the control u, and thus also that of the state y. If the desired state y_0 is regular enough, the adjoint variable p admits the highest regularity properties among all variables involved in the optimality system. Error analysis in this case then should involve the adjoint variable p and exploit its regularity properties.

If pointwise state constraints, are present, the situation is completely different. Now the adjoint variable only admits low regularity due to the presence of the multiplier μ, which in general is only a measure. The state now admits the highest regularity in the optimality system. This fact should be exploited in the error analysis. However, the presence of the complementarity system (15) requires L^∞-error estimates for the state. In the next two sections, we present error estimates for problems with state and/or control constraints. Details can be found in [28, Chap. 3]. We consider variational discretization, and piecewise constant, and also piecewise linear control approximations. For variational discretization, the approximation properties are determined by the L^∞-error of the state approximation. In the latter

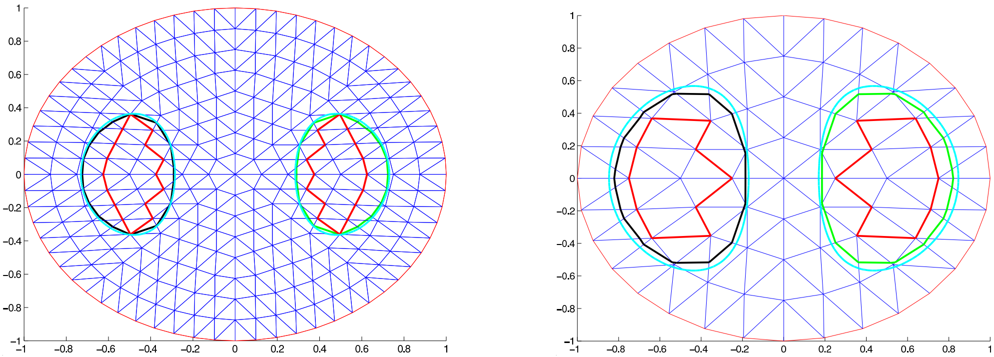

Fig. 1 Numerical comparison of active sets obtained by variational discretization, and those obtained by a conventional approach with piecewise linear, continuous controls: $h = \frac{1}{8}$ and $\alpha = 0.1$ (left), $h = \frac{1}{4}$ and $\alpha = 0.01$ (right). The red line depicts the boarder of the active set in the conventional approach, the cyan line the exact boarder, the black and green lines, respectively the boarders of the active set in variational discretization.

case, the approximation properties depend in addition on the error induced by the orthogonal projection on the set of piecewise constant controls.

2.1.3 Error bounds

For the approximation error of variational discretization we have the following theorem, whose proof can be found in [28, Chap. 3].

Theorem 2.6 *Let u and u_h be the solutions of (11) and (16) respectively. Then*

$$\alpha\|u-u_h\|_U + \|y-y_h\|_{L^2}, \ \|y-y_h\|_{H^1} \le Ch^{1-\frac{d}{4}}.$$

If in addition $Bu \in W^{1,s}(\Omega)$ for some $s \in (1, \frac{d}{d-1})$ then

$$\alpha\|u-u_h\|_U + \|y-y_h\|_{L^2}, \ \|y-y_h\|_{H^1} \le Ch^{\frac{3}{2}-\frac{d}{2s}}\sqrt{|\log h|}.$$

If $Bu, Bu_h \in L^\infty(\Omega)$ with $(Bu_h)_h$ uniformly bounded in $L^\infty(\Omega)$ also

$$\alpha\|u-u_h\|_U + \|y-y_h\|_{L^2}, \ \|y-y_h\|_{H^1} \le Ch|\log h|,$$

where the latter estimate is valid for $d = 2, 3$.

For piecewise constant control approximations and the setting of Section 2.1.2 the following theorem is proved in [17].

Theorem 2.7 *Let u and u_h be the solutions of (11) and (22) respectively with $(u_h)_h \subset L^\infty(\Omega)$ uniformly bounded. Then we have for $0 < h \le \bar{h}$*

$$\alpha\|u-u_h\| + \|y-y_h\|_{H^1} \le \begin{cases} Ch|\log h|, & \text{if } d = 2 \\ C\sqrt{h}, & \text{if } d = 3. \end{cases}$$

The two theorems above have in common that a control error estimate is only available for $\alpha > 0$. However, the appearance of α in these estimates indicates that in the *bang-bang*-case $\alpha = 0$ an error estimate for $\|y - y_h\|_{L^2}$ still is available, whereas no information for the control error $\|u - u_h\|_U$ seems to remain. In [18] a refined analysis of bang-bang controls without state constraints also provides estimates for the control error on inactive regions in the L^1-norm. We further observe that piecewise constant control approximations in 2 space dimensions deliver the same approximation quality as variational discrete controls. Only in 3 space dimensions variational discretization provides a better error estimate. This is caused by the fact that state constraints limit the regularity of the adjoint state, so that optimal error estimates can be expected by techniques which avoid its use. Currently the analysis for piecewise constant control approximations involves an inverse estimate for $\|p_h\|_{H^1}$, which explains the lower approximation order in the case $d = 3$.

Let us mention that the bottleneck in the analysis here is not formed by control constraints, but by the state constraints. In fact, if one uses $U_{ad} = U$, then variational discretization (16) delivers the same numerical solution as the approach (22) with piecewise linear, continuous control approximations. Variational discretization really pays off if only control contraints are present and the adjoint variable is smooth, compare [26],[28, Chap.. 3].

For the numerical solution of problem (16), (22) several approaches exist in the literature. Common are so called regularization methods which relax the state constraints in (11) by either substituting it by a mixed control-state constraint (Lavrentiev relaxation [41]), or by adding suitable penalty terms to the cost functional instead requiring the state constraints (barrier methods [29, 44], penalty methods [23, 25].

3 Improvement of error estimates for special classes of control problems

3.1 The control-constrained case

The numerical analysis of $(\mathbb{S})$ is well developed in the case without the pointwise state-constraints $y(x) \leq b(x)$ and simple bound constraints on the control. Let us consider the special case $U = L^2(\Omega)$, where B is the injection of $L^2(\Omega)$ into $H^1(\Omega)^*$. With real numbers $a_l < a_r$, we consider the box constraints

$$U_{ad} = \{u \in U,\, a_l \leq u(x) \leq a_r \text{ a.e. in } \Omega\}.$$

Here, Theorem 2.3 holds with $\mu = 0$, the adjoint state p belongs to $H^2(\Omega)$ and the pointwise projection formula

$$u(x) = \mathbb{P}_{[a_l,a_r]}\left(-\frac{1}{\alpha}p(x)\right) \quad \text{a.e. in } \Omega \tag{26}$$

holds for the optimal control u, where $\mathbb{P}_{[a_l,a_r]}$ is the projection from $\mathbb{R}$ onto $[a_l, a_r]$. We consider now the approximated control constrained problem

$$\min_{u \in U^h_{ad}} J_h(u) := \frac{1}{2}\int_\Omega |y_h - y_0|^2 + \frac{\alpha}{2}\int_\Omega |u|^2 \tag{27}$$

with the admissible set U^h_{ad} of piecewise constant controls defined by (21).

¿From $p \in H^2(\Omega)$ and (26) we obtain $u \in H^1(\Omega)$. The numerical approximation of u by u_h in $L^2(\Omega)$ cannot be better than that of u by $\Pi_h u$, its projection in U_h. If $u \in H^1(\Omega)$, then $\|u - \Pi_h u\|_U$ is of order h. The same order might be expected for $\|u - u_h\|_U$. Indeed, this can be shown even for semilinear elliptic equations and also for boundary control problems, [1], [11].

Can an approximation of the control u by continuous piecewise linear functions improve the estimate? The optimal control u is not regular, where it switches between activity and inactivity (u is called active in x if $u(x) = a_l$ or $u(x) = a_r$). In between, u is as smooth as $p \in H^2(\Omega)$. If the measure of the union of all triangles T of the triangulation with $u_h \notin H^2(T)$ can be estimated by $C\,h$, then for piecewise linear approximation of u the error $\|u - u_h\|_U$ is of order $h^{3/2}$, [9]. These control estimates of order h and $h^{3/2}$, respectively, are sharp and are usually observed numerically.

What about the variational discretization, where the control function u is not discretized? Here, there is no approximation error in u so that only the FEM causes an error. In view of the reasoning above, $\|u - u_h\|_U$ should then have the order of the finite element approximation. Therefore, the expected order h^2 can indeed be proven, and is also observed numerically [26]. Summarizing, under natural assumptions we have

$$\alpha\|u-u_h\|_U+\|y-y_h\|_{L^2} \le \begin{cases} C\,h & \text{for piecewise constant } u_h \\ C\,h^{3/2} & \text{for continuous and piecewise linear } u_h \\ C\,h^2 & \text{for variational discretization.} \end{cases} \tag{28}$$

These estimates are also true for Neumann boundary control problems under associated assumptions. Here, the discussion of *piecewise linear* controls is more difficult. We refer only to [10], [30] for Neumann and to [12], and [48]. Moreover, we mention [19], where the error is estimated for Dirichlet boundary control problems under variational discretization.

As observed e.g. by [11], the error $\|y - y_h\|_{L^2(\Omega)}$ for the state may exhibit the higher order h^2, as it is the case for variational discretization. This behavior was explained and proven in [39] under the assumption on the measure of ”triangles of irregularity” mentioned above. For piecewise constant control approximation, this order h^2 can be obtained by a simple postprocessing step: After having computed the optimal u_h of (22), substitute the associated discrete adjoint state p_h for p in (26) and denote the resulting u by $\tilde{u}_h$. Then $\|u-\tilde{u}_h\|_U \le c\,h^2$ holds and $\tilde{u}_h$ has the same discrete structure as the optimal control obtained by variational discretization. However, $\tilde{u}_h$ no longer is numerical solution to an optimal control problem.

The case of a semilinear elliptic equation: If the pde or the associated boundary condition is of semilinear type, say

$$Ay + \Phi(y) = u, \tag{29}$$

where $\Phi : \mathbb{R} \to \mathbb{R}$ is monotone non-decreasing and sufficiently smooth, then the situation is more delicate.

Here, the choice of $U = L^\infty(\Omega)$ is often needed to guarantee the existence of first- and second-order Fréchet derivatives of the mapping $\mathcal{G} : u \to y$ from $L^\infty(\Omega)$ to $C(\bar{\Omega})$. We also should expect locally optimal controls rather than a unique optimal control. Moreover, the reduced objective functional $\hat{J}$ should be locally convex around the selected local reference solution u. Therefore, the reference solution u is usually required to satisfy a second-order sufficient optimality condition. To formulate it, we first introduce for $\tau \geq 0$ the strongly active set

$$I_\tau(u) = \{x \in \Omega,\ |\alpha\, u(x) + p(x)| \geq \tau\}.$$

Moreover, we define the τ-critical cone $C_\tau(u)$ by the set of all $v \in L^\infty(\Omega)$ with the property

$$v(x) \begin{cases} = 0, & \text{if } x \in I_\tau(u) \\ \geq 0, & \text{if } u(x) = a_l \text{ and } x \notin I_\tau(u) \\ \leq 0, & \text{if } u(x) = a_r \text{ and } x \notin I_\tau(u). \end{cases}$$

In almost all points x with $|\alpha\, u(x) + p(x)| > 0$, by the first order condition (26), the control $u(x)$ admits either the value a_l or a_r. Here, we do not need additional second-order information. This motivates the choice of $C_\tau(u)$.

The second-order sufficient optimality condition requires that, in addition to the first-order necessary optimality conditions, there exist $\tau > 0$ and $\delta > 0$ such that

$$\hat{J}''[v, v] \geq \delta \|v\|^2_{L^2(\Omega)} \quad \forall v \in C_\tau(u).$$

The smaller $\tau > 0$ can be taken, the smaller is the set $C_\tau(u)$ and the weaker is the second-order requirement. Unfortunately, the choice $\tau = 0$ is not allowed. If the second-order sufficient condition is satisfied, then u is locally optimal in an open ball of $L^\infty(\Omega)$ centered at u. For a detailed discussion of second-order sufficient conditions and the computation of $J''[v, v]$, we refer to [1] or to the detailed exposition in [45] and the references cited therein. We have the error estimate

$$\|u - u_h\|_{L^\infty(\Omega)} \leq c\, h$$

for the selected locally optimal control u, where u_h is the related piecewise constant optimal solution of (22) without state constraints, [1], [11].

3.2 Finite-dimensional controls

Let us now return to the pointwise state constraints $y(x) \leq b$ with some real number b, but under the simplification that Bu has the form (iii) of Example 2.1,

$$(Bu)(x) = \sum_{i=1} u_i\, f_i(x) \tag{30}$$

with Hölder continuous functions $f_i : \Omega \to \mathbb{R}$, $i = 1, \ldots, n$. Then problem (12) is of semi-infinite type. Still, we have pointwise state constraints with measures as associated Lagrange multipliers. Therefore, the adjoint state exhibits the same low regularity as p in Theorem 2.3. On the other hand, the control $u = (u_1, \ldots, u_n)$ is a vector. As for variational discretization, there is no need to discretize it, hence the discretization error comes only from the FEM and the discretization of the state constraints. Does this increase the order of the error $|u - u_h|$?

An answer given in [37] for $d = 2$, which depends on the form of the active set of y. Counter examples confirm that, in general, we can only expect the order $h\sqrt{|\log h|}$ being close to the one in Theorem 2.6. Under additional assumptions, a higher order can be shown. To simplify the formulation of the next result, we assume $U_{ad} = \mathbb{R}^n$. Moreover, we denote by y_i the state associated to the control u with entries $u_j = \delta_{ij}$, $j = 1, \ldots, n$.

Theorem 3.1 *Let u and u_h be the solutions of* (12) *with $U_{ad} = \mathbb{R}^n$ in the setting* (30)*. Assume that the optimal state y has exactly n active points $x_1, \ldots, x_n$ in Ω, the Slater Assumption 2.2 is fulfilled, the Hessian matrices $y''(x_1), \ldots, y''(x_n)$ are negative definit, and the matrix $(y_i(x_j))_{i,j=1,\ldots,n}$ has full rank. Then the following error estimate is fulfilled:*

$$|u - u_h| \leq C\, h^2 |\log h|.$$

This estimate is confirmed by associated numerical examples, [37]. In the semi-infinite case, one of the main difficulties is that number and location of active points of y_h vary with h. The situation simplifies considerably, if the state constraints are required only in finitely many fixed interior points as it is pointed out next.

3.3 Finite-dimensional control and state constraints in finitely many points

Here, we consider problem (12), where $B : \mathbb{R}^n \to H^1(\Omega)^*$ has the form (30) and the set Y_{ad} of state constraints is given by

$$Y_{ad} = \{y \in C(\bar\Omega),\ y(x_j) \leq b,\ j = 1, ..., m\}$$

with $m \in \mathbb{N}$ and $x_j \in \Omega,\ j = 1, ..., m,$ given fixed. Let us allow also a semilinear equation of the form (29). Now, the mappings $\hat J$ and $g_j : u \mapsto y(x_j) = y(\mathcal{G}(Bu))(x_j)$ are real-valued and smooth functions depending on $u \in \mathbb{R}^n$ so that this optimal control problem is equivalent to a finite-dimensional nonlinear programming problem. The approximation error comes only from the FEM. In view of the pointwise state constraints, we again need $y \in C(\bar\Omega)$. In the maximum norm, the associated error has the order $h^2|\log h|$, [38]. Also here, the Lagrange multiplier μ is a measure. However, it is a linear combination of Dirac measures concentrated in the points x_j so that μ can be identified with the vector of associated nonnegative real coefficients.

This and the equivalence to finite-dimensional programming permits to estimate $\|\mu - \mu_h\|_{M(\bar\Omega)}$ by $ch^2|\log h|$ under natural assumptions. The next result is taken from [38].

Theorem 3.2 *Let u and u_h be the solutions of the optimal control problem with finite-dimensional control and state constraints in finitely many points. Let a locally optimal u satisfy a linearized Slater condition. Assume further that, in the formulation of a nonlinear programming problem, the strong second-order sufficient optimality condition and the linear independence condition of active gradients are satisfied. Then there is a $C > 0$ independent of h such that, for all sufficiently small $h > 0$, it holds*

$$|u - u_h| + \|\mu - \mu_h\|_{M(\bar\Omega)} \leq C\, h^2 |\log h|.$$

Example 3.3 ([38]) We consider the state equation (29) in $\Omega = (-1, 1) \times (-1, 1)$ with $A = -\Delta$, $\Phi(y) = y(15 + |y|)$, homogeneous Dirichlet boundary conditions and the ansatz (30) for the control. The problem is

$$\min_{u \in \mathbb{R}^5} J(y, u) = \frac{1}{2}\|y - y_0\|_U^2 + \frac{1}{2}|u - u_d|^2$$

subject to the elliptic equation (29) and the constraints

$$y(x_i) \leq 8/27, \quad i = 1, \ldots, 4, \qquad\qquad y(x_5) \geqslant 0,$$

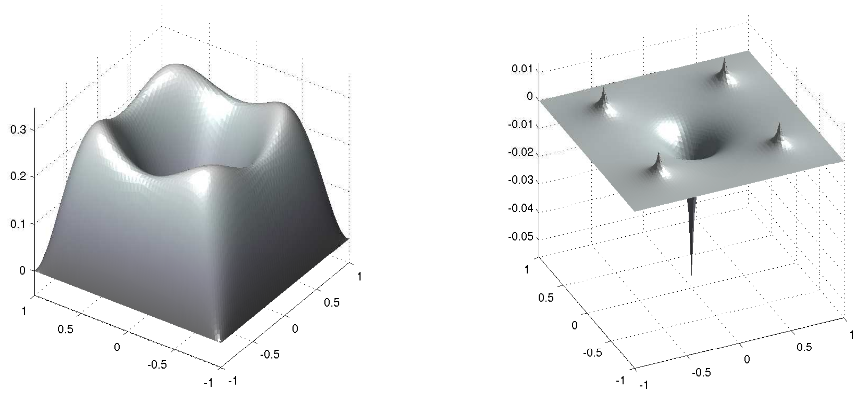

Fig. 2 Optimal state and adjoint state of Example 3.3

where $x_1, \ldots, x_4$ are defined by the 4 possible selections of $(\pm\sqrt{1/3}, \pm\sqrt{1/3})$, $x_5 = (0,0)$, and the ansatz functions are $f_1(x) = 12x_1^2x_2^2 - 2(x_1^4 + x_2^4),\ f_2(x) = x_1^2 + x_2^2,\ f_3(x) = 1,\ f_4(x) = (x_1^2 - 1)(x_2^2 - 1)(x_1^2 + x_2^2),\ f_5(x) = (x_1^2 - 1)^2(x_2^2 - 1)^2(x_1^2 + x_2^2)^2$. Further, we define $y_0(x) = (x_1^2 - 1)(x_2^2 - 1)(x_1^2 + x_2^2)$ and $u_d = (-2, 16, -4, 15, 1)^\top$.

Then $u = u_d$ is the optimal control with state $y = y_0$, which is active in $x_1, \ldots, x_5$.

The computed state y and the adjoint state are shown in Figure 3.3. The Lagrange multipliers are Dirac measures concentrated on the points x_i, hence the associated adjoint state exhibits singularities in these points. Computations with an initial mesh containing $x_1, \ldots, x_5$ confirmed the predicted error estimate, [38].

Acknowledgements The authors gratefully acknowledge the support of the DFG Priority Program 1253 entitled Optimization With Partial Differential Equations.

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