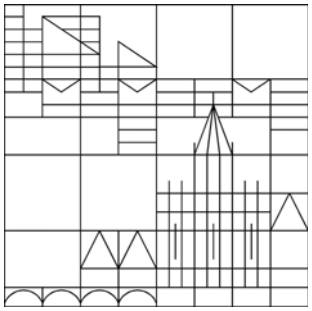

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OPTIMALITY SYSTEM POD AND A-POSTERIORI ERROR ANALYSIS FOR LINEAR-QUADRATIC PROBLEMS

S. VOLKWEIN

Abstract. In this paper an abstract linear-quadratic optimal control problem governed by an evolution equation is considered. To solve this problem numerically a reduced-order approach based on proper orthogonal decomposition (POD) is applied. The error between the POD suboptimal control and the optimal control of the original problem is controlled by an a-posteriori error analysis. However, if the POD basis has bad approximation properties, a huge number of POD basis function is required to solve the reduced-order problem with the desired accuracy. To overcome this problem optimality system POD (OS-POD) is utilized, where the POD basis is chosen with respect to the optimization criteria.

1. Introduction

Optimal control problems for partial differential equation are often hard to tackle numerically because their discretization leads to very large scale optimization problems. Therefore, different techniques of model reduction were developed to approximate these problems by smaller ones that are tractable with less effort. Among them, the method of proper orthogonal decomposition (POD) [18] and the balanced truncation method [3] seem to be most widely used in the context of optimal control. POD is based on projecting the dynamical system onto subspaces of basis elements that express characteristics of the expected solution. This is in contrast to, e.g., finite element techniques, where the elements are not correlated to the physical properties of the system they approximate.

In our present work, POD is applied to linear-quadratic optimal control problems. Linear-quadratic problems are interesting in several respects; in particular, they occur in each level of sequential quadratic programming (SQP) methods; see, e.g., [16] from a general viewpoint and [10, 18] in the context of multilevel reduced-order approximations. We continue the research on POD a-posteriori error analysis; see [10, 11, 18, 20]. Based on a perturbation argument it is derived how far the suboptimal control, computed on the basis of the POD model, is from the (unknown) exact one. Increasing the number of POD ansatz functions leads to more accurate POD suboptimal controls. This idea turns out to be numerically very efficient. It is also successfully applied for other reduced-order approximations; see [19]. However, if the POD basis is created from a reference trajectory containing features which

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are quite different from those of the optimally controlled trajectory, a rather huge number of POD ansatz functions have to be included in the reduced-order model. This fact may lead to nonefficient reduced-order models and numerical instabilities. To avoid these problems the POD basis is generated in an initialization step utilizing *optimality system POD* (OS-POD); see [14]. In OS-POD the POD basis is updated in the direction of the minimum of the cost. For other POD basis update techniques we refer to [1, 2].

The paper is organized as follows: In Section 2 we introduce the abstract linear-quadratic optimal control problem and review first-order necessary optimality conditions. The POD method, its application to the optimal control problem and the a-posteriori error estimate are explained in Section 3. In Section 4 we discuss the combination of OS-POD and a-posteriori error estimation. A numerical example is presented in Section 5, whereas some concludions are made in the last section.

2. The linear-quadratic parabolic optimal control problem

In this section, we introduce a class of linear-quadratic parabolic optimal control problems and recall the associated first-order necessary optimality conditions.

2.1. **Problem formulation.** Let V and H be real, separable Hilbert spaces and suppose that V is dense in H with compact embedding. By $\langle \cdot\,, \cdot \rangle_H$ we denote the inner product in H. The inner product in V is given by a symmetric bounded, coercive, bilinear form $a : V \times V \to \mathbb{R}$:

$$\langle \varphi, \psi \rangle_V = a(\varphi, \psi) \quad \text{for all } \varphi, \psi \in V \tag{2.1}$$

with associated norm $\|\cdot\|_V = \sqrt{a(\cdot\,,\cdot)}$. By identifying H and its dual H' it follows that $V \hookrightarrow H = H' \hookrightarrow V'$, each embedding being continuous and dense. Recall that for $T > 0$ the space $W(0,T)$

$$W(0,T) = \big\{ \varphi \in L^2(0,T;V) : \varphi_t \in L^2(0,T;V') \big\}$$

is a Hilbert space endowed with the common inner product (see, for example, [4, p. 473]). The control space is the Hilbert space $U = L^2(0,T;\mathbb{R}^m)$ with $m \in \mathbb{N}$. By $U_{\mathsf{ad}} \subset U$, we define the closed, convex and bounded subset

$$U_{\mathsf{ad}} = \big\{ u \in U \,|\, u_{a,i} \le u_i \le u_{b,i} \text{ in } (0,T) \text{ for } 1 \le i \le m \big\}$$

with $u_a, u_b \in U$ satisfying $u_{a,i} \le u_{b,i}$ almost everywhere (a.e.) in $(0,T)$ for $1 \le i \le m$. For $y_0 \in H$, $f \in L^2(0,T;V')$ and $u \in U_{\mathsf{ad}}$ we consider the linear evolution problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi \rangle_H + a(y(t), \varphi) &= \langle (f + \mathcal{B}u)(t), \varphi \rangle_{V',V} \ \text{ f.a.a. } t \in [0,T],\ \forall \varphi \in V, \\ \langle y(0), \varphi \rangle_H &= \langle y_0, \varphi \rangle_H \qquad\qquad \forall \varphi \in V, \end{aligned} \tag{2.2}$$

where $\mathcal{B} : U \to L^2(0,T;V')$ is a continuous, linear operator. Throughout we write 'f.a.a.' for 'for almost all'.

Example 2.1. Let us present an example for (2.2). Suppose that $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, is an open and bounded domain with Lipschitz-continuous boundary $\Gamma = \partial\Omega$. For $T > 0$ we set $Q = (0,T) \times \Omega$ and $\Sigma = (0,T) \times \Gamma$. Let $H = L^2(\Omega)$

and $V = H_0^1(\Omega)$. Then, for given control $u \in U$, and initial condition $y_0 \in H$ we consider the linear heat equation

$$y_t(t,\mathbf{x}) - \Delta y(t,\mathbf{x}) + c(\mathbf{x})y(t,\mathbf{x}) = f(t,\mathbf{x}) + \sum_{i=1}^{m} u_i(t)b_i(\mathbf{x}) \quad \text{f.a.a. } (t,\mathbf{x}) \in Q, \tag{2.3a}$$

$$y(t,\mathbf{s}) = 0 \qquad \text{f.a.a. } (t,\mathbf{s}) \in \Sigma, \tag{2.3b}$$

$$y(0,\mathbf{x}) = y_0(\mathbf{x}) \qquad \text{f.a.a. } \mathbf{x} \in \Omega. \tag{2.3c}$$

In (2.3a) we suppose that $c \in L^\infty(\Omega)$ with $c \geq 0$ in Ω a.e., $f \in L^2(0,T;V')$ and $b_i \in H$ for $1 \leq i \leq m$. Introducing the bilinear form $a : V \times V \to \mathbb{R}$ by

$$a(\varphi,\psi) = \int_\Omega \nabla\varphi(\mathbf{x}) \cdot \nabla\psi(\mathbf{x}) + c(\mathbf{x})\varphi(\mathbf{x})\psi(\mathbf{x})\,\mathrm{d}\mathbf{x} \quad \text{for } \varphi,\psi \in V$$

and the linear, bounded operator $\mathcal{B} : L^2(0,T;\mathbb{R}^m) \to L^2(0,T;V')$ by

$$\langle(\mathcal{B}u)(t),\phi\rangle_{V',V} = \sum_{i=1}^{m} u_i(t) \int_\Omega b_i(\mathbf{x})\varphi(\mathbf{x})\,\mathrm{d}\mathbf{x} \quad \text{for } \phi \in V,\ t \in (0,T) \text{ a.e.}$$

it follows that the weak formulation of (2.3) can be expressed in the form (2.2). ◊

It is well-known [4] that for every $f \in L^2(0,T;V')$, $u \in U$ and $y_0 \in H$ there exists a unique weak solution $y \in W(0,T)$ satisfying (2.2).

Remark 2.2. Let $\hat{y}_0 \in W(0,T)$ be the unique solution to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{y}_0(t),\varphi\rangle_H + a(\hat{y}_0(t),\varphi) &= \langle f(t),\varphi\rangle_{V',V} && \text{f.a.a. } t \in [0,T],\ \forall\varphi \in V, \\ \langle\hat{y}_0(0),\varphi\rangle_H &= \langle y_0,\varphi\rangle_H && \forall\varphi \in V. \end{aligned}$$

Moreover, we introduce the linear and bounded operator $\mathcal{S} : U \to W(0,T)$ as follows: $\tilde{y} = \mathcal{S}u \in W(0,T)$ is the unique solution to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{y}(t),\varphi\rangle_H + a(\tilde{y}(t),\varphi) &= \langle(\mathcal{B}u)(t),\varphi\rangle_{V',V} && \text{f.a.a. } t \in [0,T],\ \forall\varphi \in V, \\ \langle\tilde{y}(0),\varphi\rangle_H &= 0 && \forall\varphi \in V. \end{aligned}$$

Then, $y = \hat{y}_0 + \mathcal{S}u$ is the weak solution to (2.2). ◊

Next we introduce the cost functional $J : W(0,T) \times U \to \mathbb{R}$ by

$$J(y,u) = \frac{1}{2}\|\mathcal{C}y - z\|_W^2 + \frac{\sigma}{2}\|u\|_U^2, \tag{2.4}$$

where W is a Hilbert space, $\mathcal{C} : L^2(0,T;H) \to W$ is a bounded linear operator, and $z \in W$ holds. Furthermore, $\sigma > 0$ is a regularization parameter.

Remark 2.3. In the context of Example 2.3 we choose $W = L^2(0,T;H)$, $z \in W$, $\mathcal{C} = \mathrm{id}$ on W. Then, (2.4) yields the cost functional

$$J(y,u) = \frac{1}{2}\int_0^T \int_\Omega \big(y(t,\mathbf{x}) - z(t,\mathbf{x})\big)^2\,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{\sigma}{2}\int_0^T \|u(t)\|_{\mathbb{R}^m}^2\,\mathrm{d}t$$

for $(y,u) \in W(0,T) \times U$. ◊

The optimal control problem is given by

$$\textbf{(P)} \qquad \min J(y,u) \quad \text{subject to (s.t.)} \quad (y,u) \in W(0,T) \times U_{\mathsf{ad}} \text{ solves (2.2)}.$$

Applying standard arguments (see [15], for instance) one can prove that there exists a unique optimal solution $\bar{x} = (\bar{y},\bar{u})$ to (**P**).

2.2. **First-order optimality conditions.** First-order necessary optimality conditions for our parabolic optimal control problem are well known. We briefly recall them here. Suppose that $\bar{x} = (\bar{y}, \bar{u})$ is the optimal solution to (**P**) (in the paper, a bar indicates optimality). Then there exists a unique Lagrange-multiplier $\bar{p} \in W(0,T)$ satisfying together with $\bar{x}$ the *first-order necessary optimality conditions*, which consist of the *state equations* (2.2), the *adjoint equations*

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\langle \bar{p}(t), \varphi\rangle_H + a(\bar{p}(t), \varphi) &= \langle z - \mathcal{C}\bar{y}(t), \mathcal{C}\varphi\rangle_W \quad \text{f.a.a. } t \in [0,T], \forall \varphi \in V, \\ \langle \bar{p}(T), \varphi\rangle_H &= 0 \qquad\qquad\qquad\qquad \forall \varphi \in V, \end{aligned} \tag{2.5}$$

and of the *variational inequality*

$$\langle \sigma\bar{u} - \mathcal{B}^\star \bar{p}, u - \bar{u}\rangle_U \geq 0 \quad \forall u \in \mathcal{U}_{\mathsf{ad}}. \tag{2.6}$$

Here, the linear and bounded operator $\mathcal{B}^\star : L^2(0,T;V) \to U' \sim U$ stands for the dual operator of $\mathcal{B}$ satisfying

$$\langle \mathcal{B}u, \varphi\rangle_{L^2(0,T;V'),L^2(0,T;V)} = \langle u, \mathcal{B}^\star\varphi\rangle_U = \langle \mathcal{B}^\star\varphi, u\rangle_U \quad \forall (u,\varphi) \in U \times L^2(0,T;V).$$

Remark 2.4. We continue the discussion of Example 2.3 and Remark 2.3. The adjoint equations (2.5) are given by

$$\begin{aligned} -\bar{p}_t(t,\mathbf{x}) - \Delta\bar{p}(t,\mathbf{x}) + c(\mathbf{x})\bar{p}(t,\mathbf{x}) &= z(t,\mathbf{x}) - \bar{y}(t,\mathbf{x}) \qquad \text{f.a.a. } (t,\mathbf{x}) \in Q, \\ \bar{p}(t,\mathbf{s}) &= 0 \qquad\qquad\qquad\qquad\quad \text{f.a.a. } (t,\mathbf{s}) \in \Sigma, \\ \bar{p}(T,\mathbf{x}) &= 0 \qquad\qquad\qquad\qquad\quad \text{f.a.a. } \mathbf{x} \in \Omega. \end{aligned}$$

Moreover, the variational inequality (2.6) has the form

$$\sum_{i=1}^m \int_0^T \left(\sigma\bar{u}_i(t) - \int_\Omega b_i(\mathbf{x})\bar{p}(t,\mathbf{x})\,\mathrm{d}\mathbf{x}\right)\big(u_i(t) - \bar{u}_i(t)\big)\,\mathrm{d}t \geq 0 \quad \text{for all } u \in U_{\mathsf{ad}}$$

and $(\mathcal{B}^\star\bar{p})(t) \in \mathbb{R}^m$ is given by the components $(\mathcal{B}^\star\bar{p})_i(t) = \int_\Omega b_i(\mathbf{x})\bar{p}(t,\mathbf{x})\,\mathrm{d}\mathbf{x}$ f.a.a. $t \in [0,T]$ and for $i = 1, \ldots, m$. Consequently, we have the pointwise variational inequality:

$$\int_0^T \left(\sigma\bar{u}_i(t) - \int_\Omega b_i(\mathbf{x})\bar{p}(t,\mathbf{x})\,\mathrm{d}\mathbf{x}\right)\big(v(t) - \bar{u}_i(t)\big)\,\mathrm{d}t \geq 0, \quad 1 \leq i \leq m,$$

for all $v \in L^2(0,T)$ satisfying $u_{a,i} \leq v \leq u_{b_i}$ in $[0,T]$. ◊

Problem (**P**) is an infinite-dimensional problem. Therefore, we have to discretize (**P**) for its numerical solution. For the discretization of the spatial variable we apply a POD Galerkin approximation, which is introduced in the next section.

3. The POD Galerkin discretization

In this section we introduce the POD method and derive the reduced-order model. To keep the notation simple, we apply only a spatial discretization with POD basis functions, but no time integration by, e.g., an implicit Euler method. For the discrete version of the POD method and its relation to the continuous one we refer to [13], for instance. Let X denote either the space H or the space V.

3.1. **The POD method.** Let an arbitrary $u \in U$ be chosen such that the corresponding state variable $y = \hat{y}_0 + \mathcal{S}u \in W(0,T)$ belongs to $C([0,T];V) \hookrightarrow C([0,T];X)$. Then,

$$\mathcal{V} = \operatorname{span}\big\{ y(t) \,|\, t \in [0,T] \big\} \subseteq V \subset X. \tag{3.1}$$

If $y_0 \neq 0$ holds, then $\operatorname{span}\{y_0\} \subset \mathcal{V}$ and $d = \dim \mathcal{V} \in [1,\infty]$, but $\mathcal{V}$ may have infinite dimension. We define a bounded linear operator $\mathcal{Y} : L^2(0,T) \to X$ by

$$\mathcal{Y}\varphi = \int_0^T \varphi(t) y(t)\,\mathrm{d}t \quad \text{for } \varphi \in L^2(0,T).$$

Its Hilbert space adjoint $\mathcal{Y}^\star : X \to L^2(0,T)$ satisfying

$$\langle \mathcal{Y}\varphi, z \rangle_X = \langle \varphi, \mathcal{Y}^\star z \rangle_{L^2(0,T)} \quad \text{for } (\varphi, z) \in L^2(0,T) \times X$$

is given by $(\mathcal{Y}^\star z)(t) = \langle z, y(t) \rangle_X$ for $z \in X$ and f.a.a. $t \in [0,T]$. The bounded linear operator $\mathcal{R} = \mathcal{Y}\mathcal{Y}^\star : X \to \mathcal{V} \subset X$ has the form

$$\mathcal{R}z = \int_0^T \langle z, y(t) \rangle_X \, y(t)\,\mathrm{d}t \quad \text{for } z \in X. \tag{3.2}$$

Moreover, let $\mathcal{K} = \mathcal{Y}^\star\mathcal{Y} : L^2(0,T) \to L^2(0,T)$ be defined by

$$\big(\mathcal{K}\varphi\big)(t) = \int_0^T \langle y(s), y(t) \rangle_X \, \varphi(s)\,\mathrm{d}s \quad \text{for } \varphi \in L^2(0,T).$$

It is well-known [9, Section 3] that the operator $\mathcal{R}$ is self-adjoint, compact and nonnegative. Thus, that there exists a complete orthonormal basis $\{\psi_i\}_{i=1}^d$ for $\mathcal{V} = \operatorname{range}(\mathcal{R}) \subseteq V$ and a sequence $\{\lambda_i\}_{i=1}^d$ of real numbers such that

$$\mathcal{R}\psi_i = \lambda_i \psi_i \text{ for } i = 1, \ldots, d \quad \text{and} \quad \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d \geq 0. \tag{3.3}$$

Remark 3.1.
1) By the Riesz-Schauder theorem the spectrum of $\mathcal{R}$ is a pure point spectrum except for possibly 0; see [17, p. 203].
2) Analogously to the theory of singular value decompositions for matrices, we find that the linear, bounded, compact and self-adjoint operator $\mathcal{K}$ has the same eigenvalues $\{\lambda_i\}_{i=1}^d$ as the operator $\mathcal{R}$. For all $\lambda_i > 0$ the corresponding eigenfunctions of $\mathcal{K}$ are given by
$$v_i(t) = \frac{1}{\sqrt{\lambda_i}} \big(\mathcal{Y}^* \psi_i\big)(t) = \frac{1}{\sqrt{\lambda_i}} \langle \psi_i, y(t) \rangle_X \text{ f.a.a. } t \in [0,T] \text{ and } 1 \leq i \leq \ell.$$
3) Notice that $\mathcal{V} \subset V$ implies $\psi_i \in V$ for $1 \leq i \leq \ell$. ◊

For $\ell \leq d$ the eigenvalues and eigenfunctions of $\mathcal{R}$ solve the following minimization problem

$$\min \int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle_V \, \psi_i \Big\|_X^2 \quad \text{s.t.} \quad \langle \psi_j, \psi_i \rangle_X = \delta_{ij} \text{ for } 1 \leq i, j \leq \ell$$

In particular,

$$\int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle_V \, \psi_i \Big\|_X^2 = \sum_{i=\ell+1}^{d} \lambda_i.$$

3.2. **POD Galerkin approximation for (P).** Let $y = \hat{y}_0 + \mathcal{S}u$ be the state associated with some control $u \in U$, and let $\mathcal{V}$ be given as in (3.1). We fix ℓ with $\ell \leq d$ and compute the first ℓ POD basis functions $\psi_1, \ldots, \psi_\ell \in V$ by solving either $\mathcal{R}\psi_i = \lambda_i \psi_i$ or $\mathcal{K}v_i = \lambda v_i$ for $i = 1, \ldots, \ell$ (see Remark 3.1). Then we define the finite dimensional linear space

$$V^\ell = \operatorname{span}\{\psi_1, \ldots, \psi_\ell\} \subset V.$$

Endowed with the topology in V it follows that V^ℓ is a Hilbert space. The POD Galerkin scheme for the state equation (2.2) leads to the following linear problem: determine a function

$$y^\ell(t) = \sum_{i=1}^{\ell} y_i(t)\psi_i \in V \quad \text{for } t \in [0,T]$$

such that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle y^\ell(t), \psi\rangle_H + a(y^\ell(t), \psi) &= \langle (f + \mathcal{B}u)(t), \psi\rangle_{V',V} \text{ f.a.a. } t \in [0,T], \forall \psi \in V^\ell, \\ \langle y^\ell(0), \psi\rangle_H &= \langle y_0, \psi\rangle_H \quad \forall \psi \in V^\ell. \end{aligned} \tag{3.4}$$

For every $f \in L^2(0,T;V')$, $u \in U$, $y_0 \in H$ and for every $\ell \in \mathbb{N}$ problem (3.4) admits a unique solution $y^\ell \in H^1(0,T;V^\ell)$; see [8, Proposition 3.4]. From $V^\ell \hookrightarrow V$ it follows that $y^\ell \in W(0,T)$ holds.

The POD Galerkin approximation for (**P**) is given by the minimization problem

$$(\mathbf{P}^\ell) \qquad \min J(y^\ell, u) \quad \text{s.t.} \quad (y^\ell, u) \in H^1(0,T;V^\ell) \times U_{\mathsf{ad}} \text{ solves (3.4)}.$$

Problem ($\mathbf{P}^\ell$) admits a unique optimal solution $\bar{x}^\ell = (\bar{y}^\ell, \bar{u}^\ell)$ that is interpreted as a suboptimal solution to (**P**). First-order necessary optimality conditions for ($\mathbf{P}^\ell$) are given by the *state equation* (3.4) with $u = \bar{u}^\ell$, the *adjoint equation*

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\langle \bar{p}^\ell(t), \psi\rangle_H + a(\bar{p}^\ell(t), \psi) &= \langle z - \mathcal{C}\bar{y}^\ell(t), \mathcal{C}\psi\rangle_W, \quad t \in [0,T], \forall \psi \in V^\ell, \\ \langle \bar{p}^\ell(T), \psi\rangle_H &= 0 \quad \forall \psi \in V^\ell. \end{aligned} \tag{3.5}$$

and *the variational inequality*

$$\langle \sigma\bar{u}^\ell - \mathcal{B}^\star \bar{p}^\ell, u - \bar{u}^\ell\rangle_U \geq 0 \quad \text{for all } u \in U_{\mathsf{ad}}.$$

To solve ($\mathbf{P}^\ell$) we apply a primal-dual active set strategy, which is a locally superlinearly convergent method [5]. Its mesh-independence is proved in [6, 7].

3.3. **A-posteriori error estimate for the POD approximation.** In this subsection we present the a-posteriori error estimate for the control variable. The result is taken from [20, Theorem 4.11].

Theorem 3.2. *Suppose that $(\bar{y}, \bar{u})$ is the solution to (**P**). For $\ell \leq d$ be arbitrarily let $(\bar{y}^\ell, \bar{u}^\ell)$ be the optimal solution to ($\mathbf{P}^\ell$). Let $\tilde{y} = \hat{y}_0 + \mathcal{S}\bar{u}^\ell$ and $\tilde{p} = \tilde{p}(\bar{u}^\ell)$ be the solution to the associated adjoint equation*

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{p}(t), \varphi\rangle_H + a(\tilde{p}(t), \varphi) &= \langle z - \mathcal{C}\tilde{y}(t), \mathcal{C}\varphi\rangle_W, \quad t \in [0,T], \ \forall \varphi \in V, \\ \langle \tilde{p}(T), \varphi\rangle_H &= 0 \qquad\qquad\qquad\quad \forall \varphi \in V. \end{aligned} \tag{3.6}$$

Define the residual function $\zeta^\ell \in U$ *by*

$$\zeta^\ell(t) = \begin{cases} \big[(\sigma\bar{u}^\ell - \mathcal{B}^\star\tilde{p})(t)\big]_- & \text{on } \mathcal{A}_-^\ell = \big\{t \in (0,T) \,\big|\, \bar{u}^\ell(t) = u_a(t)\big\}, \\ \big[(\sigma\bar{u}^\ell - \mathcal{B}^\star\tilde{p})(t)\big]_+ & \text{on } \mathcal{A}_+^\ell = \big\{t \in (0,T) \,\big|\, \bar{u}^\ell(t) = u_b(t)\big\}, \\ -(\sigma\bar{u}^\ell - \mathcal{B}^\star\tilde{p})(t) & \text{on } \mathcal{I}^\ell = [0,T] \setminus (\mathcal{A}_-^\ell \cup \mathcal{A}_+^\ell) \end{cases} \tag{3.7}$$

with $[s]_- = -\min(0,s)$ *and* $[s]_+ = \max(0,s)$. *Then*

$$\|\bar{u} - \bar{u}^\ell\|_U \le \frac{1}{\sigma}\,\|\zeta^\ell\|_U.$$

Remark 3.3.
1) Notice that $\tilde{y}$ and $\tilde{p}$ must be taken as the solutions to the (full) state and adjoint equation, respectively, not of their POD-approximations.
2) In [20] sufficient conditions are presented that $\lim_{\ell\to\infty}\|\zeta^\ell\|_U = 0$. Thus, $\|\zeta^\ell\|_U$ can be expected smaller than any $\varepsilon > 0$ provided that ℓ is taken sufficiently large. Motivated by this result, we set up the Algorithm 1. $\lozenge$
3) Notice that the presented error estimate holds for time-variant, linear-quadratic optimal control problems. For recent extension to nonlinear problems we refer the diploma thesis [11] for first numerical tests in the nonlinear case and to [10, 18], where the presented error estimate are utilized in a multilevel SQP algorithm.

Algorithm 1 POD reduced-order method with a-posteriori estimator.

1: Choose an input $u \in U_{\mathsf{ad}}$, an initial number ℓ for POD ansatz functions, a maximal number $\ell^{\max} > \ell$ of POD ansatz functions, and a stopping tolerance $\varepsilon > 0$; compute $y = \hat{y}_0 + \mathcal{S}u$.
2: Determine a POD basis of rank $\ell^{\max}$ utilizing the state $y = \hat{y}_0 + \mathcal{S}u$.
3: **repeat**
4: Build the reduced-order problem $(\mathbf{P}^\ell)$ of rank $\ell \le \ell^{\max}$.
5: Compute the suboptimal control $\bar{u}^\ell$.
6: Determine $\tilde{y} = \hat{y}_0 + \mathcal{S}\bar{u}^\ell$, $\tilde{p}$ (see (3.6)) as well as ζ^ℓ (see (3.7)).
7: **if** $\|\zeta^\ell\|_U < \varepsilon$ **or** $\ell = \ell^{\max}$ **then**
8: Return ℓ, suboptimal control $\bar{u}^\ell$ and STOP.
9: **else**
10: Set $\ell = \ell + 1$.
11: **end if**
12: **until** $\ell > \ell^{\max}$

4. Optimaliy system proper orthogional decomposition

We infer from Remark 3.3 that ζ^ℓ tends to zero provided ℓ goes to infinity. It follows from [8] that we have a rate of the form

$$\|\zeta^\ell\|_U^2 = \mathcal{O}\Big(\sum_{i=\ell+1}^{d} \lambda_i\Big)$$

provided the POD basis is computed utilizing the optimal state $\bar{y}$ and associated adjoint variable $\hat{p}$. However, in real computation we do not know the optimal solution in advance so that the convergence of $\|\zeta^\ell\|_U$ can be very slow. Hence, the

a-posteriori approach may suffer from the fact that the basis elements are computed from a reference trajectory containing features which are quite different from those of the optimally controlled trajectory. In this case, Algorithm 1 requires many iterations in the **repeat**-loop. To avoid a POD basis with poor approximation properties we make use of *optimality system POD* (OS-POD) [14]. This method avoids the problem of unmodelled dynamics.

4.1. **The method.** Recall that the POD basis for $(\mathbf{P}^\ell)$ is computed from the state $y = \hat{y}_0 + \mathcal{S}u$ with some control $u \in U$. Thus, the Galerkin projection in $(\mathbf{P}^\ell)$ depends on the state variable and hence on the control u at which either the eigenvalue $\mathcal{R}\psi_i = \lambda_i\psi_i$ or $\mathcal{K}v_i = \lambda v_i$ for $i = 1, \ldots, \ell$ is solved for the basis $\{\psi_i\}_{i=1}^\ell$. This may deter from one of the main advantages of the POD approach for model reduction, which consists in the fact that unlike typical finite element basis functions the elements of the POD basis reflects the dynamics of the system. In optimal control this feature gets lost if the dynamics of the state corresponding to the referece control is significantly different from the trajectory corresponding to the optimal approach we propose to consider the extended problem [14]:

$$(\mathbf{P}^\ell_{\text{ospod}}) \quad \min J(z,u) \text{ s.t. } \begin{cases} z = (y^\ell, y, \lambda_i, \psi_i), \\ (y^\ell, u) \in H^1(0,T;V^\ell) \times U_{\mathsf{ad}} \text{ solves (3.4)}, \\ y \in W(0,T) \text{ solves (2.2)}, \ (\lambda_i, \psi_i) \in \mathbb{R} \times V \text{ satisfy} \\ \mathcal{R}(y)\psi_i = \int_0^T \langle \psi_i, y(t) \rangle_V \, y(t) \, \mathrm{d}t = \lambda_i \psi_i, \ 1 \le i \le \ell. \end{cases}$$

Notice that the second line of the constraints in $(\mathbf{P}^\ell_{\text{ospod}})$ coincide with the constraints in $(\mathbf{P}^\ell)$, the next two are the infinite-dimensional state equation and the eigenvalue problem characterizing the POD basis. For the optimal solution the problem formulation $(\mathbf{P}^\ell_{\text{ospod}})$ has the property that the associated POD reduced system is computed from the trajectory corresponding to the optimal control and thus, differently from $(\mathbf{P}^\ell)$, the problem of unmodelled dynamics is removed. Of course, $(\mathbf{P}^\ell_{\text{ospod}})$ is more complicated than $(\mathbf{P}^\ell)$. For practical realization an operator splitting approach is used in [14]. In [14] sufficient conditions are given so that $(\mathbf{P}^\ell_{\text{ospod}})$ possesses a unique optimal solution $(\bar{y}^\ell, \bar{y}, \bar{\lambda}_i, \bar{\psi}_i, \bar{u}^\ell)$, which can be characterized by first-order necessary optimality conditions. These conditions consist in the existence of Lagrange multipliers $(\bar{p}^\ell, \bar{p}, \bar{\mu}_i)$ satisfying

- *state equations*:
  (S.1) (2.2) for $\bar{y}^\ell$,
  (S.2) (3.4) for $\bar{y}$,
  (S.3) (3.3) for $(\bar{\lambda}_i, \bar{\psi}_i)$ with $\bar{\lambda}_1 > \ldots > \bar{\lambda}_\ell$ and $\|\psi_i\|_V = 1$;
- *adjoint equations*:
  (A.1) (3.5) for $\bar{p}^\ell$,
  (A.2) the variational problem

$$-\frac{\mathrm{d}}{\mathrm{d}t}\langle \bar{p}(t), \varphi \rangle_H + a(\bar{p}(t), \varphi) = \sum_{i=1}^{\ell} \big\langle \langle \bar{y}(t), \bar{\mu}_i \rangle_X \, \bar{\psi}_i + \langle \bar{y}(t), \bar{\psi}_i \rangle_X \, \bar{\mu}_i, \varphi \big\rangle_H \quad \text{f.a.a. } t \in [0,T], \ \forall \varphi \in V, \tag{4.1}$$

$$\langle \bar{p}(T), \varphi \rangle_H = 0 \quad \forall \varphi \in V,$$

  for $\bar{p}$,

(A.3) the linear system

$$(\mathcal{R}-\bar{\lambda}_i\mathcal{I})\bar{\mu}_i=\mathcal{G}_i(\bar{y}^\ell,\bar{\psi},\bar{u}^\ell,\bar{p}^\ell)\in\operatorname{span}\{\bar{\psi}_i\}^\perp,\quad 1\le i\le\ell,$$

for $\bar{\mu}_i$ with the orthogonality relation $\langle\bar{\psi}_i,\bar{\mu}_i\rangle_X=0$ and

$$\begin{aligned}\langle\mathcal{G}_i(\bar{y}^\ell,\bar{\psi},\bar{u}^\ell,\bar{p}^\ell),\psi\rangle_{X',X}&\\ =\int_0^T\bar{y}_i(t)\Big(-\frac{\mathrm{d}}{\mathrm{d}t}\langle\bar{p}^\ell(t),\psi\rangle_H+a(\bar{p}^\ell(t),\psi)-\langle z-\mathcal{C}\bar{y}^\ell(t),\mathcal{C}\psi\rangle_W\Big),\mathrm{d}t&\\ +\int_0^T\bar{p}_i(t)\Big(\frac{\mathrm{d}}{\mathrm{d}t}\langle\bar{y}^\ell(t),\psi\rangle_H+a(\bar{y}^\ell(t),\psi)-\langle(f+\mathcal{B}\bar{u})(t),\psi\rangle_{V',V}\Big)\,\mathrm{d}t&\end{aligned}$$

for $\psi\in X$ and $1\le i\le\ell$, where $\bar{y}^\ell=\sum_{j=1}^\ell\bar{y}_j(t)\psi_j$ and $\bar{p}^\ell(t)=\sum_{j=1}^\ell\bar{p}_j(t)\psi_j$.

- *variational inequality*:

$$\langle\sigma\bar{u}^\ell-\mathcal{B}^\star(\bar{p}^\ell+\bar{p}),u-\bar{u}^\ell\rangle_U\ge 0\quad\text{for all } u\in U_{\mathsf{ad}}.$$

4.2. **Combination with the POD a-posteriori error estimation.** Notice that we have to solve the full state equation both in the computation of the a-posteriori residual ζ^ℓ as well as in the OS-POD approcch to compute a new POD basis. Furthermore, comparing (3.6) and (4.1) we observe that in both cases we have to solve the same adjoint equation with different right-hand sides. This offers the possibility to combine both methods in an efficient way. The idea is to use OS-POD to generate a suitable POD basis for Algorithm 1 in an initialization step. For that purpose we make use of the reduced cost functional. The state variable $z=(y^\ell,y,\lambda_i,\psi_i)$ depends on the control via (3.4), (2.2) and (3.3). Thus, we define the reduced cost

$$\hat{J}(u)=J(z(u),u)\quad\text{for } u\in U_{\mathsf{ad}}.$$

From the first-order optimalty conditions we infer that the gradient of $\hat{J}$ is given by

$$\hat{J}'(u)=\sigma u-\mathcal{B}^\star(p^\ell+p_2)\in U,$$

where p^ℓ solves (3.5) with $y^\ell=y^\ell(u)$ and p_2 is the solution to (4.1) with $y=\hat{y}_0+\mathcal{S}u$. The new approach is described in Algorithm 2.

Remark 4.1.
1) In the numerical realization of Algorithm 2 the adjoint variables p_1 and p_2 are computed simultaneously (see Step 5). Furthermore, the computation of y^i is utilized to determine the POD basis and the adjoints (p_1,p_2); see Steps 3 and 5.
2) If we choose $k=0$, we do not perform any gradient step in the initialization step. In this case Algorithm 2 coincides with Algorithm 1.
3) Compared to Algorithm 1 the initialization step is costly. Thus we should take a small number k. In our numerical experiment we choose $k=1$. ◊

5. Numerical experiments

In this section we present numerical examples illustrating the efficiency of the combination of the POD a-posteriori error estimation with an OS-POD initialization step. All computation are performed with the MATLAB programming language.

Algorithm 2 POD a-posteriori estimator with OS-POD initialization.

1: Choose an initial $u^0 \in U_{\mathsf{ad}}$, a number of ℓ POD basis functions and the number $k \geq 0$ of projected gradient steps.
2: **for** $i = 0$ **to** $k-1$ **do**
3: Compute $y^i = \hat{y}_0 + \mathcal{S}u^i$ and a new basis $\{\psi_i(y^i)\}_{i=1}^{\ell}$.
4: Determine $y^\ell(u^i)$, $p^\ell(u^i)$, and $\{\mu_i\}_{i=1}^{\ell}$.
5: Calculate $p_1(y^i)$ with the right-hand side of (3.6) and $p_2(y^i)$ with the right-hand side of (4.1).
6: Compute ζ^ℓ using p_1 (see (3.7)).
7: **if** $\|\zeta^\ell\|_U < \varepsilon$ **or** $\ell = \ell^{\max}$ **then**
8: Return suboptimal control u^i and STOP.
9: **else**
10: Set $\hat{J}'(u^i) = \sigma u^i - \mathcal{B}^\star(p^\ell + p_2)$.
11: Perform a projected gradient step and an Armijo linesearch [12] to get a new control $u^{i+1} \in U_{\mathsf{ad}}$.
12: **end if**
13: **end for**
14: Call Algorithm 1 with initial control u^k, a maximal number $\ell^{\max} > \ell$ of POD ansatz functions, and a stopping tolerance $\varepsilon > 0$.

Let $T = 1$ be the terminal time, $\Omega = (0,1) \times (0,1) \subset \mathbb{R}^2$ be the unit square and

$$\Omega_1 = \big(0, \tfrac{1}{2}\big) \times \big(0, \tfrac{1}{2}\big), \qquad \Omega_2 = \big(\tfrac{1}{2}, 1\big) \times \big(0, \tfrac{1}{2}\big),$$
$$\Omega_3 = \big(0, \tfrac{1}{2}\big) \times \big(\tfrac{1}{2}, 1\big), \qquad \Omega_4 = \big(\tfrac{1}{2}, 1\big) \times \big(\tfrac{1}{2}, 1\big).$$

We write $\mathbf{x} = (x_1, x_2)$ for an element in Ω and set $U = L^2(0,T;\mathbb{R}^4)$ as well as $z = \chi_{\Omega_1}(\mathbf{x}) - \chi_{\Omega_3}(\mathbf{x})$. Consider the problem (compare Example 2.3, Remark 2.3 and Remark 2.4)

$$\min J(y,u) = \frac{1}{2}\int_0^T \int_\Omega \big(y(t,\mathbf{x}) - z(\mathbf{x})\big)^2 \,\mathrm{d}\mathbf{x}\mathrm{d}t + \frac{1}{40}\sum_{i=1}^4 \int_0^T u_i^2(t)\,\mathrm{d}t$$

subject to the linear parabolic equation

$$\begin{aligned} y_t(t,\mathbf{x}) - \Delta y(t,\mathbf{x}) + (x_1 + x_2)y(t,\mathbf{x}) &= \sin(\pi t) + \sum_{i=1}^4 u_i(t)\chi_{\Omega_i}(\mathbf{x}), && (t,\mathbf{x}) \in Q, \\ y(t,\mathbf{s}) &= 0, && (t,\mathbf{s}) \in \Sigma, \\ y(0,\mathbf{x}) &= 2\sin(\pi x_1)e^{-x_2}, && \mathbf{x} \in \Omega \end{aligned}$$

and the inequality constraints

$$u \in U_{\mathsf{ad}} = \big\{v \in U \mid -0.03 \leq v_i(t) \leq 0.03 \text{ for } t \in [0,T] \text{ and } 1 \leq i \leq 4\big\}.$$

Numerical solution with a finite difference approximation. In our first numerical test we solve the optimal control problem by applying the primal-daul active set strategy (see [5, 6]). The spatial variable is discretized by the classical finite difference (FD) approximation, i.e., we utilize the standard five-point stencil to discretize the Laplace operator. For the time intergration we apply the Crank-Nicolson method. We use a uniform grid in the x_1- and x_2-direction with the mesh size $h = 1/50$. In the time interval we use the uniform step size $\Delta t = 1/70$. The

optimization method requires 562 seconds CPU time. The FD optimal controls u_i^{FD}, $i = 1, \ldots, 4$, are presented in the left plot of Figure 5.1.

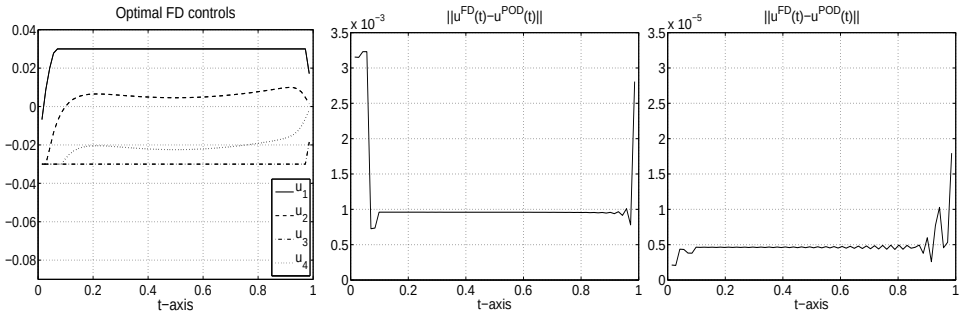

FIGURE 5.1. Optimal FD controls u^{FD} (left), $\|u^{\mathrm{FD}}(t) - u^{\mathrm{POD}}(t)\|_2$ for the results of Algorithm 1 (middle) and of Algorithm 2 (right).

Numerical solution with Algorithm 1. In the second test we solve the optimal control problem by applying a POD Galerkin approximation. For the time integration we apply again the Crank-Nicolson method. Algorithm 1 is utilized with the input variables $u = 0 \in U_{\mathsf{ad}}$, $\ell = 10$, $\ell^{\max} = 50$ and $\varepsilon = \max(\Delta t^2, h^2)/2 = h^2/2 = 2 \cdot 10^{-4}$. Notice that the value for ε is motivated by the discretization error of the Crank-Nicolson and the finite difference scheme. Algorithm stops after 36 seconds CPU time. The difference between the POD optimal control u^{POD} and the FD optimal control u^{FD} is shown in the middle plot of Figure 5.1. It turns out that the differences are bigger than the discretization error, which is of the order $\mathcal{O}(\Delta t^2 + h^2) \approx \varepsilon$ We observe that $\ell = \ell^{\max}$ holds, but $\|\zeta^\ell\|_U \approx 1.2 \cdot 10^{-3} > \varepsilon$. Taking the discretization errors into account, the estimation by ζ^ℓ is sharp: we have $\|u^{\mathrm{FD}} - u^{\mathrm{POD}}\|_U \approx 1.23 \cdot 10^{-3} \approx \|\zeta^\ell\|_U > \varepsilon$.

Numerical solution with Algorithm 2. For the time integration we use the Crank-Nicolson method again. As in the previous test we choose $u = 0 \in U_{\mathsf{ad}}$, $\ell = 10$, $\ell^{\max} = 50$ and $\varepsilon = 2 \cdot 10^{-4}$. We improve our POD basis by applying one single gradient projection step at the beginning. Algorithm 2 stops after 16 seconds CPU time. The difference between the suboptimal control u^{POD} and the finite-difference optimal control u^{FD} is presented in the right plot of Figure 5.1. We observe that coincides with the finite difference ones. It turns out that $\ell = 24$ POD ansatz function are used. Moreover,

$$\|\zeta^\ell\|_U \approx 1.583 \cdot 10^{-5} < \varepsilon \quad \text{and} \quad \|u_{\mathrm{FD}} - u^{\mathrm{POD}}\|_U \approx 1.581 \cdot 10^{-5}.$$

6. Conclusions

In this paper we present an approach for POD Galerkin approximations to optimal control problems, where the adaptation of the POD basis is combined with the adaptivity with respect to the number of POD basis functions. This strategy turns out to be very efficient with respect to the numerical example. In a future research we plan to study further combinations of OS-POD and POD a-posteriori error analysis to generate robust and accurate POD surrogate models for optimal

control problems. Let us mention that OS-POD is developped for nonlinear optimal control problems. Thus, if we can derive a POD a-posteriori error aalysis for some classes of nonlinear problems, the present approach can be also utilized for nonlinear problems.

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