A posteriori error estimation for nonlinear parabolic boundary control

Eileen Kammann
Technische Universitt Berlin
Institut für Mathematik
D-10623 Berlin, Germany
Email: kammann@math.tu-berlin.de

Fredi Tröltzsch
Technische Universitt Berlin
Institut für Mathematik
D-10623 Berlin, Germany
Email: troeltzsch@math.tu-berlin.de

***Abstract*— We consider the following problem of error estimation for the optimal control of nonlinear parabolic partial differential equations: Let an arbitrary control function be given. How far is it from the next locally optimal control? Under natural assumptions including a second order sufficient optimality condition for the (unknown) locally optimal control, we are able to estimate the distance between the two controls. To do this, we need some information on the lowest eigenvalue of the reduced Hessian. We apply this technique to a model reduced optimal control problem obtained by proper orthogonal decomposition (POD). The distance between a (suboptimal) local solution of the reduced problem to a local solution of the original problem is estimated.**

I. Introduction

We focus on the following question for the optimal control problem of semilinear parabolic equations: Let a numerical approximation u_s for a locally optimal control be given. For instance, it can be the solution to some reduced order optimization model. How far is this control from the nearest locally optimal control $\bar{u}$? We want to quantify the error $\|u_s - \bar{u}\|$ in an appropriate norm.

We will concentrate on suboptimal controls u_s obtained by proper orthogonal decomposition (POD). We extend a method suggested in [1] to the case of semilinear equations.

II. Optimal control problem and optimality conditions

We explain our method for the following special optimal control problem in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$:

$$(P) \quad \min\ J(y,u) := \frac{1}{2}\int_\Omega (y(x,T) - y_d(x))^2\,dx + \frac{\lambda}{2}\int_0^T u(t)^2\,dt$$

in $\Omega = (0,\ell)$, subject to

$$\begin{aligned} y_t(x,t) - y_{xx}(x,t) &= 0 && \text{in } \Omega \times (0,T) \\ y_x(0,t) &= 0 && \text{in } (0,T] \\ y_x(\ell,t) + y^4(\ell,t) &= u(t) && \text{in } (0,T] \\ y(x,0) &= 0 && \text{in } \Omega \end{aligned}$$

and to the control constraints $\quad |u(t)| \le 1.$

In this problem, $y_d \in L^2(\Omega)$; T, λ, $\ell > 0$ are given. For the control we require $u \in L^\infty(0,T)$, and y is defined as weak solution of the parabolic equation in $W(0,T) \cap C(\bar{Q})$; we have set $Q := \Omega \times (0,T)$.

Let u be an arbitrary control for (P). Associated with u, we have the state function y_u is the unique solution of the parabolic equation above. Moreover, we define the associated adjoint state p_u as the weak solution to the adjoint equation

$$\begin{aligned} -p_t(x,t) - p_{xx}(x,t) &= 0 && \text{in } Q \\ p_x(0,t) &= 0 && \text{in } (0,T] \\ p_x(\ell,t) + 4\,y_u^3(\ell,t)\,p(\ell,t) &= 0 && \text{in } (0,T] \\ p(x,T) &= y_u(x,T) - y_d(x) && \text{in } \Omega. \end{aligned}$$

Let now $\bar{u}$ be a locally optimal control for (P) and let $\bar{p} := p_{\bar{u}}$ be the associated adjoint state. Then the following standard necessary optimality condition must be satisfied for almost all $t \in [0,T]$:

$$(\bar{p}(\ell,t) + \lambda\bar{u}(t))(u - \bar{u}(t)) \ge 0 \quad \forall u \in [-1,1],$$

From this variational inequality, we deduce the implications

$$\begin{aligned} \bar{p}(\ell,t) + \lambda\bar{u}(t) < 0 \quad &\Rightarrow \quad \bar{u}(t) = 1, \\ \bar{p}(\ell,t) + \lambda\bar{u}(t) > 0 \quad &\Rightarrow \quad \bar{u}(t) = -1. \end{aligned}$$

On the other hand, this also implies

$$\left.\begin{aligned} \bar{u}(t) = -1 \quad &\Rightarrow \quad \bar{p}(\ell,t) + \lambda\bar{u}(t) \ge 0 \\ \bar{u}(t) \in (-1,1) \quad &\Rightarrow \quad \bar{p}(\ell,t) + \lambda\bar{u}(t) = 0 \\ \bar{u}(t) = 1 \quad &\Rightarrow \quad \bar{p}(\ell,t) + \lambda\bar{u}(t) \le 0 \end{aligned}\right\} \qquad (1)$$

a.e. in $(0,T)$. This is the basis for the *perturbation method.*

III. The perturbation method

For the optimal control of ordinary differential equations, the perturbation method was introduced by Dontchev et al. [2] and Malanowski, Büskens, and Maurer.

Let $u_s \neq \bar{u}$ be a suboptimal control, obtained by some numerical method. Then u_s will not in general satisfy the optimality conditions above. However, u_s satisfies the condition

$$(p_s(\ell,t) + \lambda u_s(t) + \zeta(t))(u - u_s(t)) \ge 0 \quad \forall u \in [-1,1],$$

978-1-4577-0914-2/11/$26.00 ©2011 IEEE

if the perturbation $\zeta \in L^2(0,T)$ is properly chosen. Following Arada et al. [3] we define

$$\zeta(t) := \begin{cases} [p_s(\ell,t) + \lambda u_s(t)]_- & \text{if } u_s(t) = -1 \\ -(p_s(\ell,t) + \lambda u_s(t)) & \text{if } u_s(t) \in (-1,1) \\ [p_s(\ell,t) + \lambda u_s(t)]_+ & \text{if } u_s(t) = 1, \end{cases} \qquad (2)$$

where, for $a \in \mathbb{R}$, $[a]_+ := \frac{1}{2}(|a| + a)$, $[a]_- := \frac{1}{2}(|a| - a)$. With this choice of ζ, u_s satisfies the necessary optimality conditions for the perturbed control problem

$$(P_\zeta) \quad \min J(y_u, u) + \int_0^T \zeta(t) u(t)\, dt$$

subject to all other constraints of (P). An easy discussion shows that ζ is defined such that u_s obeys the counterpart of the conditions (1) formulated for (P_ζ).

IV. A posteriori error estimation

A. The error estimate

Define the reduced objective functional f by

$$f(u) := J(y_u, u).$$

By our construction above, $\bar{u}$ and u_s satisfy the necessary optimality conditions for the problems (P) and (P_ζ), respectively. Therefore, we have

$$\begin{aligned} f'(\bar{u})(u_s - \bar{u}) & \geq 0 \\ f'(u_s)(\bar{u} - u_s) + \big(\zeta\,,\, \bar{u} - u_s\big) & \geq 0, \end{aligned} \qquad (3)$$

where $\big(\cdot\,,\,\cdot\big)$ denotes the inner product of $L^2(0,T)$.

To quantify the distance of u_s to $\bar{u}$, it is natural to require that $\bar{u}$ satisfies a second-order sufficient optimality condition. If this is true, then the second derivative $f''(u)$ is positive definite in a certain L^∞- neighborhood of $\bar{u}$. To get an estimate, we have to assume that u_s belongs to this neighborhood. Notice that f'' is not twice differentiable in $L^2(0,T)$, we need the space $L^\infty(0,T)$, cf. [4].

Theorem. *Suppose there are a radius $\rho > 0$ and some $\alpha > 0$ such that*

$$f''(u)h^2 \geq \alpha \, \|h\|^2_{L^2(0,T)} \quad \forall u \in B_\rho(\bar{u}), \;\; \forall h \in L^2(0,T).$$

If u_s belongs to $B_\rho(\bar{u})$, then it holds

$$\|u_s - \bar{u}\|_{L^2(0,T)} \leq \frac{1}{\alpha} \, \|\zeta\|_{L^2(0,T)}.$$

Proof. Adding the inequalities (3), we find

$$(f'(u_s) - f'(\bar{u}))(\bar{u} - u_s) + \big(\zeta\,,\, \bar{u} - u_s\big) \geq 0. \qquad (4)$$

By the mean value theorem, there exists $u_\theta \in [u_s, \bar{u}]$ so that

$$-(f'(u_s) - f'(\bar{u}))(\bar{u} - u_s) = f''(u_\theta)(u_s - \bar{u})^2.$$

Therefore (4) yields

$$f''(u_\theta)(\bar{u} - u_s)^2 \;\leq\; \big(\zeta\,,\, \bar{u} - u_s\big),$$

where u_θ belongs to $[u_s, \bar{u}]$, hence $u_\theta \in B_\rho(\bar{u})$.
Invoking the assumed second-order coercivity condition, we obtain

$$f''(u_\theta)(\bar{u} - u_s)^2 \geq \alpha \, \|\bar{u} - u_s\|^2_{L^2(0,T)}.$$

By the Cauchy-Schwarz inequality,

$$\big(\zeta\,,\, \bar{u} - u_s\big) \leq \|\zeta\|_{L^2(0,T)} \, \|\bar{u} - u_s\|_{L^2(0,T)},$$

it follows

$$\alpha \, \|\bar{u} - u_s\|^2_{L^2(0,T)} \leq \|\zeta\|_{L^2(0,T)} \, \|u_s - \bar{u}\|_{L^2(0,T)}$$

implying the statement of the theorem. □

B. Numerical application of the perturbation method

1) General remarks: A numerical application of this result requires the following information:

- The second derivative f'' is uniformly positive definite in an L^∞-ball around $\bar{u}$. This is equivalent to a second-order sufficient condition at $\bar{u}$.
- The suboptimal u_s is sufficiently close to $\bar{u}$.
- We know α, the associated coercivity constant.

In general, none of them is known in advance, except the equation is linear. Therefore, we somehow have to trust that u_s was already determined sufficiently close to $\bar{u}$ while the latter function satisfies the second-order condition. Assumptions of this type are more or less unavoidable in the numerical solution of nonlinear optimization problems. This concerns in particular the second-order sufficient optimality condition. A similar assumption is that of a constraint qualification in nonlinear optimization that guarantees the existence of Lagrange multipliers. Also this assumption can often not be verified in advance.

A serious obstacle is the estimation of the coercivity constant α. We try to estimate α by establishing the reduced Hessian associated with u_s and computing its smallest eigenvalue.

2) Application to (P): For a numerical implementation in the case of our boundary control problem (P), we take an equidistant partition of $[0,T]$ with mesh size τ and assume that u is a step function expressed by a vector $\vec{u}_\tau$ having the "step heights" as entries.

In this way, we obtain a discrete version of the reduced functional f,

$$\varphi(\vec{u}_\tau) := f(u_\tau),$$

where u_τ is the step function associated with the vector $\vec{u}_\tau$.

Denote by H_s the reduced Hessian matrix, associated with the suboptimal solution $\vec{u}_{s,\tau}$,

$$H_s = \varphi''(\vec{u}_{s,\tau})$$

and assume that H_s has the smallest eigenvalue $\sigma^s_{min} > 0$.

Then it holds

$$\vec{u}_\tau^T H_s \vec{u}_\tau \;\geq\; \sigma^s_{min} \, |\vec{u}_\tau|_2^2 \;=\; \frac{\sigma^s_{min}}{\tau} \|u_\tau\|^2_{L^2(0,T)}$$

for all vectors $\vec{u}_\tau$ associated with a corresponding step function u_τ.
If the problem (P) behaves well around the unknown $\bar{u}$, i.e.

our coercivity assumptions are satisfied, and u_s is sufficiently close to $\bar{u}$, then

$$\alpha \approx \frac{\sigma^s_{min}}{\tau}.$$

If there holds in addition $\frac{\sigma^s_{min}}{\tau} \leq \alpha$, then

$$\|u_s - \bar{u}\|_{L^2(0,T)} \leq \frac{\tau}{\sigma^s_{min}} \|\zeta\|_{L^2(0,T)}.$$

3) Numerical application: We first should mention that all arguments above were presented as if we were able to determine the state functions y and p exactly. This was tacitly assumed to keep the presentation simple. A precise estimation should also include the error due to a numerical discretization of the parabolic state equation and the associated adjoint equation. Let us therefore assume that the solution of these equations is done very precisely so that the associated error can be neglected.

To estimate the distance of a suboptimal control u_s to the unknown exact locally optimal control $\bar{u}$, one has to proceed as follows:

(i) Compute the state $y_s = y_{u_s}$ and the adjoint state p_{u_s}.
(ii) Determine the residual ζ of the optimality system according to (2).
(iii) Compute the reduced Hessian H_s for the discretized problem and determine its smallest eigenvalue σ^s_{min}.
(iv) Estimate by

$$\|u_s - \bar{u}\|_{L^2(0,T)} \approx \frac{\tau}{\sigma^s_{min}} \|\zeta\|_{L^2(0,T)}.$$

V. An application to model reduction by POD

A. Proper orthogonal decomposition

To establish a model reduced optimal control problem, we apply standard POD. We find a small Galerkin basis that well expresses the main properties of the underlying system.

Step 1. Determine snapshots.

We compute the state $y_{\tilde{u}}$ for a useful control $\tilde{u}$. For instance, $\tilde{u} = 0$ is not useful, since $y_{\tilde{u}} = 0$. We took $\tilde{u}(t) = -1 + 2t/T, \quad 0 \leq t \leq T$.

For a partition of $[0, T]$, $t_i = i/n \cdot T, i = 0, \ldots, n$, we computed the snapshots $y_i(\cdot) := y(\cdot, t_i), i = 0, \ldots, n$, of the state $y_{\tilde{u}}$. To have some typical number at hand, think of $n = 100$.

Step 2. Find a small Galerkin basis.

Define $V := H^1(\Omega)$, $V^n :=$ span $\{y_0, \ldots, y_n\}$, let $d =$ dim V^n, fix $r \in \mathbb{N}, r \leq d$. In our tests, we took $r = 3, 4, 5$.

Establish an orthonormal system $\{\Phi_1, \ldots, \Phi_r\}$ by

$$\min_{\Phi_1,\ldots,\Phi_r} \sum_{i=0}^{n} \alpha_j \Big\| y_j - \sum_{i=1}^{r} (\Phi_i \, , \, y_j) \Phi_i \Big\|_V^2$$

with certain weights $\alpha_j > 0$. This step is accomplished by solving a certain eigenvalue problem, see e.g. Kunisch and Volkwein [5] or Volkwein [6].

Step 3. Set up the reduced PDE.

With the small Galerkin basis $\{\Phi_1, \ldots, \Phi_r\}$, we apply the standard Galerkin method: Based on the ansatz

$$y(x, t) = \sum_{i=1}^{r} \eta_i(t) \Phi_i(x),$$

we obtain the system

$$\begin{aligned} \frac{d}{dt}(y(\cdot, t) \, , \, \Phi_j)_\Omega + (\nabla y(\cdot, t) \, , \, \nabla \Phi_j)_\Omega \\ +(y^4(\cdot, t) \, , \, \Phi_j)_{\partial\Omega} = (u(t) \, , \, \Phi_j)_{\partial\Omega}. \end{aligned}$$

for all $j = 1, ..., r$.

Next, the associated low-dimensional optimal control problem is solved to obtain the suboptimal control u_r with state y_r. For this purpose, we used an SQP method.

Step 4. POD a posteriori error estimation.

The a posteriori estimation of $\|\bar{u} - u_r\|_{L^2(0,T)}$ is done by our perturbation method. This requires the full state $y_r := y_{u_r}$ and the solution $p_r = p_{u_r}$ of the adjoint equation

$$\begin{aligned} -p_t(x, t) - p_{xx}(x, t) &= 0 \\ p_x(0, t) &= 0 \\ p_x(\ell, t) + 4\, y_r^3(\ell, t) p(\ell, t) &= 0, \\ p(x, T) &= y_r(x, T) - y_d(x). \end{aligned}$$

In this way, we have to solve two full size PDEs. Then we determined the associated reduced Hessian matrix and estimated as explained in Section IV. We increased the number r, if the computed estimate was too large. In this case, we solved the associated slightly larger reduced control problem.

B. Numerical test

We report on one of our numerical tests, where we considered (P) in $\Omega = (0, 1)$ with $T = 1.58$, $y_d(x) := (1 - x^2)/2$ and $\lambda = 1/10$.

The state equation and the adjoint equation were solved by a finite element scheme with $m = 400$ degrees of freedom. A semi-implicit Euler scheme was applied for solving the semidiscrete equation PDEs. Next, 200 snapshots were taken and the small Galerkin basis was set up accordingly.

As a substitute for the unknown exact locally optimal control, we solved the full discretized optimal control problem with spatial step size $h = \frac{1}{400}$ and time step size $\tau = \frac{T}{200}$ to determine the "exact" optimal solution $\bar{u}^{h,\tau}$.

Then we solved the POD reduced optimal control problem with r = 2, ..., 5 POD ansatz functions. Already for $r = 4$, the computed suboptimal control cannot be graphically distinguished from the "exact" optimal control $\bar{u}^{h,\tau}$ presented in Fig. 1.

The table below indicates that the order of the error is well expressed by our method of a posteriori estimation.

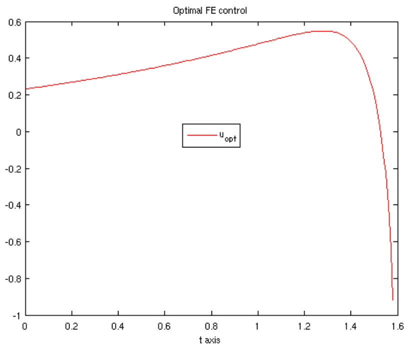

Fig. 1. Optimal control in the example

r	$\|\bar{u}^{h,\tau} - u_r\|_{L^2(0,T)}$	$\frac{\tau}{\sigma^r_{min}} \|\zeta\|_{L^2(0,T)}$
1	3.622e-1	6.440e-1
2	5.745e-2	6.471e-2
3	3.728e-3	4.606e-3
4	8.616e-4	4.749e-4
5	1.121e-3	7.407e-4
6	1.101e-3	7.095e-4

The tremendous gain in performance by the model reduction is shown in the next table:

Computational step	CPU time
FE optimization	143 s
Snapshots for $r = 4$	0.7 s
POD basis for $r = 4$	0.1 s
Optimization ROM for $r = 4$	0.4 s

VI. Conclusion

We have suggested a method of a posteriori error estimation for estimating the distance of a computed suboptimal control to a sufficiently close unknown (exact) locally optimal control. The method is based on some second-order coercivity assumption on the exact optimal control. Moreover, it requires that the suboptimal control is sufficiently close to the exact one. Assumptions of this type seem to be unavoidable for nonlinear equations. They were also needed in any method of model reduction, if a precise error estimate for the difference between the solution of the given PDE and its reduced version were available.

The application of our method to a nonlinear boundary control problem with Stefan-Boltzmann boundary condition demonstrated the applicability of our method. We have also discussed nonlinear distributed control problems with similar success. More details are presented for a general class of parabolic control problems in [7].

References

[1] F. Tröltzsch and S. Volkwein, “Pod a-posteriori error estimates for linear-quadratic optimal control problems,” *Computational Optimization and Applications*, vol. 44, pp. 83–115, 2009.

[2] A. L. Dontchev, W. W. Hager, A. B. Poore, and B. Yang, “Optimality, stability, and convergence in nonlinear control,” *Applied Math. and Optimization*, vol. 31, pp. 297–326, 1995.

[3] N. Arada, E. Casas, and F. Tröltzsch, “Error estimates for the numerical approximation of a semilinear elliptic control problem,” *Computational Optimization and Applications*, vol. 23, pp. 201–229, 2002.

[4] F. Tröltzsch, *Optimal Control of Partial Differential Equations. Theory, Methods and Applications*. Providence: American Math. Society, 2010, vol. 112.

[5] K. Kunisch and S. Volkwein, “Galerkin proper orthogonal decomposition methods for parabolic problems,” *Numerische Mathematik*, vol. 90, pp. 117–148, 2001.

[6] S. Volkwein, “Model reduction using proper orthogonal decomposition, Lecture Notes, Institute of Mathematics and Scientific Computing, University of Graz,” 2007.

[7] E. Kammann and F. Tröltzsch, “A method of a-posteriori estimation with appliction to proper orthogonal decomposition,” *Submitted*, 2011.