

Optimality System Proper Orthogonal Decomposition for Optimal Control Problems with Control and State Constraints

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Problem formulation

We consider the optimal control problem

$$\min_{y,u,w} J(y, u, w) = \int_{\Theta} \frac{1}{2} \|y(t) - y_d(t)\|_H^2 + \frac{\sigma_u}{2} \|u(t)\|_{\mathbb{R}^{N_u}}^2 + \frac{\sigma_w}{2} \|w(t)\|_{\mathbb{R}^{N_w}}^2 dt \quad (\text{OCP})$$

on the time interval $\Theta = [0, T]$ subject to the linear parabolic pde constraint

$$\begin{aligned} \langle \dot{y}(t), \varphi \rangle_{V^*, V} + \langle \mathcal{A}y(t), \varphi \rangle_{V^*, V} &= \langle \mathcal{B}u(t), \varphi \rangle_{V^*, V} & \forall \varphi \in V \\ \langle y(0), \varphi \rangle_H &= \langle y_0, \varphi \rangle_H & \forall \varphi \in H \end{aligned}$$

and the control and state constraints

$$y_a(t) \leq \varepsilon w(t) + (\mathcal{I}y)(t) \leq y_b(t) \quad \& \quad u_a(t) \leq u(t) \leq u_b(t),$$

with the operators $\mathcal{B} : L^2(\Theta, \mathbb{R}^{N_u}) \rightarrow L^2(\Theta, H)$ and $\mathcal{I} : L^2(\Theta, H) \rightarrow L^2(\Theta, \mathbb{R}^{N_w})$,

$$(\mathcal{B}u)(t, x) = \sum_{i=1}^{N_u} u_i(t) \chi_i(x), \quad (\mathcal{I}y)_i(t) = \int_{\Omega} \pi_i(x) y(t, x) dx.$$



Transformation on pure box constraints

Introducing a transformed penalty $\omega(t) = \varepsilon w(t) + \mathcal{I}y(t)$, we get the equivalent transformed optimal control problem (TOCP)

$$\min_{y, u, \omega} \tilde{J}(y, u, \omega) = \int_{\Theta} \frac{1}{2} \|y(t) - \hat{y}_d(t)\|_H^2 + \frac{\sigma_u}{2} \|u(t)\|_{\mathbb{R}^{N_u}}^2 + \frac{\sigma_w}{2\varepsilon^2} \|\omega(t) - \mathcal{I}y(t)\|_{\mathbb{R}^{N_w}}^2 dt$$

subject to the *homogeneous* pde

$$\dot{y}(t) + \mathcal{A}y(t) = \mathcal{B}u(t) \quad \& \quad y(0) = 0$$

and the *explicit* penalty and control constraints

$$\hat{y}_a(t) \leq \omega(t) \leq \hat{y}_b(t) \quad \& \quad u_a(t) \leq u(t) \leq u_b(t)$$

where $\hat{y}_d = y_d - \hat{y}$, $\hat{y}_a = y_a - \mathcal{I}\hat{y}$, $\hat{y}_b = y_b - \mathcal{I}\hat{y}$ and \hat{y} solves

$$\dot{\hat{y}}(t) + \mathcal{A}\hat{y}(t) = 0 \quad \& \quad \hat{y}(0) = y_0.$$



Well-posedness and optimality conditions

THEOREM. Assume that the closed, convex and bounded set

$$\{(y, u, \omega) \mid \dot{y} + \mathcal{A}y = \mathcal{B}u \ \& \ y(0) = 0 \ \& \ u \in [u_a, u_b] \ \& \ \omega \in [\hat{y}_a, \hat{y}_b]\}$$

is nonempty. Then there exists a unique solution $(\bar{y}, \bar{u}, \bar{\omega})$ to (TOCP).

Further, defining the *active and inactive sets*

$$\begin{aligned} \mathcal{A}_a^u &= \{t \mid \frac{1}{\sigma_u} \mathcal{B}^* \bar{p} < u_a\}, & \mathcal{A}_b^u &= \{t \mid \frac{1}{\sigma_u} \mathcal{B}^* \bar{p} > u_a\}, & \mathcal{A}_i^u &= \Theta \setminus (\mathcal{A}_a^u \cup \mathcal{A}_b^u) \\ \mathcal{A}_a^y &= \{t \mid \mathcal{I} \bar{y} < \hat{y}_a\}, & \mathcal{A}_b^y &= \{t \mid \mathcal{I} \bar{y} > \hat{y}_b\}, & \mathcal{A}_i^y &= \Theta \setminus (\mathcal{A}_a^y \cup \mathcal{A}_b^y), \end{aligned}$$

the following first-order optimality system (OS) is fulfilled:

$$\begin{aligned} \dot{\bar{y}}(t) + \mathcal{A}y(t) - \mathcal{B}\bar{u}(t) &= 0, & \bar{y}(0) &= 0, \\ -\dot{\bar{p}}(t) + \mathcal{A}p(t) + \frac{\sigma_w}{\varepsilon^2} (\mathcal{I}^* (\mathcal{I}y(t) - \omega(t))) + (y(t) - \hat{y}_d(t)) &= 0, & \bar{p}(T) &= 0, \\ \bar{u}(t) - \frac{1}{\sigma_u} \chi_i^u(t) \mathcal{B}^* \bar{p}(t) - (\chi_a^u(t) u_a(t) + \chi_b^u(t) u_b(t)) &= 0, \\ \bar{\omega}(t) - \chi_i^y(t) \mathcal{I} \bar{y}(t) - (\chi_a^y(t) \hat{y}_a(t) + \chi_b^y(t) \hat{y}_b(t)) &= 0. \end{aligned}$$



Primal-dual active set strategy (PDASS)

Algorithm (Primal-dual active set strategy)

Require: Initial state-adjoint state pair (y^0, p^0) .

1: Set $k = 0$

2: **repeat**

3: Calculate the six active and inactive sets with respect to (y^k, p^k) .

4: Solve *linear* primal-dual system (OS) with these fix sets to get (y^{k+1}, p^{k+1})

5: Set $k = k + 1$

6: **until** the current and the previous active and inactive sets coincide.

7: Return control $\bar{u} \in L^2(\Theta, \mathbb{R}^{N_u})$ and penalty $\bar{w} = \frac{1}{\varepsilon}(\omega - \mathcal{I}y) \in L^2(\Theta, \mathbb{R}^{N_w})$.



Proper orthogonal decomposition (POD)

Problem: After elimination of u, ω , the discrete linear system (OS) is still of the dimension $2N_t N_x$.

Idea: For $\ell \ll N_x$, find an *optimal* orthonormal system $\psi = (\psi_1, \dots, \psi_\ell) \in V^\ell$ such that the projection error of \bar{y} on the space $\text{span}(\psi)$ is minimal:

$$\min_{\phi \in V^\ell \text{ ONB}} \int_{\Theta} \left\| \bar{y}(t) - \sum_{i=1}^{\ell} \langle \bar{y}(t), \phi_i \rangle_V \phi_i \right\|_V^2 dt. \quad (\text{POD})$$

Realization: Perform an eigenvalue decomposition of a compact, self-adjoint, non-negative operator $\mathcal{R} : V \rightarrow V$ which includes the dynamics of the state solution.

Challenge: The *optimal* Galerkin ansatz requires the knowledge of the state solution \bar{y} which is not available.



Proper orthogonal decomposition (POD)

THEOREM. (Continuous version) Let $y \in C(0, T; V)$ be an *arbitrary* state and let $(\lambda_i, \psi_i)_{i \in \mathbb{N}}$ be an eigenvalue decomposition of

$$\mathcal{R}(y) : V \rightarrow V, \quad \mathcal{R}(y)\varphi = \int_{\Theta} \langle y(t), \varphi \rangle_V y(t) dt.$$

with $\lambda_i \geq \lambda_{i+1}$ for all $i \in \mathbb{N}$.

Then $(\psi_i)_{i \in \mathbb{N}}$ is a complete orthonormal system in V and the *rank- ℓ POD basis* $\psi^\ell = (\psi_1, \dots, \psi_\ell)$ is a solution to (POD).

A priori estimate: The projection error of y on $V^\ell = \text{span}(\psi)$ fulfills

$$\int_{\Theta} \left\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \phi_i \rangle_V \phi_i \right\|_V^2 = \sum_{i=\ell+1}^{\infty} \lambda_i.$$



Proper orthogonal decomposition (POD)

Discrete POD: Let $(t_1, \dots, t_{N_t}) \subseteq \Theta$ be a time discretization scheme with stepsize Δt and let $\varphi = (\varphi_1, \dots, \varphi_{N_x}) \subseteq V$ be a finite element basis with corresponding weights matrix $X = (\langle \varphi_i, \varphi_j \rangle_V)$.

Let $Y \in \mathbb{R}^{N_x \times N_t}$ be the coefficient matrix of a state

$$y^{\text{FE}}(t_j, x) = \sum_{i=1}^{N_x} Y_{ij} \varphi_i(x).$$

Then the coefficient matrix of a rank- ℓ POD basis $\psi \in \mathbb{R}^{N_x \times \ell}$ for y^{FE} is given by the discrete eigenvalue problem

$$\Delta t Y Y^T X \psi_l = \lambda_l \psi_l$$

and the l -th POD element in $V^{N_x} = \text{span}(\varphi)$ is represented by

$$\psi_l = \sum_{i=1}^{N_x} \psi_{il} \varphi_i.$$



Reduced order model (ROM)

1 ROM components:

- $\mathbf{M} = (\langle \psi_i, \psi_j \rangle_H) \in \mathbb{R}^{\ell \times \ell}$ and $\mathbf{A} = (\langle \mathcal{A}\psi_i, \psi_j \rangle_{V^*, V}) \in \mathbb{R}^{\ell \times \ell}$.
- $\mathbf{B} = (\langle \mathcal{B}_j^*, \psi_i \rangle_{V^*, V}) \in \mathbb{R}^{\ell \times N_u}$ and $\mathbf{I} = (\mathcal{I}_j \psi_i) \in \mathbb{R}^{N_w \times \ell}$.
- $\hat{y}_d(t) = (\langle \hat{y}_d(t), \psi_i \rangle_H) \in \mathbb{R}^{\ell}$.

2 ROM system:

$$\begin{aligned} \mathbf{M}\dot{\mathbf{y}}(t) + \mathbf{A}\mathbf{y}(t) - \mathbf{B}\mathbf{u}(t) &= 0, & \mathbf{y}(0) &= 0, \\ -\mathbf{M}\dot{\mathbf{p}}(t) + \mathbf{A}\mathbf{p}(t) + \frac{\sigma_w}{\varepsilon^2}(\mathbf{I}^T(\mathbf{I}\mathbf{y}(t) - \boldsymbol{\omega}(t))) + (\mathbf{M}\mathbf{y}(t) - \hat{y}_d(t)) &= 0, & \mathbf{p}(T) &= 0, \\ \mathbf{u}(t) - \frac{1}{\sigma_u}\boldsymbol{\chi}_i^u(t)\mathbf{B}^T\mathbf{p}(t) - (\boldsymbol{\chi}_i^u(t)\mathbf{u}_a(t) + \boldsymbol{\chi}_b^u(t)\mathbf{u}_b(t)) &= 0, \\ \boldsymbol{\omega}(t) - \boldsymbol{\chi}_i^y(t)\mathbf{I}\mathbf{y}(t) - (\boldsymbol{\chi}_a^y(t)\hat{y}_a(t) + \boldsymbol{\chi}_b^y(t)\hat{y}_b(t)) &= 0. \end{aligned}$$

3 ROM expansions:

$$\mathbf{y}^\ell(t) = \sum_{l=1}^{\ell} y_l(t)\psi_l, \quad \mathbf{p}^\ell(t) = \sum_{l=1}^{\ell} p_l(t)\psi_l, \quad \mathbf{u}^\ell = \mathbf{u}, \quad \boldsymbol{\omega}^\ell = \boldsymbol{\omega}$$



Reduced order model (ROM)

A posteriori error bound: Let (u, ω) be any suboptimal control-penalty pair. Then there exists some computable $\zeta \in L^2(\Theta, \mathbb{R}^{N_u} \times \mathbb{R}^{N_w})$ such that

$$\begin{aligned} & \int_{\Theta} \|u(t) - \bar{u}(t)\|_{\mathbb{R}^{N_u}}^2 + \|\omega(t) - \bar{\omega}(t)\|_{\mathbb{R}^{N_w}}^2 dt \\ & \leq \frac{1}{\min(\sigma_u^2, \sigma_w^2)} \int_{\Theta} \|\zeta(t)\|_{\mathbb{R}^{N_u} \times \mathbb{R}^{N_w}}^2 dt. \end{aligned}$$

In our numerical tests, the evaluation of this error estimator is *cheap* (compared to the effort of solving the optimization problem). Problems may arise here in case of *nonlinear* pdes.

In many applications, the error bounds are *sharp*, i.e. the error bound has the same order as the error itself.



Reduced order model (ROM)

Algorithm (Model reduction with iterative POD basis updates (IPOD))

Require: Initial control-penalty pair $(u^{(0)}, \omega^{(0)})$, POD basis rank ℓ , desired exactness ε , maximal iteration number k_{\max} .

1: Set $k = 0$

2: **repeat**

3: Solve the full state and adjoint state equations for $(y^{(k)}, p^{(k)})$.

4: Solve the POD eigenvalue problem for the rank- ℓ basis $\psi^{(k)}$.

5: Choose PDASS initialization $(y, p) = ((\langle y^{(k)}, \psi_l \rangle_H), (\langle p^{(k)}, \psi_l \rangle_H))$ and provide the PDASS algorithm to solve the ROM system; get feedback $(u^{(k)}, \omega^{(k)})$.

6: Set $k = k + 1$

7: **until** $\text{Aposti}(u^{(k)}, \omega^{(k)}) < \varepsilon$ or $k > k_{\max}$.

8: Return control $u^{(k)} \in L^2(\Theta, \mathbb{R}^{N_u})$ and penalty $w^{(k)} = \frac{1}{\varepsilon}(\omega^{(k)} - \mathcal{I}y) \in L^2(\Theta, \mathbb{R}^{N_w})$.



Optimality system proper orthogonal decomp. (OSPOD)

The optimal state required to determine the POD basis is known *implicitly*:

$$\min_{y, u, \omega, \psi} \tilde{J}(y, u, \omega, \psi) = \int_{\Theta} \frac{1}{2} \left\| \sum_{l=1}^{\ell} y_l \psi_l - \hat{y}_d \right\|_H^2 + \frac{\sigma_u}{2} \|u\|_{\mathbb{R}^{N_u}}^2 + \frac{\sigma_w}{2\varepsilon^2} \|\omega - \mathbf{I}(\psi)y\|_{\mathbb{R}^{N_w}}^2 dt$$

subject to the *two* state equations

$$\dot{y} + \mathcal{A}y = \mathcal{B}u, \quad y(0) = 0, \quad (1)$$

$$\mathbf{M}(\psi)\dot{y} + \mathbf{A}(\psi)y = \mathbf{B}(\psi)u, \quad y(0) = 0, \quad (2)$$

the POD eigenvalue problem

$$\mathcal{R}(y)\psi_l - \lambda_l \psi_l = 0, \quad \|\psi_l\|_V^2 = 1 \quad (3)$$

and the penalty and control constraints

$$\hat{y}_a(t) \leq \omega(t) \leq \hat{y}_b(t) \quad \& \quad u_a(t) \leq u(t) \leq u_b(t).$$



Optimality system proper orthogonal decomp. (OSPOD)

The corresponding dual system is similar to the optimality equations above:

$$-\dot{p} + \mathcal{A}p + \sum_{l=1}^{\ell} \langle y, \psi_l \rangle_V \mu_l + \sum_{l=1}^{\ell} \langle y, \mu_l \rangle_V \psi_l = 0, \quad (4)$$

$$-M\dot{p} + Ap + \frac{\sigma_w}{\varepsilon^2} \mathbf{I}^T (\mathbf{I}y - \omega) + (\mathbf{M}y - \hat{y}_d) = 0, \quad (5)$$

$$u - \frac{1}{\sigma_u} \chi_i^u (\mathcal{B}^* p + \mathbf{B}^T p) - (\chi_a^u u_a + \chi_b^u u_b) = 0, \quad (6)$$

$$\omega - \chi_i^y \mathbf{I}y - (\chi_a^y \hat{y}_a + \chi_b^y \hat{y}_b) = 0, \quad (7)$$

$$\mathcal{R}(y) \mu_l - \lambda_l \mu_l + \mathcal{N}(y, p, u, \omega, \psi) = 0. \quad (8)$$

with some nonlinear term \mathcal{N} arising by the ψ -differential and the active sets

$$\mathcal{A}_a^u = \{t \mid \frac{1}{\sigma_u} \mathcal{B}^* \bar{p} + \mathbf{B}^T p < u_a\},$$

$$\mathcal{A}_b^u = \{t \mid \frac{1}{\sigma_u} \mathcal{B}^* \bar{p} + \mathbf{B}^T p > u_a\},$$

$$\mathcal{A}_a^y = \{t \mid \mathbf{I}y < \hat{y}_a\},$$

$$\mathcal{A}_b^y = \{t \mid \mathbf{I}y > \hat{y}_b\}.$$



Optimality system proper orthogonal decomp. (OSPOD)

Algorithm (Optimality System POD (OSPOD))

Require: Initial control-penalty pair (u, ω) , POD basis rank ℓ , desired exactness ε .

- 1: **repeat**
 - 2: Solve the full state equation (1) for y .
 - 3: Solve the eigenvalue problem (3) for ψ .
 - 4: Solve the ROM problem (2), (5), (6), (7) for (y, p, u, ω) .
 - 5: Solve the eigenvalue problem (8) for μ .
 - 6: Solve the full adjoint equation (4) for p .
 - 7: Provide a descent step in direction $-\sigma_u u + \mathcal{B}^* p + \mathbf{B}^T p$ for u
 - 8: Provide a descent step in direction $-\frac{\sigma_w}{\varepsilon}(\omega - \mathbf{I}y)$ for ω .
 - 9: **until** $\text{Aposti}(u, \omega) < \varepsilon$.
 - 10: Return control $u \in L^2(\Theta, \mathbb{R}^{N_u})$ and penalty $w = \frac{1}{\varepsilon}(\omega - \mathbf{I}y) \in L^2(\Theta, \mathbb{R}^{N_w})$.
-



Conclusion: POD & OSPOD

POD: Use a *problem specific* Galerkin ansatz with respect to some reference trajectory y .

OSPOD: Use the trajectory of the optimal state \bar{y} to get the *optimal* Galerkin basis.



Run 1: 1d state constraints, iterative POD updates

desired state y_Q & state constraint u_b

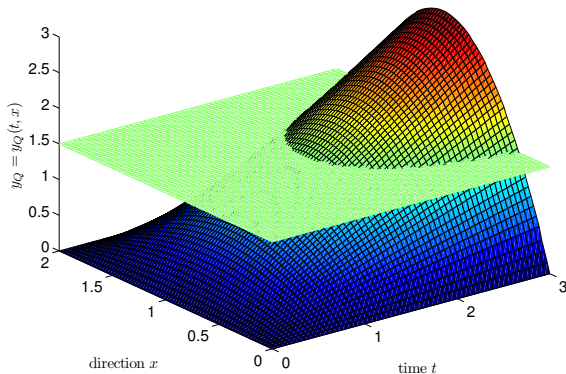


Fig. 1. The desired state $y_d \in L^2(0, T; H)$ and the upper mixed control-state bound y_b , interpreted as a pure pointwise state constraint. Here we apply a Lavrentiev regularization, i.e. we choose $w = u$ instead of introducing a new penalty variable.

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Run 1: 1d state constraints, iterative POD updates

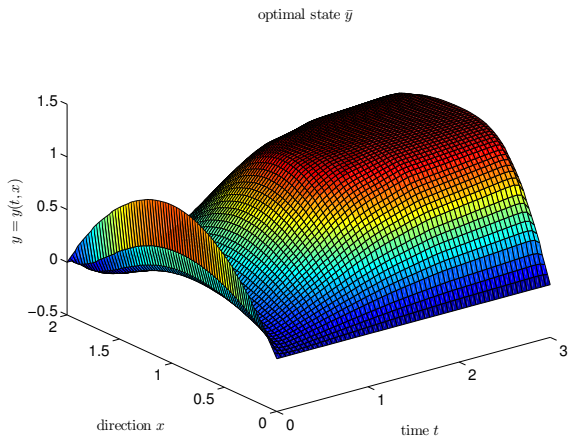


Fig. 2. The optimal state solution \bar{y} satisfying the state constraints. Regarding y_d , the optimal control \bar{u} has to be negative at $t = 0$ to tear down the initial value, then to be positive to achieve $\bar{y} \approx y_d$ and to be zero where \bar{y} hits the upper bound y_b .



Run 1: 1d state constraints, iterative POD updates

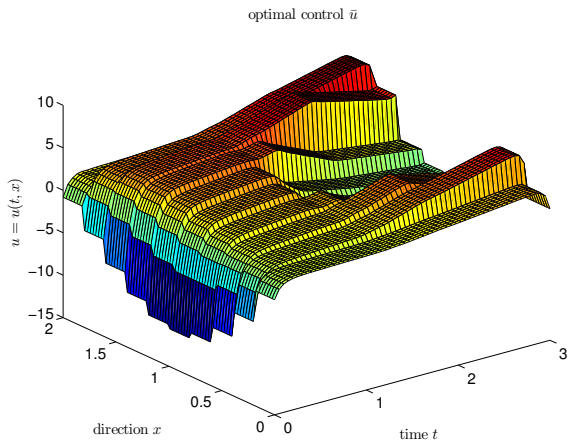


Fig. 3. The optimal control term $\mathcal{B}\bar{u} \in L^2(0, T; H)$ controlling the state equation and regularizing the state constraint. If the regularization parameter σ_u is chosen close to zero, one observes that $\mathcal{B}\bar{u}$ develops singularities between the active and inactive sets.



Run 1: 1d state constraints, iterative POD updates

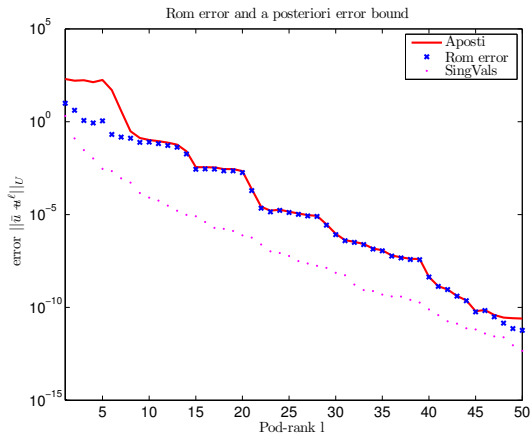
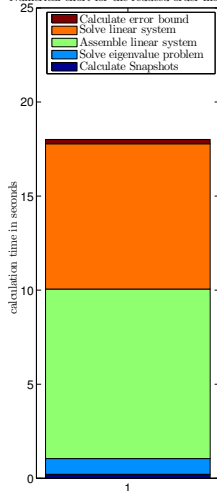


Fig. 4. The ROM errors of the control u^ℓ for different ranks $\ell = 1, \dots, 50$ of an updated POD basis, the error bound provided by the a posteriori error estimator and the singular values (squares of the eigenvalues) of the operator \mathcal{R} which can be used as a costless error indicator.



Run 1: 1d state constraints, iterative POD updates

Numerical effort for the reduced order model



Process	Time	#	Total
Assemble full system	0.66 sec	9×	5.97 sec
Solve full system	22.27 sec	9×	200.43 sec
Total			206.40 sec
Solve full snapshots equations	0.11 sec	2×	0.21 sec
Solve eigenvalue problem	0.42 sec	2×	0.84 sec
Assemble ROM system	0.53 sec	17×	9.01 sec
Solve ROM system	0.45 sec	17×	7.72 sec
Evaluate error estimator	0.11 sec	2×	0.23 sec
Total			18.01 sec

Tab. 1. The calculation times for solving the optimization problem with and without model reduction. With 25 POD elements, the ROM problem has to be solved two times; solvings of two eigenvalue problems are required in addition to update the POD basis. Nevertheless, 91.27% of the calculation time is spared in total.

Fig. 5. The numerical effort of the single algorithm processes for solving the ROM problem on an Intel(R) Core(TM) i5 2.40GHz processor.



Run 2: 1d sparse controls, IPOD vs. OSPOD

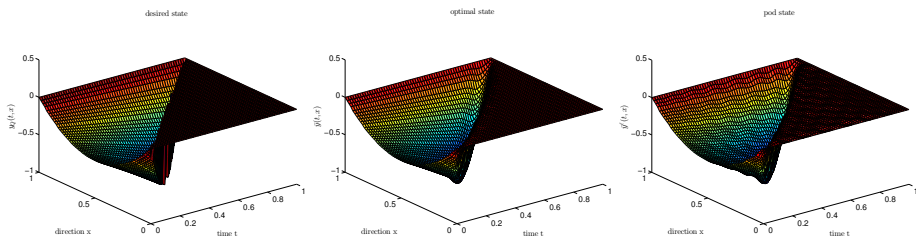


Fig. 6.1: The desired state $y_d \in L^2(0, T; H)$ which is chosen discontinuous in time and space. We choose $\sigma_H = 5.0e-10$ and generous control bounds $[u_a, u_b] = [-100, +100]$, but no state bounds.

Fig. 6.2: The full-order state solution \bar{y} which is slightly smoother at the crack of y_d , but fulfills $\bar{y} \approx y_d$.

Fig. 6.3: The rank-16 POD state y^ℓ for a well chosen POD basis and fulfills $y^\ell \approx \bar{y}$, but covers oscillations of small amplitude.



Run 2: 1d sparse controls, IPOD vs. OSPOD

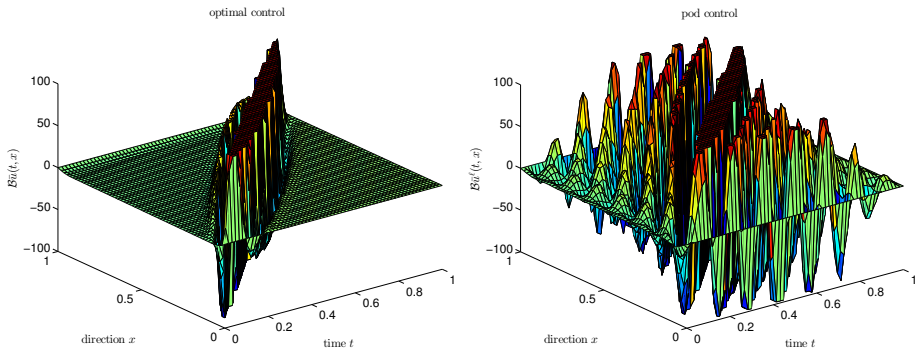


Fig. 7.1: The optimal control \bar{u} of the full order model resembles a *distribution* which has no L^2 representation (but is at least a Borel measure), a so-called *sparse control*.

Fig. 7.2: The rank-16 POD control u^ℓ causes the ridiculous control error $\|\bar{u} - u^\ell\| = 5.83e+02$ although the corresponding state fulfills $\|\bar{y} - y^\ell\| = 9.95e-03$. Notice that the objective functional is not strictly convex any more, so multiple optimal controls may appear.



Run 2: 1d sparse controls, IPOD vs. OSPOD

Process	Ospod initialization			Iterative updates		
	Time	#	Total	Time	#	Total
Determine snapshots	0.14 sec	25×	3.46 sec	0.15 sec	9×	1.37 sec
Provide gradient step	2.58 sec	20×	51.54 sec	0.00 sec	0×	0.00 sec
Solve eigenvalue problem	2.30 sec	25×	57.56 sec	2.45 sec	9×	22.03 sec
Assemble reduced system	1.39 sec	38×	88.88 sec	2.48 sec	136×	337.81 sec
Solve reduced system	0.40 sec	38×	15.01 sec	0.42 sec	136×	56.57 sec
Evaluate error estimator	0.46 sec	5×	2.31 sec	0.51 sec	9×	4.55 sec
Total			222.48 sec			427.69 sec

Tab. 2: With OSPOD initialization, the number of Newton steps within the optimization routine is decreased significantly compared to the IPOD basis updates. However, due to the expensive computations for the gradient steps, just around 50% of the computation time is spared in total.



Run 3: 1d control & state constraints, IPOD vs. OSPOD

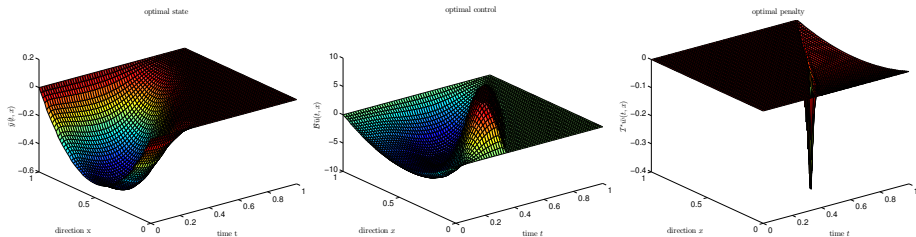


Fig. 8.1: The optimal state \bar{y} in case of regularization, but both with state constraints $y \in [-1, 0]$.

Fig. 8.2: The corresponding optimal control \bar{u} in the admissible interval $u \in [-7.5, +7.5]$.

Fig. 8.3: The corresponding optimal penalty \bar{w} which is nonzero just on the active set of the state solution and shows string activity only on the boundary of this set.



Run 3: 1d control & state constraints, IPOD vs. OSPOD

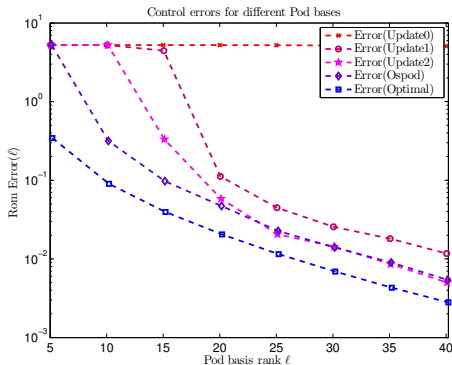


Fig. 9. The control errors vs. the pod basis ranks ℓ for different model reduction techniques. One observes that without basis updates \times , the errors stagnate while the different basis update strategies – solving the reduced optimization problem two times \circ , three times \star or applying one gradient step at the beginning \diamond , respectively – lead to comparable decay orders similar to those of the optimal pod basis choice \square where the control errors deduce to the order $1.0e-02$. For larger pod basis lengths than $\ell_{\max} = 40$, the model reduction does not pay compared to the effort of the full order optimization problem.



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