Universität
Münster

Be greedy and learn: efficient and certified algorithms for parametrized optimal control problems

YMMOR – Young Mathematicians in Model Order Reduction

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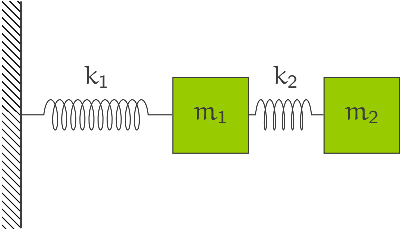
Optimal control of parametrized linear control systems

Example of a spring-mass system



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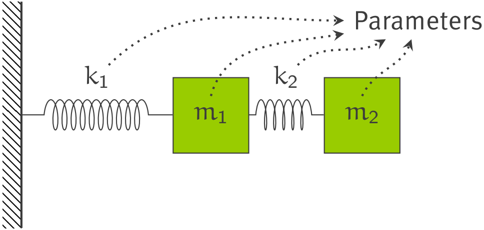

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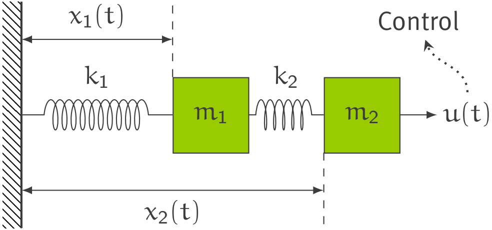

Goal: Given a parameter value,

- try to steer the system state close to a prescribed target state
- without using too much control energy.

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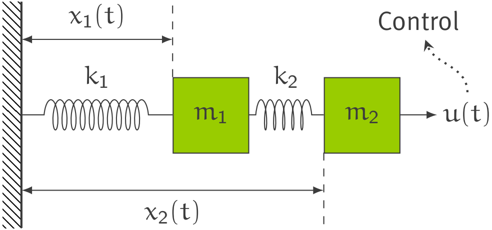

Goal: Given a parameter value,

- try to steer the system state close to a prescribed target state
- without using too much control energy.

Issue: We would like to solve this problem for many different values of the parameter!

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Parameter dependent dynamical system and cost functional

Parametrized linear time-invariant control system

$$\overset{\text{derivative of the state}}{\dot{x}_\mu}(t) = A_\mu \underset{\text{state}}{x_\mu}(t) + B_\mu \underset{\text{control}}{u_\mu}(t), \qquad t \in [0, T],$$

$$x_\mu(0) = x_\mu^0$$

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state

control

Cost functional $\mathcal{J}_\mu \colon G \to \mathbb{R}_+$

$$\mathcal{J}_\mu(u) := \frac{1}{2}\left[\underbrace{\langle x_\mu(T) - x_\mu^T, M\left(x_\mu(T) - x_\mu^T\right)\rangle}_{\text{deviation from the target state } x_\mu^T \in X} + \underbrace{\int_0^T \langle u(t), Ru(t)\rangle \, dt}_{\text{energy of the control}}\right]$$

Parametrized optimal control problem

Given a parameter $\mu \in \mathcal{P}$, solve the following optimization problem:

$$\min_{u \in G} \mathcal{J}_\mu(u), \qquad \text{s.t. } \dot{x}_\mu(t) = A_\mu x_\mu(t) + B_\mu u(t) \text{ for } t \in [0, T], \quad x_\mu(0) = x_\mu^0.$$

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Optimality system for the optimal control problem

Theorem 1 (Optimality system)

Let $\mu \in \mathcal{P}$ be a parameter, $u_\mu^* \in G$ an optimal control and $x_\mu^* \in H$ the associated state trajectory. Then there exists an adjoint solution $\varphi_\mu^* \in H$, such that the problem

$$\begin{aligned} \dot{x}_\mu(t) &= A_\mu x_\mu(t) + B_\mu u_\mu(t), \\ -\dot{\varphi}_\mu(t) &= A_\mu^* \varphi_\mu(t), \\ u_\mu(t) &= -R^{-1} B_\mu^* \varphi_\mu(t), \end{aligned}$$

for $t \in [0, T]$ with initial respectively terminal conditions

$$x_\mu(0) = x_\mu^0, \qquad \varphi_\mu(T) = M\left(x_\mu(T) - x_\mu^T\right),$$

is solved by $x_\mu = x_\mu^*$, $\varphi_\mu = \varphi_\mu^*$ and $u_\mu = u_\mu^*$.

Solving the optimality system

Optimality system

$$\begin{aligned} \dot{x}_\mu^*(t) &= A_\mu x_\mu^*(t) + B_\mu u_\mu^*(t), \\ -\dot{\varphi}_\mu^*(t) &= A_\mu^* \varphi_\mu^*(t), \\ u_\mu^*(t) &= -R^{-1} B_\mu^* \varphi_\mu^*(t), \\ x_\mu^*(0) &= x_\mu^0 \end{aligned}$$

$$\begin{cases} \varphi_\mu^*(t) = e^{A_\mu^*(T-t)} \varphi_\mu^*(T), \\ u_\mu^*(t) = -R^{-1} B_\mu^* \varphi_\mu^*(t), \\ x_\mu^*(t) = \underbrace{e^{A_\mu t} x_\mu^0}_{\text{free dynamics}} + \underbrace{\int_0^t e^{A_\mu(t-s)} B_\mu u_\mu^*(s)\,ds}_{\text{contribution by the control}} \end{cases}$$

Solving the optimality system

Optimality system

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State, control and adjoint already uniquely determined by optimal final time adjoint $\varphi_\mu^*(T)$!

Weighted controllability Gramian

Define the weighted controllability Gramian $\Lambda_\mu^R \in \mathcal{L}(X,X)$ as

$$\Lambda_\mu^R := \int\limits_0^T e^{A_\mu (T-s)} B_\mu R^{-1} B_\mu^* e^{A_\mu^* (T-s)} \, ds.$$

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Then we have

$$x_\mu^*(T) = e^{A_\mu T} x_\mu^0 - \Lambda_\mu^R \varphi_\mu^*(T).$$

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Combining this with the terminal condition

$$\varphi_\mu^*(T) = M\left(x_\mu^*(T) - x_\mu^T\right)$$

from the optimality system gives the following linear system for $\varphi_\mu^*(T)$.

Linear system for the optimal final time adjoint

Lemma 1 (Linear system)

Let $\varphi_\mu^*(T)$ denote the optimal adjoint state at time T that determines the solution of the optimality system. Then it holds

$$\left(I + M\Lambda_\mu^R\right) \varphi_\mu^*(T) = M\left(e^{A_\mu T}x_\mu^0 - x_\mu^T\right),$$

where $I \in \mathcal{L}(X, X)$ denotes the identity.

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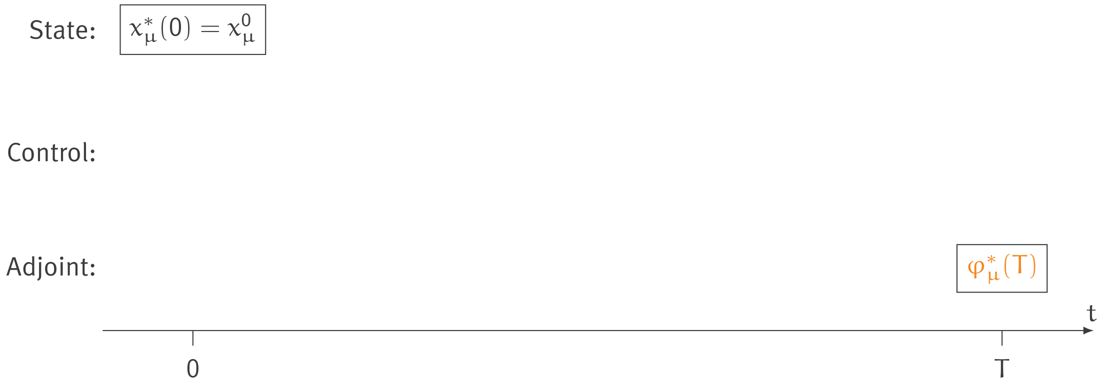
where $I \in \mathcal{L}(X, X)$ denotes the identity.

$\Longrightarrow$ We have to solve a linear system with $I + M\Lambda_\mu^R$ for every new parameter μ!

Assumption: Let $M\Lambda_\mu^R$ be positive-semidefinite for all parameters $\mu \in \mathcal{P}$.

Visualization

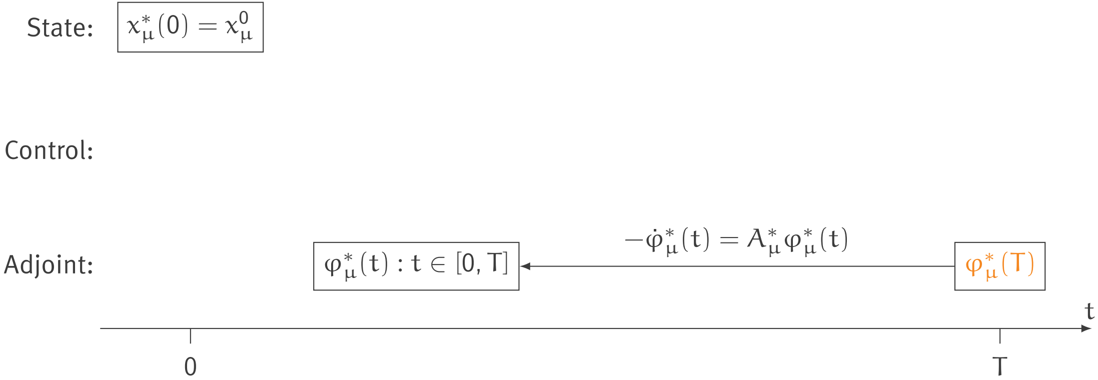


State: $\boxed{x_\mu^*(0) = x_\mu^0}$

Control:

Adjoint: $\boxed{\varphi_\mu^*(T)}$

Visualization



State: $\boxed{x_\mu^*(0) = x_\mu^0}$

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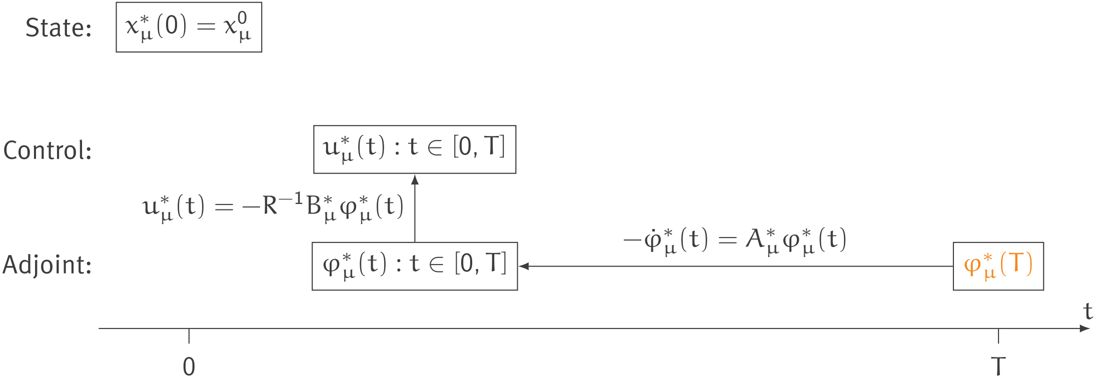

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Control: $\boxed{u_\mu^*(t) : t \in [0, T]}$

$u_\mu^*(t) = -R^{-1}B_\mu^*\varphi_\mu^*(t)$

Adjoint: $\boxed{\varphi_\mu^*(t) : t \in [0, T]}$

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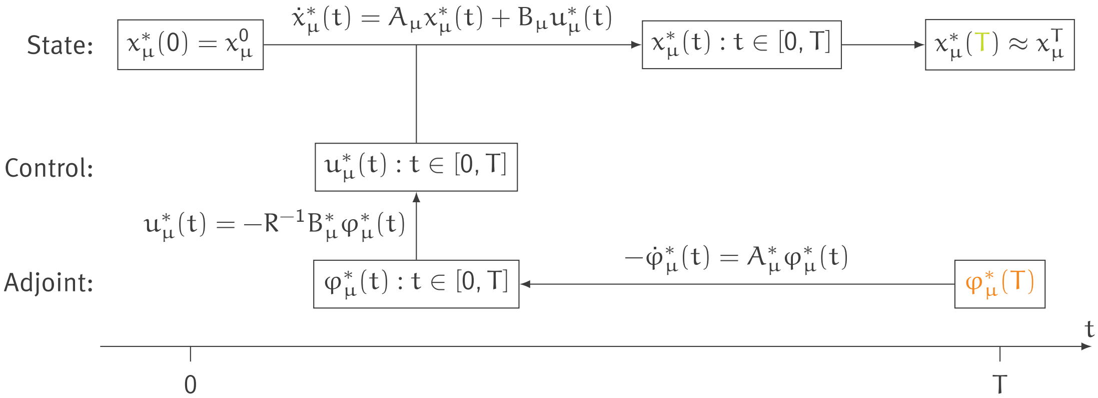

State: $x_\mu^*(0) = x_\mu^0$

$\dot{x}_\mu^*(t) = A_\mu x_\mu^*(t) + B_\mu u_\mu^*(t)$

$x_\mu^*(t) : t \in [0, T]$

$x_\mu^*(T) \approx x_\mu^T$

Control: $u_\mu^*(t) : t \in [0, T]$

$u_\mu^*(t) = -R^{-1} B_\mu^* \varphi_\mu^*(t)$

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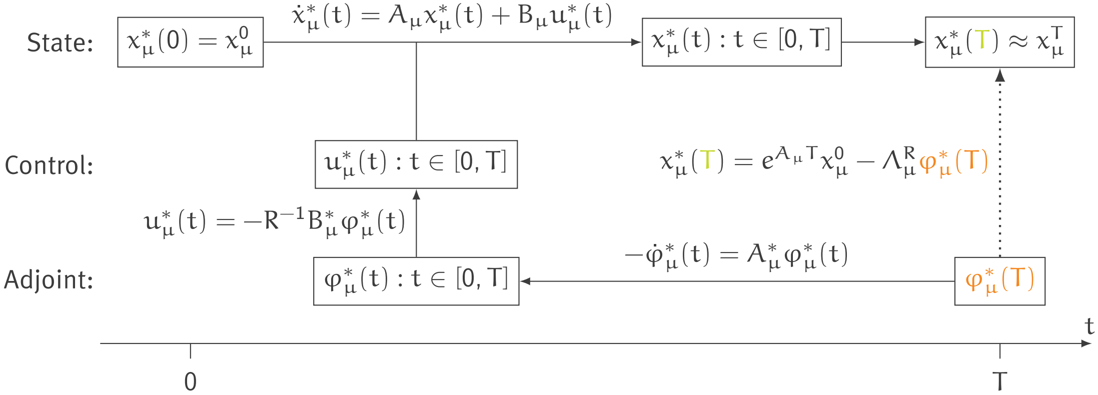
$\varphi_\mu^*(T)$

t

0

T

Visualization



State: $x^*_\mu(0) = x^0_\mu$

$\dot{x}^*_\mu(t) = A_\mu x^*_\mu(t) + B_\mu u^*_\mu(t)$

$x^*_\mu(t) : t \in [0, T]$

$x^*_\mu(T) \approx x^T_\mu$

Control: $u^*_\mu(t) : t \in [0, T]$

$x^*_\mu(T) = e^{A_\mu T} x^0_\mu - \Lambda^R_\mu \varphi^*_\mu(T)$

$u^*_\mu(t) = -R^{-1} B^*_\mu \varphi^*_\mu(t)$

$-\dot{\varphi}^*_\mu(t) = A^*_\mu \varphi^*_\mu(t)$

Adjoint: $\varphi^*_\mu(t) : t \in [0, T]$

$\varphi^*_\mu(T)$

Main ideas of the reduced order model

- Approximate the optimal final time adjoint state $\varphi_\mu^*(T)$.

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- Compute reduced solution by projecting the right hand side of the linear system onto the subspace of states reachable from the reduced space of final time adjoints.
- Later: Accelerate online phase using machine learning with error certification.

Error estimation using the residual

Given an approximate final time adjoint p, consider the residual of the linear system as error estimator:

$$\eta_\mu(p) \coloneqq \left\| M \left(e^{A_\mu T} x_\mu^0 - x_\mu^T \right) - (I + M \Lambda_\mu^R) p \right\|_X .$$

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Theorem 2 (Error estimator for an approximate final time adjoint)

Then it holds:

$$\left\| \varphi_\mu^*(T) - p \right\|_X \quad \leqslant \quad \eta_\mu(p) \quad \leqslant \quad \left\| I + M\Lambda_\mu^R \right\|_{\mathcal{L}(X,X)} \left\| \varphi_\mu^*(T) - p \right\|_X .$$

Approximating the solution manifold by linear subspaces

- Manifold $\mathcal{M} \coloneqq \{\varphi_\mu^*(T) : \mu \in \mathcal{P}\} \subset X$
- Approximation tolerance $\varepsilon > 0$

Goal of the greedy algorithm

Find a reduced space $X^N \subset X$ of (small) dimension N such that

$$\mathrm{dist}(X^N, \mathcal{M}) \leqslant \varepsilon.$$

Greedy procedure for the optimal control problem I

- Given a reduced space $X^N = \mathrm{span}\{\varphi_1, \dots, \varphi_N\} \subset X$ and a parameter $\mu \in \mathcal{P}$, minimize the residual by projecting onto $Y_\mu^N = (I + M\Lambda_\mu^R)X^N$:

$$P_{Y_\mu^N}\left(M(e^{A_\mu T}x_\mu^0 - x_\mu^T)\right) = \sum_{i=1}^{N} \alpha_i^\mu x_i^\mu,$$

where $x_i^\mu = (I + M\Lambda_\mu^R)\varphi_i$, i.e. $Y_\mu^N = \mathrm{span}\{x_1^\mu, \dots, x_N^\mu\}$.

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- Set for the reduced approximation $X^N \ni \tilde{\varphi}_\mu^N \approx \varphi_\mu^*(T) \in X$:

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- Set for the reduced approximation $X^N \ni \tilde{\varphi}_\mu^N \approx \varphi_\mu^*(T) \in X$:

$$\tilde{\varphi}_\mu^N = \sum_{i=1}^{N} \alpha_i^\mu \varphi_i.$$

- Thus, $\tilde{\varphi}_\mu^N$ is the least squares solution to the linear system in the space X^N, i.e. it holds

$$\tilde{\varphi}_\mu^N = \operatorname*{arg\,min}_{\varphi \in X^N} \eta_\mu(\varphi) = \operatorname*{arg\,min}_{\varphi \in X^N} \left\| M\left(e^{A_\mu T}x_\mu^0 - x_\mu^T\right) - (I + M\Lambda_\mu^R)\varphi \right\|_X^2.$$

Greedy procedure for the optimal control problem II

- We therefore have

$$(I+M\Lambda_\mu^R)\tilde{\varphi}_\mu^N = P_{Y_\mu^N}\left(M(e^{A_\mu T}x_\mu^0 - x_\mu^T)\right)$$

and

$$\eta_\mu(\tilde{\varphi}_\mu^N) = \left\| M(e^{A_\mu T}x_\mu^0 - x_\mu^T) - (I+M\Lambda_\mu^R)\tilde{\varphi}_\mu^N \right\| = \mathrm{dist}\left(Y_\mu^N, \{M(e^{A_\mu T}x_\mu^0 - x_\mu^T)\}\right).$$

Greedy procedure for the optimal control problem II

- We therefore have
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Theorem 3 (Error estimator for a reduced space)

Then it holds:

$$\mathrm{dist}(X^N, \{\varphi_\mu^*(T)\}) \quad \leqslant \quad \eta_\mu(\tilde{\varphi}_\mu^N) \quad \leqslant \quad \left\| I + M\Lambda_\mu^R \right\| \cdot \mathrm{dist}(X^N, \{\varphi_\mu^*(T)\}).$$

Analysis of the greedy algorithm

Theorem 3 (Weak greedy algorithm and approximation error)

The greedy procedure presented above is a weak greedy algorithm with constant

$$\gamma \coloneqq \frac{1}{C_{\varphi^*} + C_\Lambda} \leqslant 1,$$

where C_{φ^*} is the Lipschitz constant of the mapping $\mu \mapsto \varphi_\mu^*(T)$ and $C_\Lambda \coloneqq \sup_{\mu \in \mathcal{P}} \left\| I + M\Lambda_\mu^R \right\|$. It further holds for all $\mu \in \mathcal{P}$ that

$$\operatorname{dist}(X^N, \{\varphi_\mu^*(T)\}) \leqslant \varepsilon.$$

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Machine learning of reduced coefficients

- Costly part in the online phase of the reduced order model:
  Computation of $x_i^\mu = (I + M\Lambda_\mu^R)\varphi_i \qquad$ for $i = 1, \dots, N$.

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Machine learning of reduced coefficients

- Costly part in the online phase of the reduced order model:
  Computation of $\quad x_i^{\mu} = (I + M\Lambda_{\mu}^{R})\varphi_i \qquad \text{for } i = 1, \dots, N.$
- Instead: Learn the map from parameters to coefficients, i.e. approximate the map

$$\mu \quad \mapsto \quad \pi_N(\mu) \coloneqq [\alpha_i^{\mu}]_{i=1}^{N}$$

by machine learning surrogate $\hat{\pi}_N \colon \mathcal{P} \to \mathbb{R}^N$.

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- Approximate the final time adjoint as

$$\hat{\varphi}_{\mu}^{N} = \sum_{i=1}^{N} [\hat{\pi}_N(\mu)]_i \varphi_i .$$

Error estimates for machine learning approximation

- A priori bound (assuming that the reduced basis is orthonormal):

$$\| \varphi_\mu^*(T) - \hat{\varphi}_\mu^N \| \quad \leqslant \quad C_\Lambda \underbrace{\varepsilon}_{\text{greedy tolerance}} + \underbrace{\| \pi_N(\mu) - \hat{\pi}_N(\mu) \|}_{\text{approximation error of machine learning}}.$$

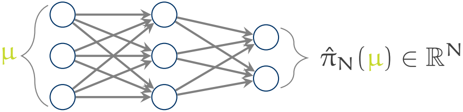
- A posteriori bound:

$$\| \varphi_\mu^*(T) - \hat{\varphi}_\mu^N \| \quad \leqslant \quad \eta_\mu(\hat{\varphi}_\mu^N) \quad \leqslant \quad \| I + M\Lambda_\mu \| \| \varphi_\mu^*(T) - \hat{\varphi}_\mu^N \|.$$

Machine learning approaches

Various machine learning methods can be applied here, we considered:

- Deep neural networks (DNN), see for instance [Petersen, Voigtlaender'18].



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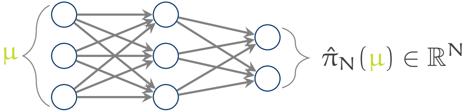

- Kernel methods (VKOGA), see for instance [Santin, Haasdonk'21].

kernel

$$\hat{\pi}_N(\mu) = \sum_{i \in \Xi} \alpha_i k_N(\mu, x_i)$$

centers

subset of selected centers

coefficients

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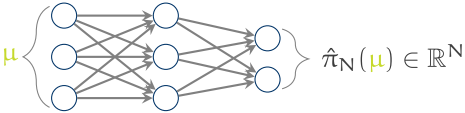


- Kernel methods (VKOGA), see for instance [Santin, Haasdonk'21].

$$\hat{\pi}_N(\mu) = \sum_{i \in \Xi} \alpha_i k_N(\mu, x_i)$$

- Gaussian process regression (GPR), see for instance [Rasmussen, Williams'06].

$$\hat{\pi}_N(\mu) = \mathbb{E}_y[P(y|\mu, X, Y)]$$

input data

output data

Numerical example: Parametrized heat equation

- Problem definition:

$$\begin{aligned} \partial_t v_\mu(t,y) - \mu_1 \Delta v_\mu(t,y) &= 0 && \text{for } t \in [0,T], y \in \Omega, \\ v_\mu(t,0) &= u_{\mu,1}(t) && \text{for } t \in [0,T], \\ v_\mu(t,1) &= u_{\mu,2}(t) && \text{for } t \in [0,T], \\ v_\mu(0,y) = v_\mu^0(y) &= \sin(\pi y) && \text{for } y \in \Omega. \end{aligned}$$

- Target state:

$$v_\mu^T(y) = \mu_2 y$$

- Details: $\Omega = [0,1]$, $T = 0.1$, $\mathcal{P} = [1,2] \times [0.5, 1.5]$

Numerical example: Details

- Spatial discretization: Second order central finite difference scheme

$$A_\mu = \frac{\mu_1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \in \mathbb{R}^{n\times n} \qquad \text{and} \qquad B_\mu = \frac{\mu_1}{h^2}\begin{bmatrix} 1 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{n\times 2}$$

- Temporal discretization: Crank-Nicolson scheme (implicit)
- Weighting matrices:

$$M = I \in \mathbb{R}^{n\times n} \qquad \text{and} \qquad R = \begin{bmatrix} 0.125 & 0 \\ 0 & 0.25 \end{bmatrix}$$

Numerical example: Parametrized heat equation

Optimal, initial and target state

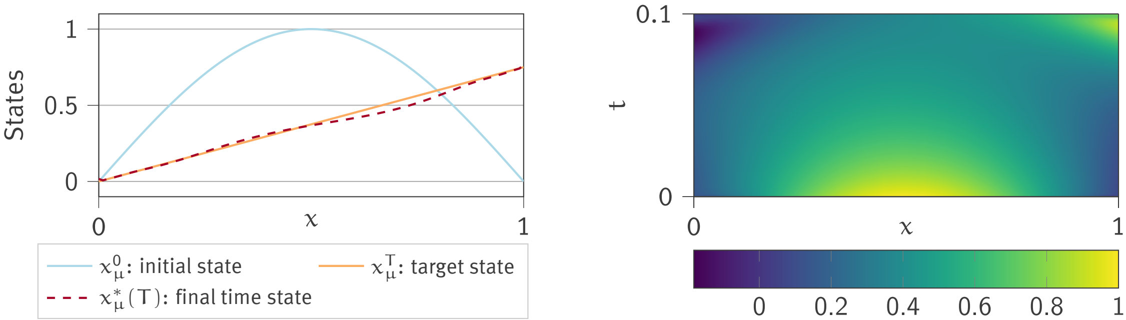


Figure: Optimal state x_μ^* in a space-time plot (left) and initial x_μ^0, final $x_\mu^*(T)$ and target x_μ^T states (right) for the parameter $\mu = (1.5, 0.75)$ in the heat equation example.

Numerical example: Parametrized heat equation

Optimal control and adjoint state

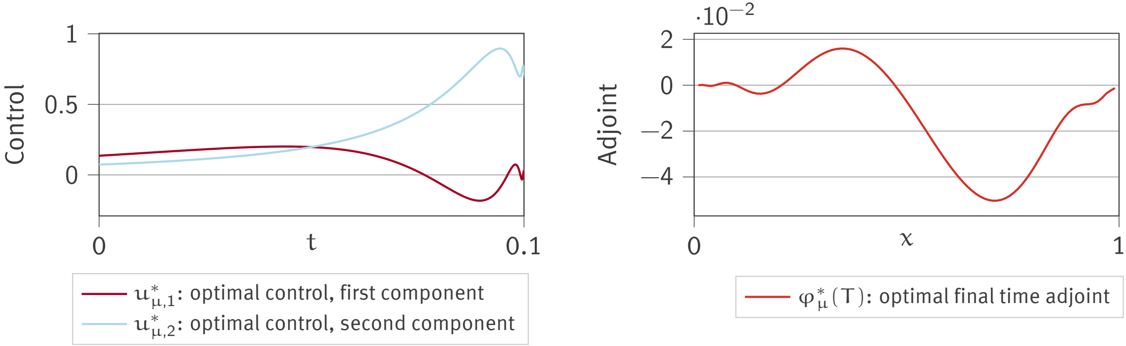
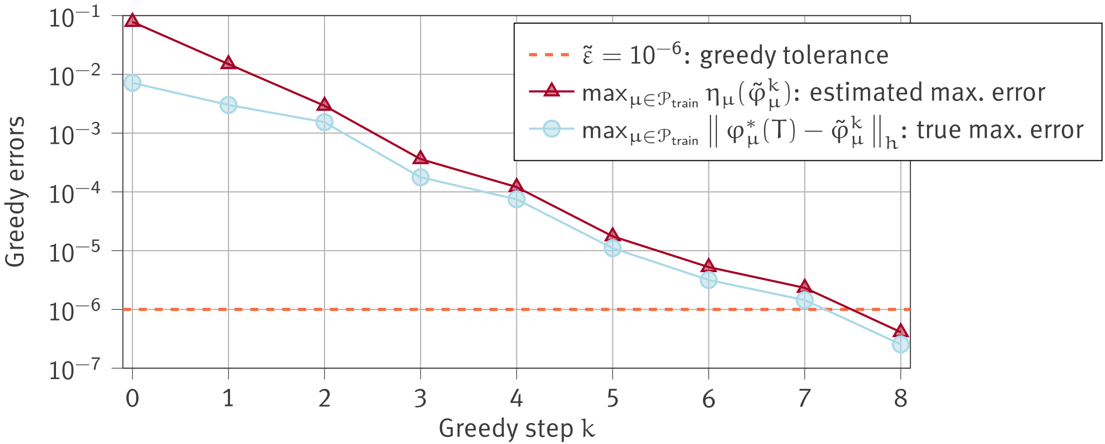


Figure: Optimal control u^*_μ (left) and optimal final time adjoint $\varphi^*_\mu(T)$ (right) for the parameter $\mu = (1.5, 0.75)$ in the heat equation example.

Numerical example: Parametrized heat equation

Greedy algorithm

Results of running the greedy algorithm with 64 uniformly distributed training parameters:



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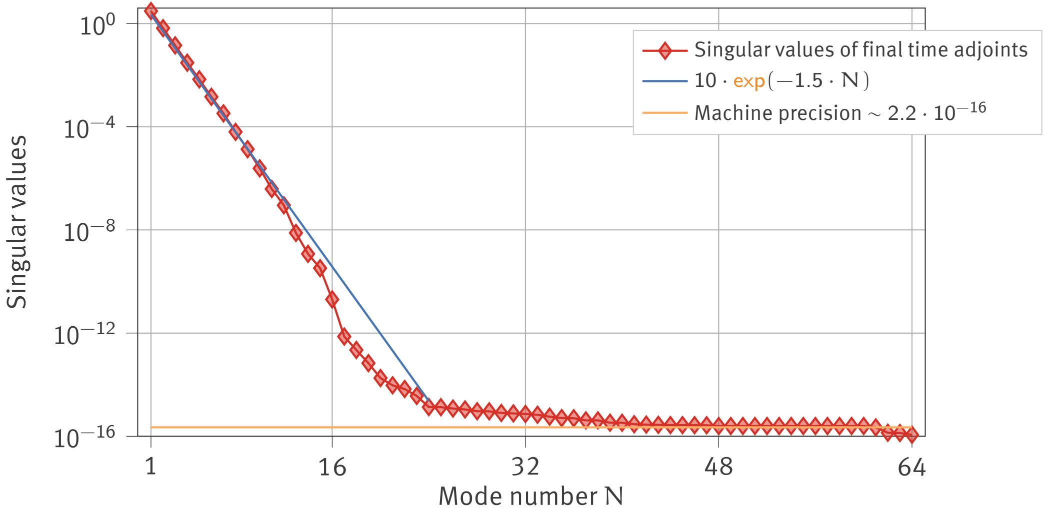
Numerical example: Parametrized heat equation

Singular value decay of optimal final time adjoints



Numerical example: Parametrized heat equation

Machine learning approaches

Results on a set of 100 randomly drawn test parameters:

Method	Avg. error adjoint	Avg. error control	Avg. runtime (s)	Avg. speedup
Exact solution	—	—	6.2760	—
RB-ROM	$5.3 \cdot 10^{-8}$	$5.4 \cdot 10^{-9}$	2.6526	2.37
DNN-ROM	$5.8 \cdot 10^{-6}$	$2.0 \cdot 10^{-6}$	0.1623	40.33
VKOGA-ROM	$1.8 \cdot 10^{-5}$	$6.9 \cdot 10^{-6}$	0.1580	41.03
GPR-ROM	$2.2 \cdot 10^{-6}$	$7.6 \cdot 10^{-7}$	0.1572	41.40

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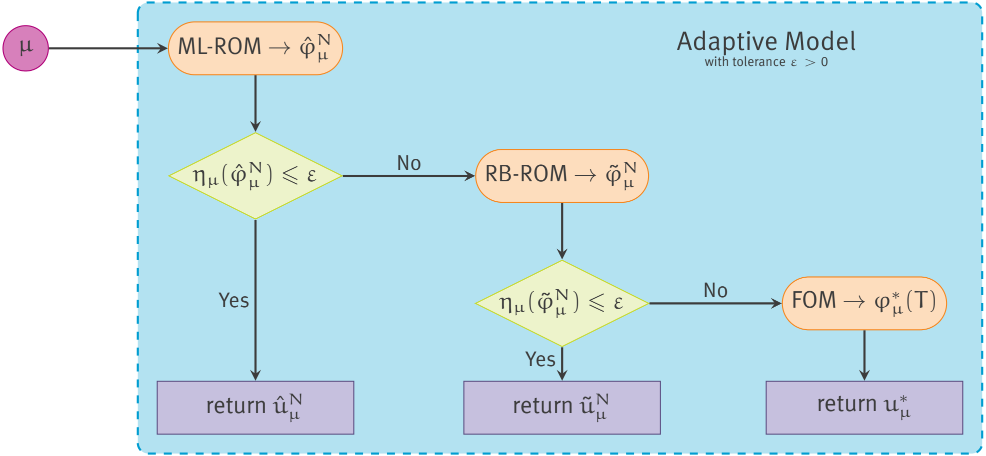
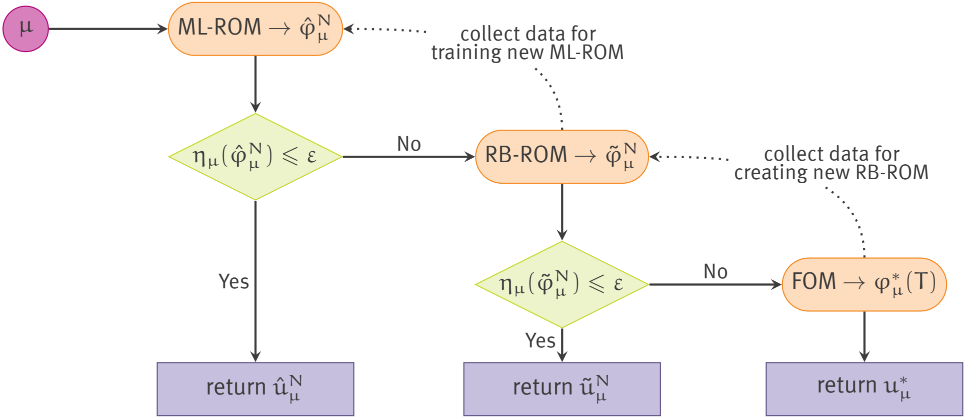
Adaptive model hierarchy [Haasdonk et al'23, Kleikamp'24]

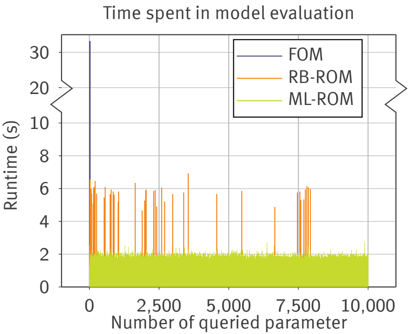


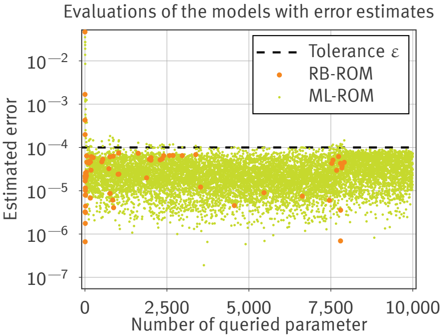
Adaptive model hierarchy [Haasdonk et al'23, Kleikamp'24]



Numerical example: Adaptive model hierarchy

Parametrized heat equation





Model	Number of solves	Number of error estimates	Total time for error est. and solving (s)	Average time for error est. and solving per solve (s)
FOM	4	—	112.24	28.06
RB-ROM	65	69	299.26	4.60
ML-ROM	9,931	10,000	16,655.78	1.68

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Future research

- Advection-diffusion-reaction equations in higher space dimensions as test cases.

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- Advection-diffusion-reaction equations in higher space dimensions as test cases.
- Incorporation of theoretical approximation results for the machine learning methods.
- Additional speedup by applying model order reduction to the parametrized control system, i.e. approximation of the state and adjoint dynamics.
- Extension to other classes of optimal control problems, such as linear time-varying systems or problems with constraints on the control.

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Thank you for your attention!

For more details, see:

H. Kleikamp, M. Lazar, C. Molinari.
Be greedy and learn: efficient and certified algorithms for parametrized optimal control problems, (2023).
`https://arxiv.org/abs/2307.15590`

H. Kleikamp.
Application of an adaptive model hierarchy to parametrized optimal control problems, (2024).
`https://arxiv.org/abs/2402.10708`

The source code for the papers is available open source:

- `https://github.com/HenKlei/ML-OPT-CONTROL`
- `https://github.com/HenKlei/ADAPTIVE-ML-OPT-CONTROL`

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