



MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG



COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Parametric Model Order Reduction for Linear Control Systems

Peter Benner

HRZZ Project

“Control of Dynamical Systems (ConDys)”

— second project meeting —

Zagreb, 2–3 November 2017



1. Introduction
2. PMOR Methods based on Moment Matching
3. Optimal PMOR using Rational Interpolation?
4. Conclusions and Outlook

1. Introduction

Parametric Dynamical Systems

The Parametric Model Order Reduction (PMOR) Problem

Error Measures

2. PMOR Methods based on Moment Matching

3. Optimal PMOR using Rational Interpolation?

4. Conclusions and Outlook



Parametric Dynamical Systems

$$\Sigma(p) : \begin{cases} E(p)\dot{x}(t; p) = f(t, x(t; p), u(t), p), & x(t_0) = x_0, & \text{(a)} \\ y(t; p) = g(t, x(t; p), u(t), p) & & \text{(b)} \end{cases}$$

with

- (generalized) **states** $x(t; p) \in \mathbb{R}^n$ ($E \in \mathbb{R}^{n \times n}$),
- **inputs (controls)** $u(t) \in \mathbb{R}^m$,
- **outputs (measurements, quantity of interest)** $y(t; p) \in \mathbb{R}^q$,
(b) is called **output equation**,
- $p \in \Omega \subset \mathbb{R}^d$ is a **parameter vector**, Ω is bounded.

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$E(p)$ singular \Rightarrow (a) is system of differential-algebraic equations (DAEs)
 otherwise \Rightarrow (a) is system of ordinary differential equations (ODEs)

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Applications:

- Repeated simulation for varying material or geometry parameters, boundary conditions,
- control, optimization and design,
- of models, often generated by FE software (e.g., ANSYS, NASTRAN, ...) or automatic tools (e.g., Modelica).



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Underlying PDE and boundary conditions often not accessible!

Parametric discretized model often not available,
but matrices for certain parameter values can be extracted
(or output data for given u and p can be generated!)



Linear, Time-Invariant (Parametric) Systems

$$\begin{aligned} E(p)\dot{x}(t; p) &= A(p)x(t; p) + B(p)u(t), & A(p), E(p) &\in \mathbb{R}^{n \times n}, \\ y(t; p) &= C(p)x(t; p), & B(p) &\in \mathbb{R}^{n \times m}, C(p) \in \mathbb{R}^{q \times n}. \end{aligned}$$



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Laplace Transformation / Frequency Domain

Application of Laplace transformation

$$x(t; p) \mapsto x(s; p), \quad \dot{x}(t; p) \mapsto sx(s; p)$$

to linear system with $x(0; p) \equiv 0$:

$$sE(p)x(s; p) = A(p)x(s; p) + B(p)u(s), \quad y(s; p) = C(p)x(s; p),$$

yields I/O-relation in frequency domain:

$$y(s; p) = \underbrace{\left(C(p)(sE(p) - A(p))^{-1}B(p) \right)}_{=: G(s, p)} u(s).$$

$G(s, p)$ is the parameter-dependent **transfer function** of $\Sigma(p)$.



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Goal: Fast evaluation of mapping $(u, p) \rightarrow y(s; p)$.



Problem

Approximate the dynamical system

$$\begin{aligned} E(p)\dot{x} &= A(p)x + B(p)u, & E(p), A(p) &\in \mathbb{R}^{n \times n}, \\ y &= C(p)x, & B(p) &\in \mathbb{R}^{n \times m}, C(p) \in \mathbb{R}^{q \times n}, \end{aligned}$$

by reduced-order system

$$\begin{aligned} \hat{E}(p)\dot{\hat{x}} &= \hat{A}(p)\hat{x} + \hat{B}(p)u, & \hat{E}(p), \hat{A}(p) &\in \mathbb{R}^{r \times r}, \\ \hat{y} &= \hat{C}(p)\hat{x}, & \hat{B}(p) &\in \mathbb{R}^{r \times m}, \hat{C}(p) \in \mathbb{R}^{q \times r}, \end{aligned}$$

of order $r \ll n$, such that

$$\|y - \hat{y}\| = \|Gu - \hat{G}u\| \leq \|G - \hat{G}\| \cdot \|u\| < \text{tolerance} \cdot \|u\| \quad \forall p \in \Omega.$$

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⇒ Approximation problem: $\min_{\text{order}(\hat{G}) \leq r} \|G - \hat{G}\|.$

Structure Preservation

Parametric System

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Parametric model reduction goal:

preserve parameters as *symbolic quantities* in reduced-order model:

$$\hat{\Sigma}(p) : \begin{cases} \hat{E}(p)\hat{\dot{x}}(t; p) & = \hat{A}(p)\hat{x}(t; p) + \hat{B}(p)u(t), \\ \hat{y}(t; p) & = \hat{C}(p)\hat{x}(t; p) \end{cases}$$

with states $\hat{x}(t; p) \in \mathbb{R}^r$ and $r \ll n$.

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Assuming **parameter-affine** representation:

$$\begin{aligned} E(p) &= E_0 + e_1(p)E_1 + \dots + e_{q_E}(p)E_{q_E}, \\ A(p) &= A_0 + a_1(p)A_1 + \dots + a_{q_A}(p)A_{q_A}, \\ B(p) &= B_0 + b_1(p)B_1 + \dots + b_{q_B}(p)B_{q_B}, \\ C(p) &= C_0 + c_1(p)C_1 + \dots + c_{q_C}(p)C_{q_C}, \end{aligned}$$

allows easy parameter preservation for projection based model reduction.



Structure Preservation

Petrov-Galerkin-type projection

For given projection matrices $V, W \in \mathbb{R}^{n \times r}$ with $W^T V = I_r$
 ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector), compute

$$\hat{E}(p) = W^T E_0 V + e_1(p) W^T E_1 V + \dots + e_{q_E}(p) W^T E_{q_E} V$$

$$\hat{A}(p) = W^T A_0 V + a_1(p) W^T A_1 V + \dots + a_{q_A}(p) W^T A_{q_A} V$$

$$\hat{B}(p) = W^T B_0 + b_1(p) W^T B_1 + \dots + b_{q_B}(p) W^T B_{q_B}$$

$$\hat{C}(p) = C_0 V + c_1(p) C_1 V + \dots + c_{q_C}(p) C_{q_C} V$$



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$$\begin{aligned} \hat{E}(p) &= W^T E_0 V + e_1(p) W^T E_1 V + \dots + e_{q_E}(p) W^T E_{q_E} V \\ &= \hat{E}_0 + e_1(p) \hat{E}_1 + \dots + e_{q_E}(p) \hat{E}_{q_E} \\ \hat{A}(p) &= W^T A_0 V + a_1(p) W^T A_1 V + \dots + a_{q_A}(p) W^T A_{q_A} V \\ &= \hat{A}_0 + a_1(p) \hat{A}_1 + \dots + a_{q_A}(p) \hat{A}_{q_A} \\ \hat{B}(p) &= W^T B_0 + b_1(p) W^T B_1 + \dots + b_{q_B}(p) W^T B_{q_B} \\ &= \hat{B}_0 + b_1(p) \hat{B}_1 + \dots + b_{q_B}(p) \hat{B}_{q_B} \\ \hat{C}(p) &= C_0 V + c_1(p) C_1 V + \dots + c_{q_C}(p) C_{q_C} V \\ &= \hat{C}_0 + c_1(p) \hat{C}_1 + \dots + c_{q_C}(p) \hat{C}_{q_C} \end{aligned}$$



Basis Generation — Global vs. Local

Local Bases

Obtain $V_k, W_k \in \mathbb{R}^{n \times r_k}$ using any non-parametric linear MOR method for a number of full-order models $\Sigma(p^{(k)})$, $k = 1, \dots, \ell$. Then compute reduced-order model by



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no need for affine parametrization, requires only system matrices $A(p^{(k)}), B(p^{(k)}), \dots$

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3. matrix interpolation: different models obtained in different coordinate systems \rightsquigarrow Procrustes problem \rightsquigarrow potential loss of accuracy; efficiency in "online" phase suffers from evaluating the interpolation operator.



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Global Basis

Obtain $V, W \in \mathbb{R}^{n \times r_k}$ such that $V^T W = I_r$ and perform structure-preserving (Petrov-) Galerkin projection, exploiting affine parametrization of the linear parametric system.



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1. concatenation of local basis matrices:

$$V := [V_1, \dots, V_\ell], \quad W := [W_1, \dots, W_\ell]$$

and orthogonalization (truncation), using, e.g., SVD;



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Avoids most of the problems encountered with local bases, but requires parameter-affine representation of system.

Empirical Matrix Interpolation Method

[B./GUGERCIN/WILLCOX 2015]

Given $V, W \in \mathbb{R}^{n \times r}$ and suppose only that $M(p) \in \mathbb{R}^{n \times t}$ can be evaluated at specific parameter values.

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- Goal: approximate $m(p) \approx \tilde{m}(p) = \Psi\alpha(p)$, where $\Psi \in \mathbb{R}^{nt \times \ell}$ and $\alpha(p) \in \mathbb{R}^{\ell}$ with $\ell \ll n$.

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- Then $\hat{m}(p) = \text{vec}(\hat{M}(p)) \in \mathbb{R}^{nt}$ (or \mathbb{R}^{r^2} if $t = n$) can be computed cheaply and independent of n as

$$\begin{aligned} \hat{m}(p) &= \text{vec}\left(W^T M(p) V\right) \\ &= (V^T \otimes W^T) m(p) \approx (V^T \otimes W^T) \tilde{m}(p) = (V^T \otimes W^T) \Psi \alpha(p) = \tilde{\tilde{m}}(p). \end{aligned}$$

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- This is achieved by sampling $M(p)$ at $p = p^{(j)}$, $j = 1, \dots, \ell$, yielding

$$\psi_j = \text{vec}(M(p^{(j)})) \quad \text{and} \quad \Psi = [\psi_1, \dots, \psi_\ell].$$

Then apply (Q,D)EIM (or alike) to determine $\alpha(p)$ s.t. selected entries of $\tilde{m}(p)$ interpolate those entries of $m(p)$.

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- Apply (Q,D)EIM (or alike) to determine $\alpha(p)$ s.t. selected entries of $\tilde{m}(p)$ interpolate those entries of $m(p)$.

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- Undoing the vectorization yields the reduced model matrix

$$\hat{M}(p) := \text{vec}^{-1}(\tilde{m}(p)) = \text{vec}^{-1}\left((V^T \otimes W^T) \Psi \alpha(p)\right) = \sum_{j=1}^{\ell} \alpha_j(p) \underbrace{W^T M(p^{(j)}) V}_{\text{precomputable!}}$$

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Parametric Systems Norms

Mean-square error norm:

$$\|G - \hat{G}\|_{\mathcal{H}_2 \otimes L_2(\Omega)}^2 := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{\Omega} \|G(j\omega, p) - \hat{G}(j\omega, p)\|_F^2 dp_1 \dots dp_d d\omega,$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

Worst-case error norm:

$$\|G - \hat{G}\|_{\mathcal{H}_\infty \otimes L_\infty(\Omega)} := \sup_{\omega \in \mathbb{R}, p \in \Omega} \|G(j\omega, p) - \hat{G}(j\omega, p)\|_2.$$

1. Introduction
2. PMOR Methods based on Moment Matching
 - Interpolatory Model Reduction
 - PMOR based on Multi-Moment Matching
3. Optimal PMOR using Rational Interpolation?
4. Conclusions and Outlook

Computation of reduced-order model by projection

Given a linear (descriptor) system $E\dot{x} = Ax + Bu, y = Cx$ with transfer function $G(s) = C(sE - A)^{-1}B$, a reduced-order model is obtained using truncation matrices $V, W \in \mathbb{R}^{n \times r}$ with $W^T V = I_r$ ($\rightsquigarrow (VW^T)^2 = VW^T$ is projector) by computing

$$\hat{E} = W^T E V, \hat{A} = W^T A V, \hat{B} = W^T B, \hat{C} = C V.$$

Petrov-Galerkin-type (two-sided) projection: $W \neq V$,

Galerkin-type (one-sided) projection: $W = V$.

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Rational Interpolation/Moment-Matching

Choose V, W such that

$$G(s_j) = \hat{G}(s_j), \quad j = 1, \dots, k,$$

and

$$\frac{d^i}{ds^i} G(s_j) = \frac{d^i}{ds^i} \hat{G}(s_j), \quad i = 1, \dots, K_j, \quad j = 1, \dots, k.$$

Theorem (simplified) [GRIMME 1997, VILLEMAGNE/SKELTON 1987]

If

$$\begin{aligned} \text{span} \{ (s_1 E - A)^{-1} B, \dots, (s_k E - A)^{-1} B \} &\subset \text{range}(V), \\ \text{span} \{ (s_1 E - A)^{-T} C^T, \dots, (s_k E - A)^{-T} C^T \} &\subset \text{range}(W), \end{aligned}$$

then

$$G(s_j) = \hat{G}(s_j), \quad \frac{d}{ds} G(s_j) = \frac{d}{ds} \hat{G}(s_j), \quad \text{for } j = 1, \dots, k.$$



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Remarks:

computation of V, W from **rational Krylov subspaces**, e.g.,

- dual rational Arnoldi/Lanczos [GRIMME 1997],
- **Iter. Rational Krylov-Alg. (IRKA)** [ANTOULAS/BEATTIE/GUGERCIN 2006/08].



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using Galerkin/one-sided projection ($W \equiv V$) yields $G(s_j) = \hat{G}(s_j)$, but in general

$$\frac{d}{ds} G(s_j) \neq \frac{d}{ds} \hat{G}(s_j).$$

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Remarks:

$k = 1$, standard Krylov subspace(**s**) of dimension K :

$$\text{range}(V) = \mathcal{K}_K((s_1 E - A)^{-1}, (s_1 E - A)^{-1} B).$$

↪ **moment-matching methods**/Padé approximation,

$$\frac{d^i}{ds^i} G(s_1) = \frac{d^i}{ds^i} \hat{G}(s_1), \quad i = 0, \dots, K - 1(+K).$$

Numerical Example: A Printed Circuit Board (PCB)

- System in time domain:

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t). \end{aligned}$$

- System in frequency domain:

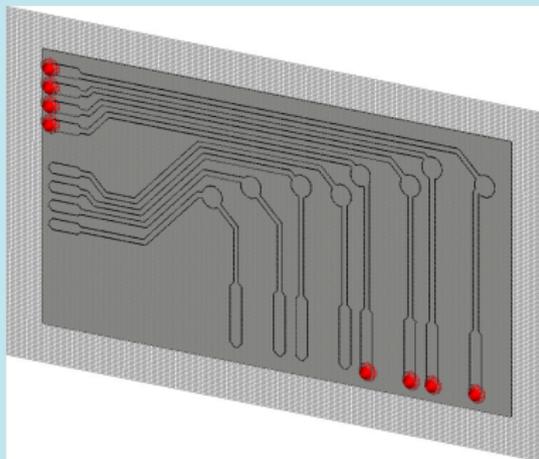
$$\begin{aligned} sEx(s) &= Ax(s) + Bu(s), \\ y(s) &= Cx(s). \end{aligned}$$

- Reduced basis method considers s as a parameter, and uses the system in frequency domain to compute

$$\text{range}(V) = \text{span}\{x(s_1), \dots, x(s_m)\}.$$

The ROM is obtained by Galerkin projection with V .

Printed circuit board

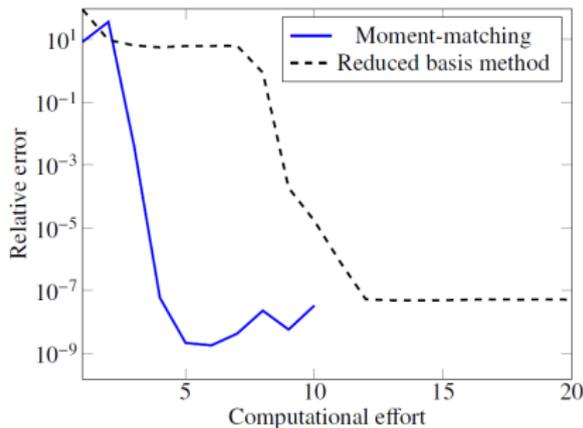
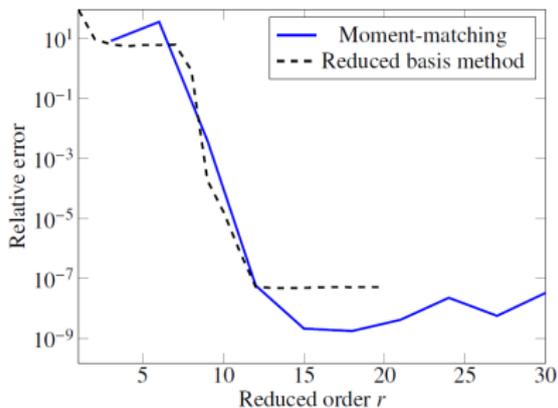


$$n = 233,060, \quad m = q = 1.$$

Courtesy of TEMF, TU Darmstadt.

Numerical Example: A Printed Circuit Board (PCB)

Moment-matching vs. reduced basis method





Idea: choose appropriate frequency parameter \hat{s} and parameter vector \hat{p} , expand into multivariate power series about (\hat{s}, \hat{p}) and compute reduced-order model, so that

$$G(s, p) = \hat{G}(s, p) + \mathcal{O}\left(|s - \hat{s}|^K + \|p - \hat{p}\|^L + |s - \hat{s}|^k \|p - \hat{p}\|^l\right),$$

i.e., first $K, L, k + l$ (mostly: $K = L = k + l$) coefficients (**multi-moments**) of Taylor/Laurent series coincide.

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Algorithms:

- [1] [DANIEL ET AL. 2004]: explicit computation of moments, numerically unstable.
- [2] [FARLE ET AL. 2006/07]: Krylov subspace approach, only polynomial param.-dependence, numerical properties not clear, but appears to be robust.
- [3] [WEILE ET AL. 1999, FENG/B. 2007/14]: Arnoldi-MGS method, employ recursive dependence of multi-moments, numerically robust, r often larger as for [2].
- [4] **New:** employ dual-weighted residual error bound and greedy procedure to define interpolation points an $\#$ of multi-moments matched [ANTOULAS/B./FENG 2014/17].

Parametric System

Again, consider linear parametric system

$$\Sigma(p) : \begin{cases} E(p)\dot{x}(t; p) & = A(p)x(t; p) + B(p)u(t), \\ y(t; p) & = C(p)x(t; p) \end{cases}$$

together with its transfer function $G(s, p)$.

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For simplicity, assume $B(\mu) \equiv B$, and re-parameterize — $\mu := [s, p^T, \dots]^T \in \mathbb{C}^\ell$ such that with

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In frequency domain, we may then re-write the parametric system as

$$\mathcal{A}(\mu)x(\mu) = Bu(s), \quad y(\mu) = C(\mu)x(\mu).$$



Multivariate Power Series Expansion I

Choose an expansion point $\mu^{(0)}$, and write

$$\begin{aligned}\mathcal{A}(\mu) &= \mathcal{A}_0 + \mu_1 \mathcal{A}_1 + \dots + \mu_\ell \mathcal{A}_m \\ &= \underbrace{(\mathcal{A}_0 + \mu_1^{(0)} \mathcal{A}_1 + \dots + \mu_\ell^{(0)} \mathcal{A}_m)}_{:=\mathcal{M}_0} + \left((\mu_1 - \mu_1^{(0)}) \mathcal{A}_1 + \dots + (\mu_\ell - \mu_\ell^{(0)}) \mathcal{A}_\ell \right)\end{aligned}$$



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Using the **Neumann lemma** ($(I - F)^{-1} = \sum_{j=0}^{\infty} F^j$ if $\|F\| < 1$), we obtain

$$\begin{aligned} \mathcal{A}(\mu)^{-1} &= \sum_{j=0}^{\infty} (-1)^j \left((\mu_1 - \mu_1^{(0)}) \mathcal{M}_0^{-1} \mathcal{A}_1 + \dots + (\mu_\ell - \mu_\ell^{(0)}) \mathcal{M}_0^{-1} \mathcal{A}_\ell \right)^j \mathcal{M}_0^{-1} \\ &= \sum_{j=0}^{\infty} (\sigma_1 \mathcal{M}_1 + \dots + \sigma_\ell \mathcal{M}_\ell)^j \mathcal{M}_0^{-1}, \end{aligned}$$

where $\sigma_i = \mu_i - \mu_i^{(0)}$ and $\mathcal{M}_i = -\mathcal{M}_0^{-1} \mathcal{A}_i$ for $i = 1, \dots, \ell$.

Multivariate Power Series Expansion II

We have

$$\mathcal{A}(\mu)x(\mu) = Bu(s).$$

and

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- Approximation is only valid locally (convergence radius of Neumann series!) \rightsquigarrow use several expansion points $\mu^{(0)}, \dots, \mu^{(h)}$, and concatenate (and truncate) the local bases to obtain a global basis.



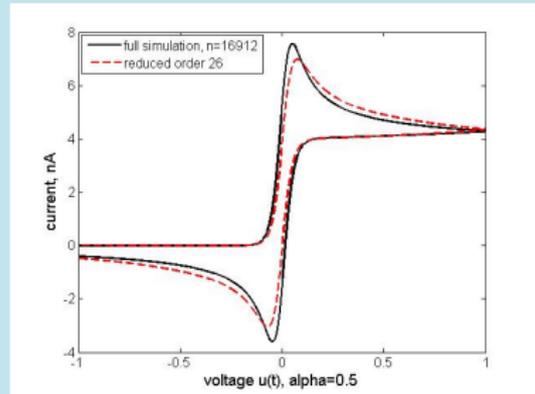
Numerical Examples: Electro-Chemical SEM

Compute cyclic voltammogram based on FE model

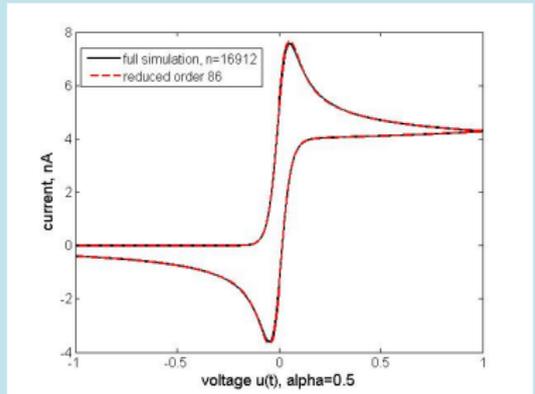
$$E\dot{x}(t) = (A_0 + p_1A_1 + p_2A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

where $n = 16,912$, $m = 3$, A_1, A_2 diagonal.

$K = L = k + l = 4 \Rightarrow r = 26$



$K = L = k + l = 9 \Rightarrow r = 86$



Source: MOR Wiki: http://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Scanning_Electrochemical_Microscopy

Open question

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And how many partial derivatives to be matched at each interpolation point?

Open question

How to adaptively choose $\mu^{(i)}$?

And how many partial derivatives to be matched at each interpolation point?

Possible approach: adopt ideas from Reduced Basis Methods, i.e., let

$$\|G(\mu) - \hat{G}(\mu)\| \leq \Delta(\mu) \quad \text{or} \quad \|y(\mu) - \hat{y}(\mu)\| \leq \Delta_o(\mu)$$

guide the selection of $\mu^{(i)}$ for computable *a posteriori* error bounds for the state or the output.

Theorem (SISO case)

[FENG/ANTOULAS/B. 2015/17]

Assume that $\sigma_{\min}(G(s, p)) =: \beta(s, p) > 0 \quad \forall \operatorname{Re}(s) \geq 0, \forall p \in \Omega$, then

$$|H(s, p) - \hat{H}(s, p)| \leq \tilde{\Delta}(s, p) + |(\hat{x}^{du})^H r^{pr}(s, p)| =: \Delta(s, p),$$

where

$$\tilde{\Delta}(s, p) = \frac{\|r^{du}(s, p)\|_2 \|r^{pr}(s, p)\|_2}{\beta(s, p)},$$

with the primal and dual residuals r^{pr}, r^{du} and the reduced "dual state" \hat{x}^{du} :

$$r^{pr}(s, p) = \|(B - (sE(p) - A(p))) (V(s\hat{E}(p) - \hat{A}(p))^{-1} \hat{B})\|,$$

$$r^{du}(s, p) = \|(C^T - (\bar{s}E(p) - A(p))^T) \hat{x}^{du}\|,$$

$$\hat{x}^{du} = -V^{du}(\bar{s}\hat{E}^{du}(p) - \hat{A}^{du}(p))^{-T} \hat{C}^{du}.$$

The dual reduced-order system is computed using Galerkin projection with V^{du} obtained by applying multi-moment matching algorithm to "dual" system $(\bar{s}E(p)^T - A(p)^T, C^T)$.

Remarks

- For application in "RBM fashion", $r^{du}(\mu)$, $r^{pr}(\mu)$ can be efficiently computed, need to solve sparse linear systems on training set, i.e., one sparse factorization for each sampling point.
- $\beta(s, p) = \sigma_{\min}(G(s, p))$ easily computable on the training set — system solves for evaluation of the transfer function readily available from residual computation!
- Extension to MIMO case possible taking max over all I/O channels.
- Can use Petrov-Galerkin framework using $W = V^{du}$ at no extra cost!

Algorithm 1 Automatic generation of the ROM: adaptively selecting $\mu^{(i)}$

Input: $V = []$; $\epsilon > \epsilon_{tol}$; Initial expansion point: $\hat{\mu}$; $i := -1$;
 Ξ_{train} : a set of samples of μ covering the parameter domain.

Output: V .

- 1: **while** $\epsilon > \epsilon_{tol}$ **do**
 - 2: $i = i + 1$;
 - 3: $\mu^{(i)} = \hat{\mu}$;
 - 4: $V_{\mu^{(i)}} = \text{orthogonal basis of } \mathcal{K}_{k+1}((\sigma_1^{(i)} \mathcal{M}_1 + \dots + \sigma_\ell^{(i)} \mathcal{M}_\ell), \mathcal{B})$;
 - 5: $V = \text{orth}([V, V_{\mu^{(i)}}])$;
 - 6: $\hat{\mu} = \arg \max_{\mu \in \Xi_{train}} \Delta(\mu)$;
 - 7: $\epsilon = \Delta(\hat{\mu})$;
 - 8: **end while**
-

Numerical Example: Silicon Nitride Membrane

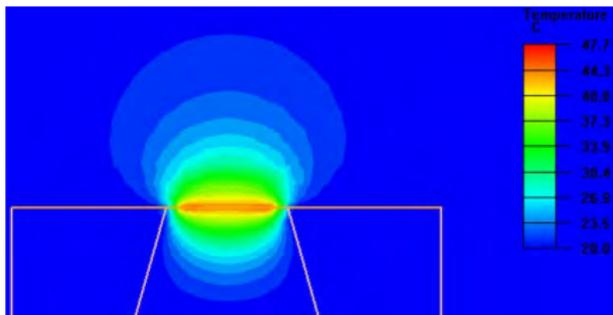
A SiN membrane can be a part of a gas sensor, an infra-red sensor, a microthruster, etc. Heat transfer in the membrane is described by

$$\begin{aligned} (E_0 + \rho c_p E_1) \dot{x}(t) &= -(K_0 + \kappa K_1 + h K_2) x(t) + bu(t) \\ y(t) &= Cx(t), \end{aligned}$$

with parameters

- density $\rho \in [3000, 3200]$,
- specific heat capacity $c_p \in [400, 750]$,
- thermal conductivity $\kappa \in [2.5, 4]$,
- membrane heat transfer coefficient $h \in [10, 12]$.

and frequency $f \in [0, 25] Hz$.



Source: MOR Wiki: http://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Silicon_nitride_membrane



Numerical Examples: Silicon Nitride Membrane

Setting

- Training set: $\Xi_{train} = 5$ random samples for ρ and c_p , 3 random samples for κ and h , respectively, 10 samples of Laplace variable s .

- Error measures:

$$\varepsilon_{true}^{rel} = \max_{\mu \in \Xi_{train}} |G(\mu) - \hat{G}(\mu)| / |G(\mu)|,$$

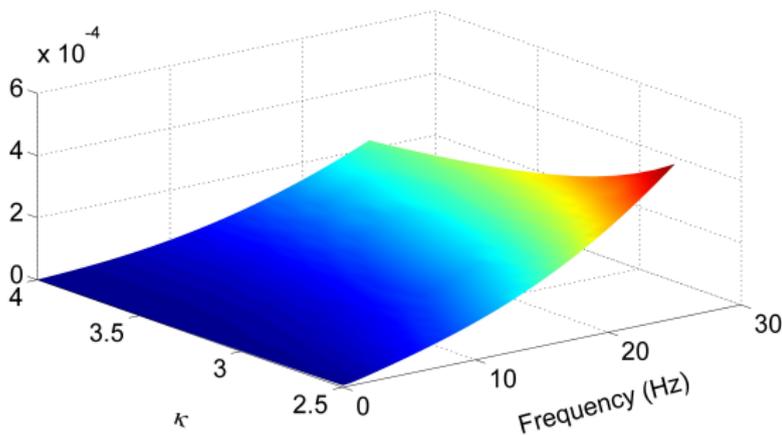
$$\Delta^{rel}(\mu) = \Delta(\mu) / |\hat{G}(\mu)|$$

- $V_{\mu^{(i)}} = \text{span}\{\mathcal{B}, (\sigma_1^{(i)} \mathcal{M}_1 + \dots + \sigma_\ell^{(i)} \mathcal{M}_\ell) \mathcal{B}\}$, $\epsilon_{tol}^{re} = 10^{-2}$, $n = 60,020$, $r = 8$.

| iter. | ε_{true}^{rel} | $\Delta^{rel}(\mu^{(i)})$ | s | ρc_p | κ | h |
|-------|----------------------------|---------------------------|-------|--------------------|----------|-------|
| 1 | 1×10^{-3} | 3.44 | 18.94 | 1.37×10^6 | 2.74 | 10.97 |
| 2 | 1×10^{-4} | 4.59×10^{-2} | 0.89 | 1.31×10^6 | 3.96 | 11.60 |
| 3 | 2.80×10^{-5} | 4.07×10^{-2} | 23.98 | 2.35×10^6 | 3.94 | 10.28 |
| 4 | 2.58×10^{-6} | 2.62×10^{-5} | 0.89 | 2.31×10^6 | 2.74 | 10.28 |

Numerical Examples: Silicon Nitride Membrane

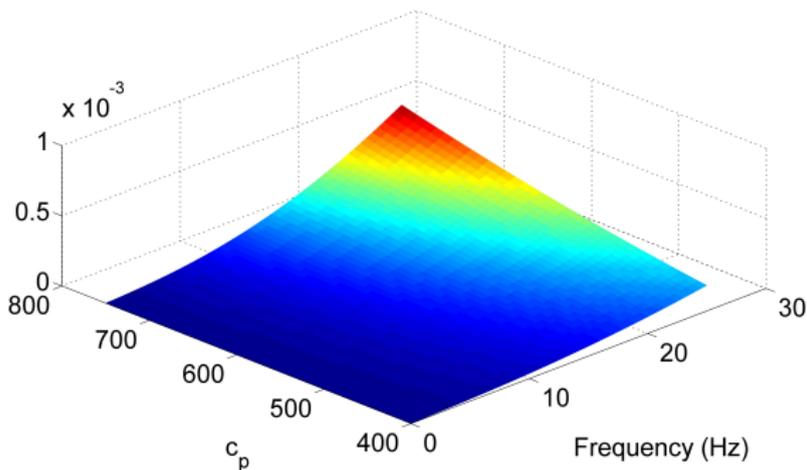
Verification of the accuracy of the ROM for κ over set Ξ_{fine} with 16 equidistant samples of κ , 51 equidistant samples of the frequency f , while the other parameters are fixed.



Relative error of the final ROM changing with κ and frequency.

Numerical Examples: Silicon Nitride Membrane

Verification of the accuracy of the ROM for c_p over set Ξ_{fine} with 36 equidistant samples of c_p , 51 equidistant samples of the frequency f , while the other parameters are fixed.

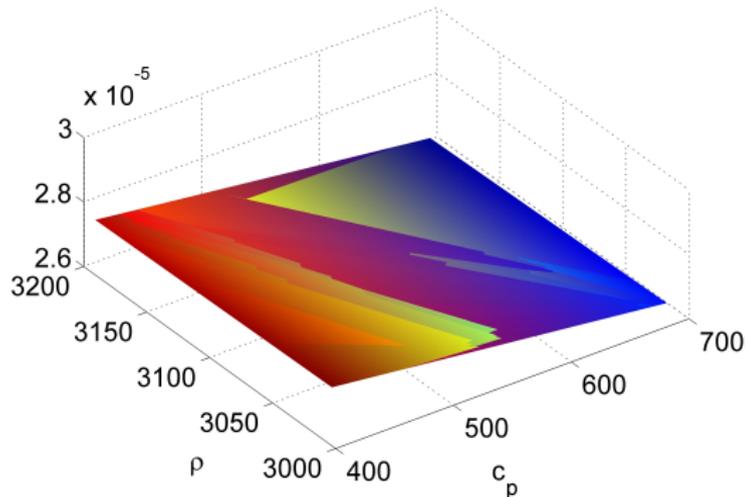


Relative error of the final ROM changing with c_p and frequency.



Numerical Examples: Silicon Nitride Membrane

Verification of the accuracy of the ROM for ρ, c_p over set Ξ_{fine} with 50 random samples of ρ, c_p , respectively, the other parameters are fixed.



Relative error of the final ROM changing with c_p and κ .

1. Introduction

2. PMOR Methods based on Moment Matching

3. Optimal PMOR using Rational Interpolation?

\mathcal{H}_2 -optimal Model Reduction for Linear Systems

\mathcal{H}_2 -(sub)optimal Model Reduction for Linear Parametric Systems

\mathcal{H}_2 -optimal Model Reduction for Special Linear Parametric Systems

A Comparison of PMOR Methods

4. Conclusions and Outlook



PMOR based on Multi-Moment Matching

Greedy expansion point selection has a heuristic nature and relies on a training set.

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How to determine the right number of partial derivatives to be matched at the expansion points is an open problem (for potential solutions in the non-parametric case, see [FENG/KORVINK/B. 2015, BONIN/FASSBENDER/SOPPA/ZÄH 2016, LEE/CHU/FENG 2006, ...]).

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Can we find (necessary) optimality conditions similar to the LTI case, leading to an IRKA-like procedure?

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Hence, we investigate the problem: for a given order r of the reduced-order model, can we provide necessary conditions for a rational interpolant to minimize

$$\|G - \hat{G}\|_{\mathcal{H}_2 \otimes L_2(\Omega)}^2 := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{\Omega} \|G(j\omega, p) - \hat{G}(j\omega, p)\|_F^2 dp_1 \dots dp_d d\omega ?$$

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Following the non-parametric case, one would need:

- Projection-based framework for tangential rational interpolation. [✓]

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Following the non-parametric case, one would need:

- Projection-based framework for tangential rational interpolation. [✓]
- Iterative procedure for selecting interpolation points. [x] ... [✓] for special case.

\mathcal{H}_2 -Model Reduction for Linear Systems

Consider **stable** (i.e. $\Lambda(A) \subset \mathbb{C}^-$) linear systems Σ ,

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t) \quad \simeq \quad y(s) = \underbrace{C(sl - A)^{-1}B}_{=:G(s)} u(s)$$

System norms

Recall: two common system norms for measuring approximation quality are

- \mathcal{H}_2 -norm, $\|\Sigma\|_{\mathcal{H}_2} = \left(\frac{1}{2\pi} \int_0^{2\pi} \text{tr}((G^T(-j\omega)G(j\omega))) d\omega \right)^{\frac{1}{2}}$,
- \mathcal{H}_∞ -norm, $\|\Sigma\|_{\mathcal{H}_\infty} = \sup_{\omega \in \mathbb{R}} \sigma_{\max}(G(j\omega))$,

where

$$G(s) = C(sl - A)^{-1}B.$$

In order to find an \mathcal{H}_2 -optimal reduced system, consider the **error system** $G(s) - \hat{G}(s)$ which can be realized by

$$A^{err} = \begin{bmatrix} A & 0 \\ 0 & \hat{A} \end{bmatrix}, \quad B^{err} = \begin{bmatrix} B \\ \hat{B} \end{bmatrix}, \quad C^{err} = [C \quad -\hat{C}].$$

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Assuming a coordinate system in which \hat{A} is diagonal and taking derivatives of

$$\|G(\cdot) - \hat{G}(\cdot)\|_{\mathcal{H}_2}^2$$

with respect to free parameters in $\Lambda(\hat{A}), \hat{B}, \hat{C} \rightsquigarrow$ **first-order necessary \mathcal{H}_2 -optimality conditions (SISO)**

$$G(-\hat{\lambda}_i) = \hat{G}(-\hat{\lambda}_i),$$

$$G'(-\hat{\lambda}_i) = \hat{G}'(-\hat{\lambda}_i),$$

where $\hat{\lambda}_i$ are the poles of the reduced system $\hat{\Sigma}$.



In order to find an \mathcal{H}_2 -optimal reduced system, consider the **error system** $G(s) - \hat{G}(s)$ which can be realized by

$$A^{err} = \begin{bmatrix} A & 0 \\ 0 & \hat{A} \end{bmatrix}, \quad B^{err} = \begin{bmatrix} B \\ \hat{B} \end{bmatrix}, \quad C^{err} = [C \quad -\hat{C}].$$

First-order necessary \mathcal{H}_2 -optimality conditions (MIMO):

$$\begin{aligned} G(-\hat{\lambda}_i)\tilde{B}_i &= \hat{G}(-\hat{\lambda}_i)\tilde{B}_i, & \text{for } i = 1, \dots, r, \\ \tilde{C}_i^T G(-\hat{\lambda}_i) &= \tilde{C}_i^T \hat{G}(-\hat{\lambda}_i), & \text{for } i = 1, \dots, r, \\ \tilde{C}_i^T H'(-\hat{\lambda}_i)\tilde{B}_i &= \tilde{C}_i^T \hat{G}'(-\hat{\lambda}_i)\tilde{B}_i & \text{for } i = 1, \dots, r, \end{aligned}$$

where $\hat{A} = R\hat{\Lambda}R^{-T}$ is the spectral decomposition of the reduced system and $\tilde{B} = \hat{B}^T R^{-T}$, $\tilde{C} = \hat{C}R$.



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$$\begin{aligned} \Leftrightarrow \text{vec}(I_q)^T \left(e_j e_i^T \otimes C \right) \left(-\hat{\Lambda} \otimes I_n - I_r \otimes A \right)^{-1} \left(\tilde{B}^T \otimes B \right) \text{vec}(I_m) \\ = \text{vec}(I_q)^T \left(e_j e_i^T \otimes \hat{C} \right) \left(-\hat{\Lambda} \otimes I_r - I_r \otimes \hat{A} \right)^{-1} \left(\tilde{B}^T \otimes \hat{B} \right) \text{vec}(I_m), \\ \text{for } i = 1, \dots, r \text{ and } j = 1, \dots, q. \end{aligned}$$

Interpolation of the Transfer Function [GRIMME 1997]

Construct reduced transfer function by **Petrov-Galerkin** projection $\mathcal{P} = VW^T$, i.e.

$$\hat{G}(s) = CV (sI - W^T AV)^{-1} W^T B,$$

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where V and W are given as

$$V = [(-\mu_1 I - A)^{-1} B, \dots, (-\mu_r I - A)^{-1} B],$$

$$W = [(-\mu_1 I - A^T)^{-1} C^T, \dots, (-\mu_r I - A^T)^{-1} C^T].$$

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Starting with an initial guess for $\hat{\Lambda}$ and setting $\mu_i \equiv \hat{\lambda}_i \rightsquigarrow$ iterative algorithms (IRKA/MIRIAM) that yield \mathcal{H}_2 -optimal models.

[GUGERCIN ET AL. 2006/08], [BUNSE-GERSTNER ET AL. 2007],
[VAN DOOREN ET AL. 2008]

The Basic IRKA Algorithm

Algorithm 2 IRKA (MIMO version/MIRIAM)

Input: A stable, B, C, \hat{A} stable, $\hat{B}, \hat{C}, \delta > 0$.

Output: $A^{opt}, B^{opt}, C^{opt}$

- 1: **while** $(\max_{j=1, \dots, r} \left\{ \frac{|\mu_j - \mu_j^{old}|}{|\mu_j|} \right\} > \delta)$ **do**
- 2: $\text{diag}(\mu_1, \dots, \mu_r) := R^{-1} \hat{A} R = \text{spectral decomposition.}$
- 3: $\tilde{B} = \hat{B}^H R^{-T}, \tilde{C} = \hat{C} R.$
- 4: $V = [(-\mu_1 I - A)^{-1} B \tilde{b}_1, \dots, (-\mu_r I - A)^{-1} B \tilde{b}_r]$
- 5: $W = [(-\mu_1 I - A^T)^{-1} C^T \tilde{c}_1, \dots, (-\mu_r I - A^T)^{-1} C^T \tilde{c}_r]$
- 6: $V = \text{orth}(V), W = \text{orth}(W), W = W(V^H W)^{-1}$
- 7: $\hat{A} = W^H A V, \hat{B} = W^H B, \hat{C} = C V.$
- 8: **end while**
- 9: $A^{opt} = \hat{A}, B^{opt} = \hat{B}, C^{opt} = \hat{C}.$

Theory: Interpolation of the Transfer Function

Theorem

[BAUR/BEATTIE/B./GUGERCIN 2007/11]

Let

$$\begin{aligned} \hat{G}(s, p) &:= \hat{C}(p)(s\hat{E}(p) - \hat{A}(p))^{-1}\hat{B}(p) \\ &= C(p)V(sW^T E(p)V - W^T A(p)V)^{-1}W^T B(p). \end{aligned}$$

Suppose $\hat{p} = [\hat{p}_1, \dots, \hat{p}_d]^T$ and $\hat{s} \in \mathbb{C}$ are chosen such that both $\hat{s} E(\hat{p}) - A(\hat{p})$ and $\hat{s} \hat{E}(\hat{p}) - \hat{A}(\hat{p})$ are invertible. If

$$(\hat{s} E(\hat{p}) - A(\hat{p}))^{-1} B(\hat{p}) \in \text{range}(V)$$

or

$$\left(C(\hat{p}) (\hat{s} E(\hat{p}) - A(\hat{p}))^{-1} \right)^T \in \text{range}(W),$$

then $G(\hat{s}, \hat{p}) = \hat{G}(\hat{s}, \hat{p})$.

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then $G(\hat{s}, \hat{p}) = \hat{G}(\hat{s}, \hat{p})$.

Extension to MIMO case using **tangential interpolation**: let $0 \neq b \in \mathbb{R}^m$, $0 \neq c \in \mathbb{R}^q$.

- If $(\hat{s}E(\hat{p}) - A(\hat{p}))^{-1}B(\hat{p})b \in \text{range}(V)$, then $G(\hat{s}, \hat{p})b = \hat{G}(\hat{s}, \hat{p})b$.
- If $\left(c^T C(\hat{p})(\hat{s}E(\hat{p}) - A(\hat{p}))^{-1}\right)^T \in \text{range}(W)$, then $c^T G(\hat{s}, \hat{p}) = c^T \hat{G}(\hat{s}, \hat{p})$.



Theory: Interpolation of the Parameter Gradient

Theorem

[BAUR/BEATTIE/B./GUGERCIN 2007/11]

Suppose that $E(p)$, $A(p)$, $B(p)$, $C(p)$ are C^1 in a neighborhood of $\hat{p} = [\hat{p}_1, \dots, \hat{p}_d]^T$ and that both $\hat{s}E(\hat{p}) - A(\hat{p})$ and $\hat{s}\hat{E}(\hat{p}) - \hat{A}(\hat{p})$ are invertible.

If

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and

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then

$$\nabla_p G(\hat{s}, \hat{p}) = \nabla_p G_r(\hat{s}, \hat{p}), \quad \frac{\partial}{\partial s} G(\hat{s}, \hat{p}) = \frac{\partial}{\partial s} \hat{G}(\hat{s}, \hat{p}).$$

Theory: Interpolation of the Parameter Gradient

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Note: result extends to MIMO case using **tangential interpolation**:

Let $0 \neq b \in \mathbb{R}^m$, $0 \neq c \in \mathbb{R}^q$ be arbitrary. If $(\hat{s}E(\hat{p}) - A(\hat{p}))^{-1} B(\hat{p})b \in \text{range}(V)$ and $(c^T C(\hat{p}) (\hat{s}E(\hat{p}) - A(\hat{p}))^{-1})^T \in \text{range}(W)$, then $\nabla_p c^T G(\hat{s}, \hat{p})b = \nabla_p c^T \hat{G}(\hat{s}, \hat{p})b$.

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then

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1. Reduced-order model satisfies necessary conditions for surrogate models in trust region methods [ALEXANDROV/DENNIS/LEWIS/TORCZON 1998].
2. Approximation of gradient allows use of reduced-order model for sensitivity analysis.



Generic implementation of interpolatory PMOR

Define $\mathcal{A}(s, p) := sE(p) - A(p)$.

1. Select “frequencies” $s_1, \dots, s_k \in \mathbb{C}$ and parameter vectors $p^{(1)}, \dots, p^{(\ell)} \in \Omega \subset \mathbb{R}^d$.
2. Compute (orthonormal) basis of

$$\mathcal{V} = \text{span} \{ \mathcal{A}(s_1, p^{(1)})^{-1} B(p^{(1)}), \dots, \mathcal{A}(s_k, p^{(\ell)})^{-1} B(p^{(\ell)}) \}.$$

3. Compute (orthonormal) basis of

$$\mathcal{W} = \text{span} \{ \mathcal{A}(s_1, p^{(1)})^{-T} C(p^{(1)})^T, \dots, \mathcal{A}(s_k, p^{(\ell)})^{-T} C(p^{(\ell)})^T \}.$$

4. Set $V := [v_1, \dots, v_{k\ell}]$, $\tilde{W} := [w_1, \dots, w_{k\ell}]$, and $W := \tilde{W}(\tilde{W}^T V)^{-1}$.
(Note: $r = k\ell$).

5. Compute
$$\begin{cases} \hat{A}(p) := W^T A(p) V, & \hat{B}(p) := W^T B(p) V, \\ \hat{C}(p) := W^T C(p) V, & \hat{E}(p) := W^T E(p) V. \end{cases}$$



Remarks

- If directional derivatives w.r.t. p are included in $\text{range}(V)$, $\text{range}(W)$, then also the Hessian of $G(\hat{s}, \hat{p})$ is interpolated by the Hessian of $\hat{G}(\hat{s}, \hat{p})$.



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- For prescribed parameter vectors $p^{(k)}$, we can use corresponding \mathcal{H}_2 -optimal frequencies $s_{k,\ell}$, $\ell = 1, \dots, r_k$ computed by IRKA, i.e., reduced-order systems $\hat{G}_*^{(k)}$ so that

$$\|G(\cdot, p^{(k)}) - \hat{G}_*^{(k)}(\cdot)\|_{\mathcal{H}_2} = \min_{\substack{\text{order}(\hat{G})=r_k \\ \hat{G} \text{ stable}}} \|G(\cdot, p^{(k)}) - \hat{G}^{(k)}(\cdot)\|_{\mathcal{H}_2},$$

where

$$\|G\|_{\mathcal{H}_2} := \left(\frac{1}{2\pi} \int_{-\infty}^{+\infty} \|G(j\omega)\|_{\text{F}}^2 d\omega \right)^{1/2}.$$



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- Optimal choice of interpolation frequencies s_k and parameter vectors $p^{(k)}$ possible for special cases.

Numerical Example: Thermal Conduction in a Semiconductor Chip

- Important requirement for a compact model of thermal conduction is boundary condition independence.
- The thermal problem is modeled by the heat equation, where heat exchange through device interfaces is modeled by convection boundary conditions containing **film coefficients** $\{p_i\}_{i=1}^3$ describing the heat exchange at i th interface.
- Spatial semi-discretization leads to

$$E\dot{x}(t) = (A_0 + \sum_{i=1}^3 p_i A_i)x(t) + bu(t), \quad y(t) = c^T x(t),$$

where $n = 4, 257$, A_i , $i = 1, 2, 3$, are diagonal.

Source: C.J.M Lasance, *Two benchmarks to facilitate the study of compact thermal modeling phenomena*, IEEE Transactions on Components and Packaging Technologies, 24(4):559–565, 2001.

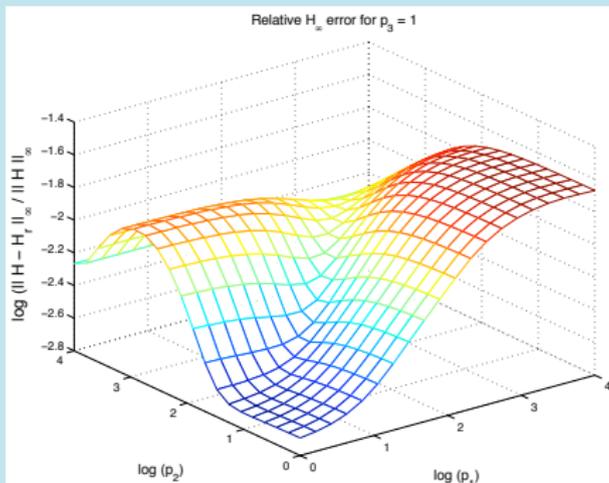
MOR Wiki: http://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Microthruster_Unit



Numerical Example: Thermal Conduction in a Semiconductor Chip

Choose 2 interpolation points for parameters (“important” configurations), 8/7 H_2 -optimal interpolation frequencies selected by IRKA. $\Rightarrow k = 2, \ell = 8, 7$, hence $r = 15$.

$p_3 = 1, p_1, p_2 \in [1, 10^4]$.





Optimality of Interpolation Points

Theorem

[BAUR/BEATTIE/B./GUGERCIN 2011]

For special parameterized SISO systems,

$$A(p) \equiv A_0, \quad E(p) \equiv E_0, \quad B(p) = B_0 + p_1 B_1, \quad C(p) = C_0 + p_2 C_1,$$

optimal choice possible, **necessary conditions**:

If \hat{G} minimizes the approximation error w.r.t. $\|G - \hat{G}\|_{\mathcal{H}_2 \times L_2(\Omega)}$, $p \in \Omega \subset \mathbb{R}^d$, and $\Lambda(\hat{A}, \hat{E}) = \{\hat{\lambda}_1, \dots, \hat{\lambda}_r\}$ (all simple), then the **interpolation frequencies** satisfy

$$s_i = -\hat{\lambda}_i, \quad i = 1, \dots, r,$$

and the **parameter interpolation points** $\{p^{(1)}, \dots, p^{(r)}\}$ satisfy the **interpolation conditions**

$$\begin{aligned} G(-\hat{\lambda}_k, p^{(k)}) &= \hat{G}(-\hat{\lambda}, p^{(k)}), \\ \frac{\partial}{\partial s} G(-\hat{\lambda}, p^{(k)}) &= \frac{\partial}{\partial s} \hat{G}(-\hat{\lambda}, p^{(k)}), \quad \nabla_p G(-\hat{\lambda}, p^{(k)}) = \nabla_p \hat{G}(-\hat{\lambda}, p^{(k)}). \end{aligned}$$

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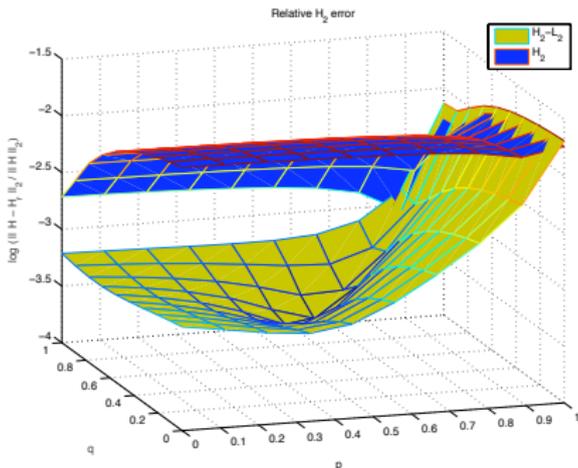
Proof:

$$\|G\|_{\mathcal{H}_2 \times L_2(\Omega)} = \|L^T \tilde{G} L\|_{\mathcal{H}_2}, \quad \text{where } \tilde{G}(s) = \begin{bmatrix} C_0 \\ C_1 \end{bmatrix} (sE - A)^{-1} [B_0, B_1], \quad L = \begin{bmatrix} 1 & 0 \\ \frac{1}{2} & \frac{1}{2\sqrt{3}} \end{bmatrix}.$$

\implies **Computation via IRKA applied to \tilde{G} .**

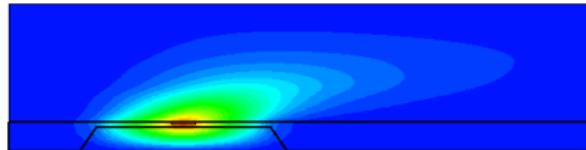
Optimality of Interpolation Points — Numerical Example

- Model for evolution of temperature distribution on a plate, described by the heat equation.
- FDM SISO model of order $n = 197$.
- Parameter $p_1 \in [0, 1]$ encodes movement of heat source from B_0 to $B_0 + B_1$, analogous for relocation of measurement.



Relative $\mathcal{H}_2 \otimes L_2(\Omega)$ error: 7.5×10^{-4} .

Consider an **anemometer**, a flow sensing device located on a membrane used in the context of minimizing heat dissipation.



Source: [BAUR/B./GREINER/KORVINK/LIENEMANN/MOOSMANN 2011]

- FE model:

$$E\dot{x}(t) = (A + pA_1)x(t) + Bu(t), \quad y(t) = Cx(t), \quad x(0) = 0,$$

- $n = 29,008$, $m = 1$, $q = 3$, $p_1 \in [0, 1]$ fluid velocity.

Source: MOR Wiki: <http://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Anemometer>

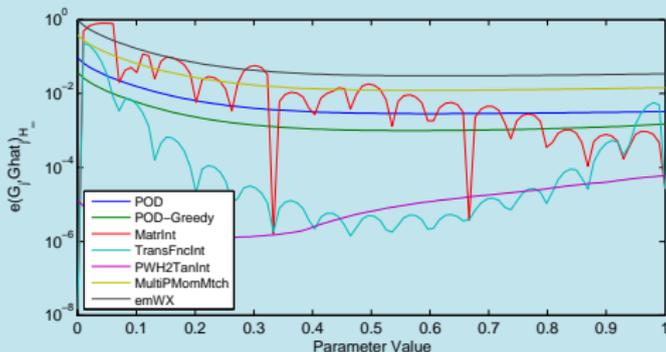
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\mathcal{H}_∞ error



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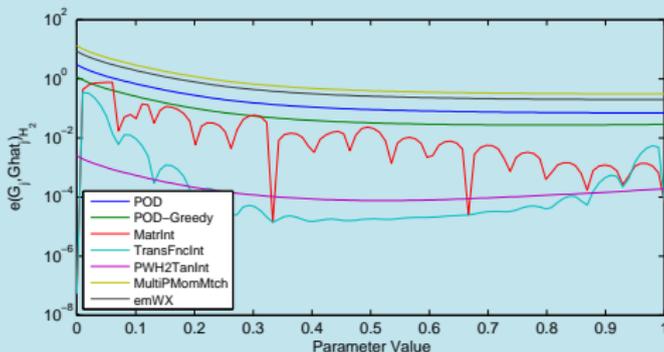
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\mathcal{H}_2 error



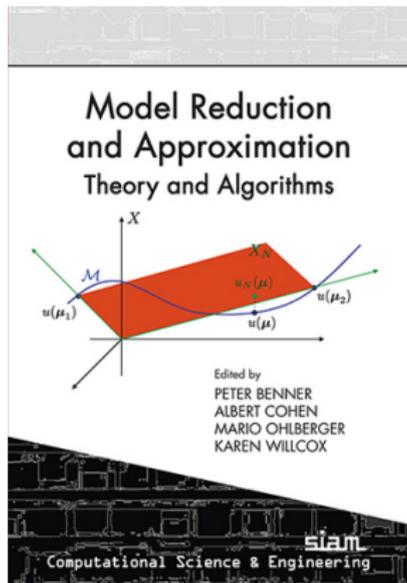
Source: MOR Wiki: <http://morwiki.mpi-magdeburg.mpg.de/morwiki/index.php/Anemometer>

For more details of this comparisons, and other tests, see



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Chapter 9 in





1. Introduction
2. PMOR Methods based on Moment Matching
3. Optimal PMOR using Rational Interpolation?
4. Conclusions and Outlook



Conclusions and Outlook

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- New direction: **data-enhanced approaches**, merging ideas from Loewner framework with model-based methods.
- Most of the methods can be used to significantly accelerate UQ by Monte Carlo or Stochastic Collocation methods!

- 

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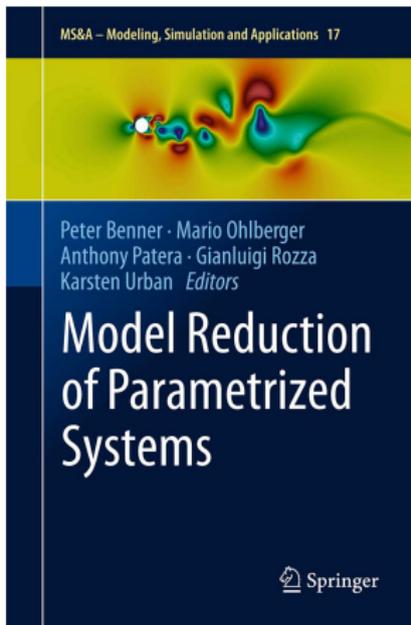
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