Université du Littoral Côte d'Opale, Calais
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PARAMETRIC MODEL REDUCTION
(Just) Another Instance of Multivariate Function Approximation!?

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Joint work with U. Baur, T. Breiten, L. Feng, J. Saak (MPI DktS),
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Overview

Introduction

Model Reduction

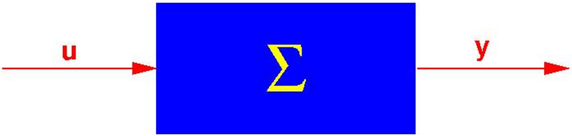
Dynamical Systems

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

with

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

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



Model Reduction for Dynamical Systems

Original System

$$\Sigma(p):\left\{\begin{aligned} E(p)\dot{x} &= f(t,x,u,p),\\ y &= g(t,x,u,p).\end{aligned}\right.$$

- states $x(t;p) \in \mathbb{R}^n$,
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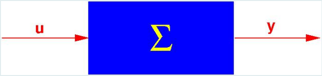

Reduced-Order System

$$\widehat{\Sigma}(p):\left\{\begin{aligned} \hat{E}(p)\dot{\hat{x}} &= \widehat{f}(t,\hat{x},u,p),\\ \hat{y} &= \widehat{g}(t,\hat{x},u,p).\end{aligned}\right.$$

- states $\hat{x}(t;p) \in \mathbb{R}^r$, $r \ll n$
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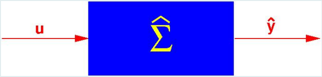

Goal:

$\|y - \hat{y}\| <$ tolerance $\cdot \|u\|$ for all admissible input signals and relevant parameter settings.

Model Reduction for Dynamical Systems

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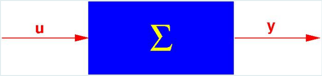

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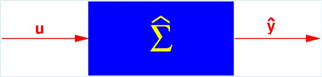

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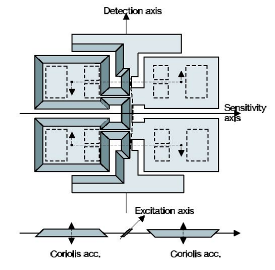
Motivation

Applications in Microsystems/MEMS Design

Microgyroscope (butterfly gyro)

- Application: inertial navigation.



- Voltage applied to electrodes induces vibration of wings, resulting rotation due to Coriolis force yields sensor data.
- FE model of second order:
  $N = 17.361 \rightsquigarrow n = 34.722,\ m = 1,\ p = 12.$
- Sensor for position control based on acceleration and rotation.

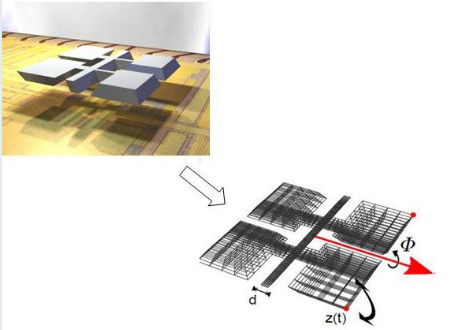
Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark

Motivation

Applications in Microsystems/MEMS Design

Microgyroscope (butterfly gyro)

Parametric FE model: $M(d)\ddot{x}(t) + D(\Phi, d, \alpha, \beta)\dot{x}(t) + T(d)x(t) = Bu(t).$



[Feng/B./Korvink '10]

Supported by DFG Projekt BE2174/7-1 *Automatic, Parameter-Preserving Model Reduction for Applications in Microsystems Technology* with IMTEK, Freiburg.

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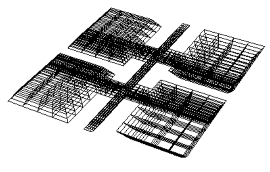
Parametric FE model:

$$M(d)\ddot{x}(t) + D(\Phi, d, \alpha, \beta)\dot{x}(t) + T(d)x(t) = Bu(t),$$

wobei

$$\begin{aligned} M(d) &= M_1 + dM_2, \\ D(\Phi, d, \alpha, \beta) &= \Phi(D_1 + dD_2) + \alpha M(d) + \beta T(d), \\ T(d) &= T_1 + \frac{1}{d}T_2 + dT_3, \end{aligned}$$



with

- width of bearing: d,
- angular velocity: Φ,
- Rayleigh damping parameters: α, β.

[Feng/B./Korvink '10]

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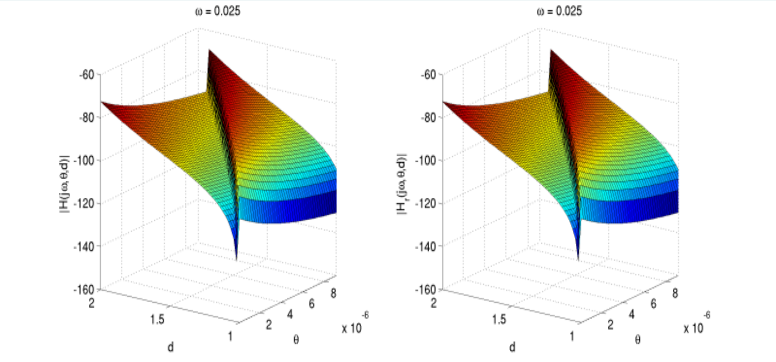
Motivation

Applications in Microsystems/MEMS Design

Microgyroscope (butterfly gyro)

Original... and reduced-order model.



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Motivation

Applications in Microsystems/MEMS Design

Electro-chemical scanning electron microscope (SEM)

- Used for high resolution measurements of chemical reactivity and topography of surfaces, in particular for biological systems and nano-structures.
- Based on measuring current through a micro-electrode which is moved through electrolyte along surface.
- Measurements lead to cyclic voltammogram, plotting the current vs. applied potential.
- Mathematical model: Multi-species diffusion equations with mixed boundary conditions, defined by Butler-Volmer equation.

  Film coefficient depending on the applied potential is to be preserved.

Motivation

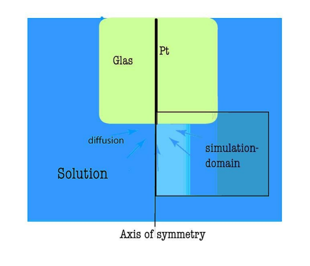
Applications in Microsystems/MEMS Design

Electro-chemical scanning electron microscope (SEM)

Example: 2 film coefficients $\Longrightarrow$

$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t).$$

FE model: $n = 16,912$, $m = 3$ inputs, A_1, A_2 diagonal.



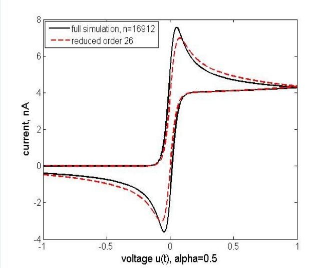


Figure: Schematic diagram of experimental set-up and corresponding voltammogram.

Motivation

Applications in Microsystems/MEMS Design

Flow sensor (anemometer)

- Sensor measuring flow rates of fluids or gas.
- Based on one heater with thermo-sensors on both sides.
- Design process requires compact model, in which flow velocity and, possibly, material parameters (viscosity, density) appear as symbolic quantities.
- Mathematical model: Linear convection-diffusion equation.

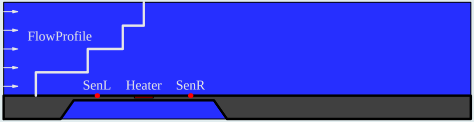


Figure: Anemometer model generated using ANSYS.

Motivation

Applications in Microsystems/MEMS Design

Flow sensor (anemometer)

Parameter study based on reduced-order model:

- Full model: $n = 29,008$.
- Reduced-order Model: $r = 75$
  12 parameter interpolation points,
  BT $(tol = 10^{-4}) \Rightarrow\ 2 \leq r_j \leq 9$,
  $\max_{\omega,p} |R(\jmath\omega, p)| \leq 6.5 \cdot 10^{-4}$
  $(R := G - \hat{G})$.
- Visualize frequency-response for $p \in [0, 1]$ (100 frequencies, 1000 parameter values).
- Generation of movie:

  $>$ 11 days with full model;
  93 sec. with reduced-order model!

[Baur/B., AT 2009]

Model Reduction Basics

Simulation-Free Methods

1. Modal Truncation
2. Guyan-Reduction/Substructuring
3. Padé-Approximation, Moment-Matching, and Krylov Subspace Methods ($\rightsquigarrow$ interpolatory methods)
4. Balanced Truncation ($\rightsquigarrow$ system-theoretic methods)
5. many more...

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Joint feature of many methods: Galerkin or Petrov-Galerkin-type projection of state-space onto low-dimensional subspace $\mathcal{V}$ along $\mathcal{W}$: assume $x \approx VW^T x =: \tilde{x}$, where

$$\mathrm{range}\,(V) = \mathcal{V}, \quad \mathrm{range}\,(W) = \mathcal{W}, \quad W^T V = I_r.$$

Then, with $\hat{x} = W^T x$, we obtain $x \approx V\hat{x}$ and

$$\|x - \tilde{x}\| = \|x - V\hat{x}\|.$$

Linear Parametric Systems

Linear, time-invariant systems depending on parameters

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

Laplace Transformation / Frequency Domain

Application of Laplace transformation ($x(t;p) \mapsto x(s;p)$, $\dot{x}(t;p) \mapsto sx(s;p)$) to linear system with $x(0) = 0$:

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

yields I/O-relation in frequency domain:

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

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

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Model Reduction for Linear Parametric Systems

Problem

Approximate the dynamical system

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

by reduced-order system

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

of order $r \ll n$, such that

$$\|y - \hat{y}\| = \|Gu - \hat{G}u\| \leq \|G - \hat{G}\|\|u\| < \text{tolerance} \cdot \|u\|.$$

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

Model Reduction for Linear Parametric Systems

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Approximate the dynamical system

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Appropriate representation:

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

allows easy parameter preservation for projection based model reduction.

Model Reduction for Linear Parametric Systems

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Applications:

- Repeated simulation for varying material or geometry parameters, boundary conditions,
- Optimization and design.

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Additional model reduction goal:

preserve parameters as symbolic quantities in reduced-order model:

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

Parametric Model Redution (PMOR) . . .

just another instance of multivariate function approximation?

- Yes — want to approximate (for fast evaluation) function G, defined on $\mathbb{C}^{q+1}$.
- But:

$$\begin{aligned} G : \mathbb{C} \times \Omega &\rightarrow \mathbb{C}^{p\times m}, \quad \Omega = [\alpha_1, \beta_1] \times \ldots \times [\alpha_q, \beta_q], \\ G(s; p_1, \ldots, p_q) &\in \mathbb{C}^{p\times m}. \end{aligned}$$

$\rightsquigarrow$ Variables s and p_j have different "meaning" for G.
Dynamical system is in the background!

$\rightsquigarrow$ Matrix-valued function, require matrix- not entry-wise approximation!

- G is rational in s, $n \sim$ degree of denominator polynomial.
  $\rightsquigarrow$ Require approximation to be rational in s.
- Require structure-preserving approximation, e.g., for control design.
  $\rightsquigarrow$ Need realization as linear parametric system!
- Also would like to be able to reproduce system dynamics (stability, passivity).

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Therefore: at least not "just"!

Interpolatory Model Reduction

Short Introduction

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 projection 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

$$\hat{E} = W^T EV,\ \hat{A} = W^T AV,\ \hat{B} = W^T B,\ \hat{C} = CV.$$

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

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

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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 projection 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

$$\hat{E} = W^T EV,\ \hat{A} = W^T AV,\ \hat{B} = W^T B,\ \hat{C} = CV.$$

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

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

Rational Interpolation/Moment-Matching

Choose V, W such that

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

and

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

Interpolatory Model Reduction

Short Introduction

Theorem (simplified) [Grimme '97, Villemagne/Skelton '87]

If

$$\begin{aligned} \operatorname{span}\left\{(s_1 E - A)^{-1}B, \ldots, (s_k E - A)^{-1}B\right\} &\subset \operatorname{Ran}(V), \\ \operatorname{span}\left\{(s_1 E - A)^{-T}C^T, \ldots, (s_k E - A)^{-T}C^T\right\} &\subset \operatorname{Ran}(W), \end{aligned}$$

then

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

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

Remarks:

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

- dual rational Arnoldi/Lanczos [Grimme '97],
- Iterative Rational Krylov-Algo. [Antoulas/Beattie/Gugercin '07].

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Remarks:

using Galerkin/one-sided projection 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 $\rightsquigarrow$ moment-matching methods/Padé approximation,

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

Interpolatory Model Reduction

Notation

Parametric Systems

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

Assume

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

Interpolatory Model Reduction

Structure-Preservation

Petrov-Galerkin-type projection

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

$$
\begin{aligned}
\hat{E}(p) &= W^TE_0V + e_1(p)W^TE_1V + \ldots + e_{q_E}(p)W^TE_{q_E}V, \\
&= \hat{E}_0 + e_1(p)\hat{E}_1 + \ldots + e_{q_E}(p)\hat{E}_{q_E}, \\
\hat{A}(p) &= W^TA_0V + a_1(p)W^TA_1V + \ldots + a_{q_A}(p)W^TA_{q_A}V, \\
&= \hat{A}_0 + a_1(p)\hat{A}_1 + \ldots + a_{q_A}(p)\hat{A}_{q_A}, \\
\hat{B}(p) &= W^TB_0 + b_1(p)W^TB_1 + \ldots + b_{q_B}(p)W^TB_{q_B}, \\
&= \hat{B}_0 + b_1(p)\hat{B}_1 + \ldots + b_{q_B}(p)\hat{B}_{q_B}, \\
\hat{C}(p) &= C_0V + c_1(p)C_1V + \ldots + c_{q_C}(p)C_{q_C}V, \\
&= \hat{C}_0 + c_1(p)\hat{C}_1 + \ldots + c_{q_C}(p)\hat{C}_{q_C}.
\end{aligned}
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Interpolatory Model Reduction

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

PMOR based on Multi-Moment Matching

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

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

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

Algorithms:

- [Daniel et al. '04]: explicit computation of moments, numerically unstable.
- [Farle et al. '06/'07]: Krylov subspace approach, only polynomial parameter-dependance, numerical properties not clear, but appears to be robust.
- [Feng/B. '07–'10]: Arnoldi-MGS method, employ recursive dependance of multi-moments, numerically robust, r often larger as with [Farle et al.].

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PMOR based on Multi-Moment Matching

Numerical Examples

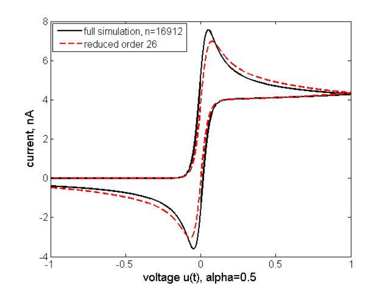
Electro-chemical SEM:

compute cyclic voltammogram based on FEM model

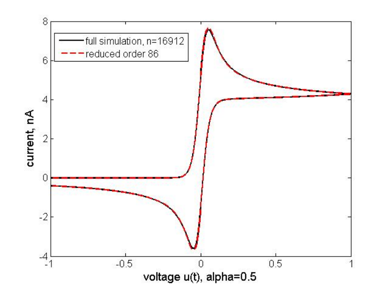
$$E\dot{x}(t) = (A_0 + p_1 A_1 + p_2 A_2)x(t) + Bu(t), \quad y(t) = c^T x(t),$$

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

$K = L = k + \ell = 4 \;\Rightarrow\; r = 26$



$K = L = k + \ell = 9 \;\Rightarrow\; r = 86$



PMOR based on Multi-Moment Matching

Numerical Examples

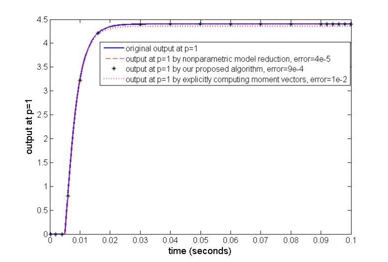
Anemometer:

FE model

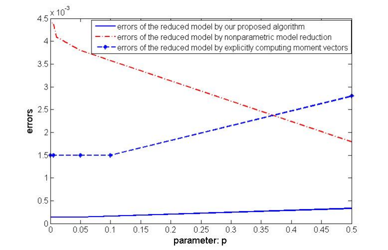
$$E\dot{x}(t) = (A_0 + p_1 A_1)x(t) + bu(t), \quad y(t) = c^T x(t),$$

where $n = 29,008$, $m = q = 1$.

Outputs for $p = 1$



Output errors for $p = 1$



PMOR based on Rational Interpolation

Theory: Interpolation of the Transfer Function

Theorem 1 [Baur/Beattie/B./Gugercin '07/'09]

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

and 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
$$(\hat{s}\,E(\hat{p})-A(\hat{p}))^{-1}B(\hat{p})\in\mathrm{Ran}(V)$$

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

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

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.

a) If $(\hat{s}\,E(\hat{p})-A(\hat{p}))^{-1}B(\hat{p})b\in\mathrm{Ran}(V)$, then $G(\hat{s},\hat{p})b=\hat{G}(\hat{s},\hat{p})b$;

b) If $\left(c^TC(\hat{p})\,(\hat{s}\,E(\hat{p})-A(\hat{p}))^{-1}\right)^T\in\mathrm{Ran}(W)$, then $c^TG(\hat{s},\hat{p})=c^T\hat{G}(\hat{s},\hat{p})$.

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PMOR based on Rational Interpolation

Theory: Interpolation of the Parameter Gradient

Theorem 2 [Baur/Beattie/B./Gugercin '07/'09]

Suppose that $E(p)$, $A(p)$, $B(p)$, $C(p)$ are C^1 in a neighborhood of $\hat{p} = [\hat{p}_1, \ldots, \hat{p}_d]^T$ 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

$$(\hat{s}\,E(\hat{p}) - A(\hat{p}))^{-1}\,B(\hat{p}) \in \mathrm{Ran}(V)$$

and

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

then

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

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

PMOR based on Rational Interpolation

Theory: Interpolation of the Parameter Gradient

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

1. Assertion of theorem satisfies necessary conditions for surrogate models in trust region methods [Alexandrov/Dennis/Lewis/Torczon '98].
2. Approximation of gradient allows use of reduced-order model for sensitivity analysis.

PMOR based on Rational Interpolation

Algorithm

Generic implementation of interpolatory PMOR

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

1. Select "frequencies" $s_1, \ldots, s_k \in \mathbb{C}$ and parameter vectors $p^{(1)}, \ldots, p^{(\ell)} \in \mathbb{R}^d$.
2. Compute (orthonormal) basis of
$$\mathcal{V} = \operatorname{span}\left\{\mathcal{A}(s_1, p^{(1)})^{-1} B(p^{(1)}), \ldots, \mathcal{A}(s_k, p^{(\ell)})^{-1} B(p^{(\ell)})\right\}.$$
3. Compute (orthonormal) basis of
$$\mathcal{W} = \operatorname{span}\left\{\mathcal{A}(s_1, p^{(1)})^{-H} C(p^{(1)})^T, \ldots, \mathcal{A}(s_k, p^{(\ell)})^{-T} C(p^{(\ell)})^T\right\}.$$
4. Set $V := [v_1, \ldots, v_{k\ell}]$, $\tilde{W} := [w_1, \ldots, w_{k\ell}]$, and $W := \tilde{W}(\tilde{W}^T V)^{-1}$. (Note: $r = k\ell$).
5. Compute $\begin{cases} \hat{A}(p) := W^T A(p) V, & \hat{B}(p) := W^T B(p) V, \\ \hat{C}(p) := W^T C(p) V, & \hat{E}(p) := W^T E(p) V. \end{cases}$

PMOR based on Rational Interpolation

Remarks

- If directional derivatives w.r.t. p are included in $\mathrm{Ran}(V)$, $\mathrm{Ran}(W)$, then also the Hessian of $G(\hat{s}, \hat{p})$ is interpolated by the Hessian of $\hat{G}(\hat{s}, \hat{p})$.
- Choice of optimal interpolation frequencies s_k and parameter vectors $p^{(k)}$ in general is an open problem.
- For prescribed parameter vectors $p^{(k)}$, we can use corresponding $\mathcal{H}_2$-optimal frequencies $s_{k,\ell}$, $\ell = 1, \ldots, r_k$ computed by IRKA, i.e., reduced-order systems $\hat{G}_*^{(k)}$ so that

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

  where

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

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

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PMOR based on Rational Interpolation

Optimality of Interpolation Points

Theorem 3 [Baur/Beattie/B./Gugercin '09]

For special parameterized SISO systems,

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

optimal choice possible, necessary conditions:
If $\hat{G}$ minimizes the approximation error w.r.t.

$$\|G - \hat{G}\|_{\mathcal{H}_2 \times \mathcal{L}_2(\Omega)}, \qquad p \in \Omega \subset \mathbb{R}^d,$$

and $\Lambda(\hat{A}, \hat{E}) = \{\hat{\lambda}_1, \ldots, \hat{\lambda}_r\}$ (all simple), then the interpolation frequencies satisfy

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

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

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

PMOR based on Rational Interpolation

Optimality of Interpolation Points

Theorem 3 [Baur/Beattie/B./Gugercin '09]

For special parameterized SISO systems,

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

optimal choice possible, necessary conditions:
If $\hat{G}$ minimizes the approximation error w.r.t.

$$\|G - \hat{G}\|_{\mathcal{H}_2 \times \mathcal{L}_2(\Omega)}, \qquad p \in \Omega \subset \mathbb{R}^d,$$

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

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Proof:

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

$\Longrightarrow$ Computation via IRKA applied to $\tilde{G}$.

PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

- FD discretization ($n = 400$, $m = q = 1$) yields

$$\dot{x}(t) = (p_0 A_0 + p_1 A_1 + p_2 A_2)\, x(t) + B\, u(t),$$

  where p_0 = diffusion coefficient; p_i, $i = 1, 2$, convection in x_i direction, $p \in [0, 1]^3$.

- Parameter vectors for interpolation:

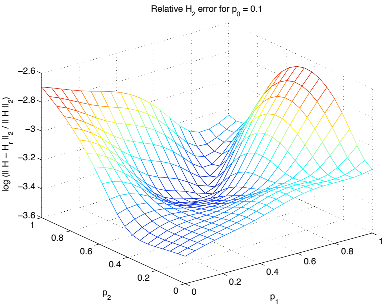
$$\begin{array}{lll} p^{(1)} = (0.8, 0.5, 0.5), & p^{(2)} = (0.8, 0, 0.5), & p^{(3)} = (0.8, 1, 0.5), \\ p^{(4)} = (0.1, 0.5, 0.5), & p^{(5)} = (0.1, 0, 1), & p^{(6)} = (0.1, 1, 1). \end{array}$$

- Compare implementations:
  - generic rational PMOR ($\equiv$ fix interpolation frequencies),
  - IRKA-based rational PMOR ($\equiv$ optimize interpolation frequencies).
- Reduced-order model: $r_1 = r_2 = r_3 = 3$, $r_4 = r_5 = r_6 = 4 \Rightarrow r = 21.$

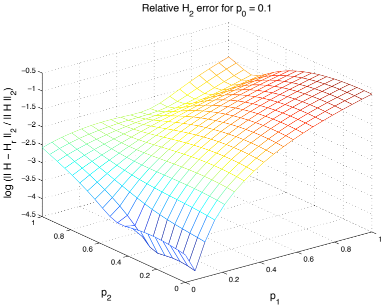
PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

Relative $\mathcal{H}_2$ Error for $p_0 = 0.1$



IRKA, 5 steps

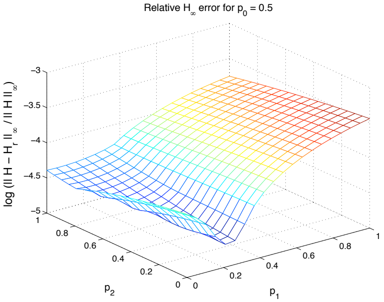


generic

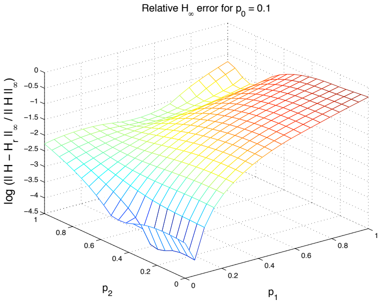
PMOR based on Rational Interpolation

Numerical Example: 2D Convection-Diffusion Equation

Relative $\mathcal{H}_\infty$ Error for $p_0 = 0.1$



IRKA, 5 steps



generic

PMOR based on Rational Interpolation

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 $\{p_i\}_{i=1}^3$, to describe the heat exchange at the ith 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.

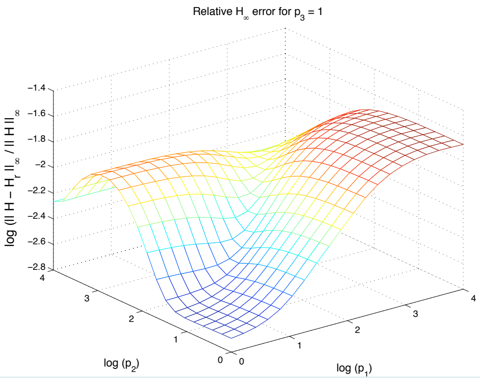
Source: C.J.M Lasance, *Two benchmarks to facilitate the study of compact thermal modeling phenomena*, IEEE. Trans. Components and Packaging Technologies, Vol. 24, No. 4, pp. 559–565, 2001.

PMOR based on Rational Interpolation

Numerical Example: Thermal Conduction in a Semiconductor Chip

Choose 2 interpolation points for parameters ("important" configurations), 8/7 interpolation frequencies are picked H_2 optimal by IRKA. $\Longrightarrow$ $k = 2, \ell = 8, 7$, hence $r = 15$.

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



Model Reduction for Linear Parameter-Varying Systems

LPV Systems

Linear parameter-varying (LPV) systems = linear parametric systems with time-dependent parameters:

$$\Sigma : \quad \begin{cases} \dot{x}(t) = A_0 x(t) + \sum_{i=1}^{q} p_i(t) A_i x(t) + B_0 u(t), \\ y(t) = C x(t), \quad x(0) = x_0, \end{cases}$$

Model Reduction for Linear Parameter-Varying Systems

LPV Systems: A Special Class of Bilinear Systems

Note that LPV systems

$$\dot{x}(t) = A_0 x(t) + \sum_{i=1}^{q} p_i(t) A_i x(t) + B_0 u_0(t), \quad y = Cx,$$

can be incorporated into the class of bilinear systems

$$\Sigma : \quad \begin{cases} \dot{x}(t) = Ax(t) + \sum_{i=1}^{q} A_i x(t) u_i(t) + Bu(t), \\ y(t) = Cx(t), \quad x(0) = x_0, \end{cases}$$

where $A_i \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{p \times n}$. For this, the parameter dependent terms $p_i(t)$ are interpreted as additional inputs, resulting in a MIMO bilinear system with $q + k$ input variables:

$$u(t) := \begin{bmatrix} p_1(t) & \ldots & p_q(t) & u_0(t) \end{bmatrix},$$
$$B := \begin{bmatrix} \mathbf{0} & \ldots & \mathbf{0} & B_0 \end{bmatrix}.$$

Remark: Applying bilinear MOR, this automatically yields structure-preserving MOR techniques for LPV systems!

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Model Reduction for Linear Parameter-Varying Systems

$\mathcal{H}_2$-Norm for Bilinear Systems

Similar to the linear case, there exist generalized transfer functions, i.e. for the SISO case:

$$H_k(s_1,\ldots,s_i) = C(s_kI - A_0)^{-1}A_1 \cdots (s_2I - A_0)^{-1}A_1(s_1I - A_0)^{-1}B.$$

Hence, we may define the $\mathcal{H}_2$-norm for bilinear systems:

$$||\Sigma||^2_{\mathcal{H}_2} := \operatorname{tr}\left(\sum_{k=1}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\frac{1}{(2\pi)^k}\,\overline{H_k(i\omega_1,\ldots,i\omega_k)}H_k^T(i\omega_1,\ldots,i\omega_k)\right),$$

which can be computed via the solution of the generalized Lyapunov eq.:

$$\begin{aligned}||\Sigma||^2_{\mathcal{H}_2} &= CPC^T\\ &= (\operatorname{vec}(I_p))^T\,(C\otimes C)\left(-A_0\otimes I - I\otimes A_0 - \sum_{k=1}^{q}A_k\otimes A_k\right)^{-1}(B\otimes B)\operatorname{vec}(I_m).\end{aligned}$$

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Model Reduction for Linear Parameter-Varying Systems

Interpolation-Based MOR for Bilinear Systems

Studying $\mathcal{H}_2$-norm of the error system leads to an iterative procedure:

Algorithm 1 Bilinear IRKA

Input: A_0, A_k, B, C, $\hat{A}_0$, $\hat{A}_k$, $\hat{B}$, $\hat{C}$

Output: A_0^{opt}, A_k^{opt}, B^{opt}, C^{opt}

1: **while** (change in $\Lambda > \epsilon$) **do**

2: $\quad R\Lambda R^{-1} = \hat{A}_0$, $\tilde{B} = R^{-1}\hat{B}$, $\tilde{C} = \hat{C}R$, $\tilde{A}_k = R^{-1}\hat{A}_k R$

3: $\quad \mathrm{vec}(V) = \left(-\Lambda \otimes I_n - I_{\hat{n}} \otimes A_0 - \sum_{k=1}^{m} \tilde{A}_k \otimes A_k\right)^{-1} \left(\tilde{B} \otimes B\right) \mathrm{vec}(I_m)$

4: $\quad \mathrm{vec}(W) = \left(-\Lambda \otimes I_n - I_{\hat{n}} \otimes A_0^T - \sum_{k=1}^{m} \tilde{A}_k^T \otimes A_k^T\right)^{-1} \left(\tilde{C}^T \otimes C^T\right) \mathrm{vec}(I_p)$

5: $\quad V = \mathrm{orth}(V)$, $W = \mathrm{orth}(W)$

6: $\quad \hat{A}_0 = \left(W^T V\right)^{-1} W^T A_0 V$, $\hat{A}_k = \left(W^T V\right)^{-1} W^T A_k V$,
$\quad \hat{B} = \left(W^T V\right)^{-1} W^T B$, $\hat{C} = CV$

7: **end while**

8: $A_0^{opt} = \hat{A}_0$, $A_k^{opt} = \hat{A}_k$, $B^{opt} = \hat{B}$, $C^{opt} = \hat{C}$

Conclusions and Outlook

- We have presented a general framework for interpolation-based model reduction of parametric systems.
- Applications: microsystems technology in particular, but also applicable to other areas where design and optimization are important.
- Approximation results for partial derivatives w.r.t. parameters $\rightsquigarrow$ sensitivities for process variations, optimization can be computed based on reduced-order model.
- Implementation of parametric model reduction based on multi-moment matching or rational Krylov methods (requires discretization w.r.t. frequency parameter).
- Efficiency of parametric model reduction methods can be enhanced when combined with sparse grid ideas.
- Wide variety of algorithmic possibilities, further need for optimization of interpolation point selection and error bounds, numerous possible applications.
  $\mathcal{H}_2$ optimization for bilinear systems very promising!
- Ideas from multivariate function approximation useful?

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