Finding the Characteristics: Radial Basis Function Interpolation for Parametric Model Order Reduction

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Linear time-invariant systems

Definition and stability

Let

- $A \in \mathbb{R}^{d \times d}$
- $B \in \mathbb{R}^{d}$
- $C \in \mathbb{R}^{1 \times d}$

A *linear time-invariant* (LTI) system

$$\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ y(t) = Cx(t) \end{cases} \quad (1)$$

is called *stable* if A has eigenvalues only in the left half plane.

Model order reduction

Model order reduction methods try to find a *reduced LTI system*

$$\hat{\Sigma} : \begin{cases} \dot{x}(t) = \hat{A}x(t) + \hat{B}u(t) \\ \hat{y}(t) = \hat{C}x(t) \end{cases} \tag{2}$$

where

- $r \ll d$
- $\hat{A} \in \mathbb{R}^{r\times r}$, $\hat{B} \in \mathbb{R}^{r}$, $\hat{C} \in \mathbb{C}^{1\times r}$

and $\hat{A}$ has eigenvalues only in the left half plane.

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Linear time-invariant systems

Transfer function

The input-output map $y(u)$ of (1) is characterized by the *transfer function*

$$H : \mathbb{C} \to \mathbb{C}, \quad H(\omega) = C(\omega I - A)^{-1} B$$

in frequency space. $\hat{H}$ is defined accordingly for (2).

Error estimate

Let $y(t)$ and $\hat{y}(t)$ be the output of (1) and (2). Then the *error of $y(t)$* is bounded by

$$\max_{t>0} |y(t) - \hat{y}(t)| \leq \|H - \hat{H}\|_{\mathcal{H}_2} \|u\|_{\mathcal{L}_2},$$

where the *$\mathcal{H}_2$-norm* is defined as

$$\|H - \hat{H}\|^2_{\mathcal{H}_2} = \frac{1}{2\pi} \int_{-\infty}^{\infty} |H(\imath\omega) - \hat{H}(\imath\omega)|^2 d\omega$$

$\mathcal{H}_2$ optimality

Given

- a stable dynamical system (1),
- a reduced order system (2).

If the reduced system (2) *minimizes $\|H - \hat{H}\|_{\mathcal{H}_2}$*, it Hermite interpolates (1) at its mirror poles $\sigma_1, \ldots, \sigma_r$.

Petrov-Galerkin projection

Let

- r fixed, $\sigma_1, \ldots, \sigma_r$ given
- V, W such that

$$(\sigma_i I - A)^{-1} B \in \text{span}(V)$$
$$(\sigma_i I - A)^{-T} C^T \in \text{span}(W)$$
$$V^T W = I$$

Then the reduced order model by *Petrov-Galerkin projection*

$$\hat{A} = V^T A W, \quad \hat{B} = V^T B, \quad \hat{C} = CW$$

Hermite interpolates (1) at $\sigma_1, \ldots, \sigma_r$.

Remark

- $\hat{A}$ is unique up to matrix similarity

Iterative Rational Krylov Algorithm (IRKA)

- *Problem:* Find $\sigma_1, \ldots, \sigma_r$ for (1)
- *Solution by IRKA:* Local optimum
  - Initial $\sigma_1, \ldots, \sigma_r$ given
  - Fixed-point iteration
  - Locally convergent if local optimum is attractive (e. g. for state-space-symmetric systems)

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Parametric LTI system

Given a compact domain $\Omega \subset \mathbb{R}^n$. Let

- A, B and C as in (1)
- A, B and C depend (smoothly) on some $p \in \Omega$

Then

- $A(p), B(p)$ and $C(p)$ define a *parametric LTI system*

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

- Each value of p defines an LTI system, which can be reduced as before

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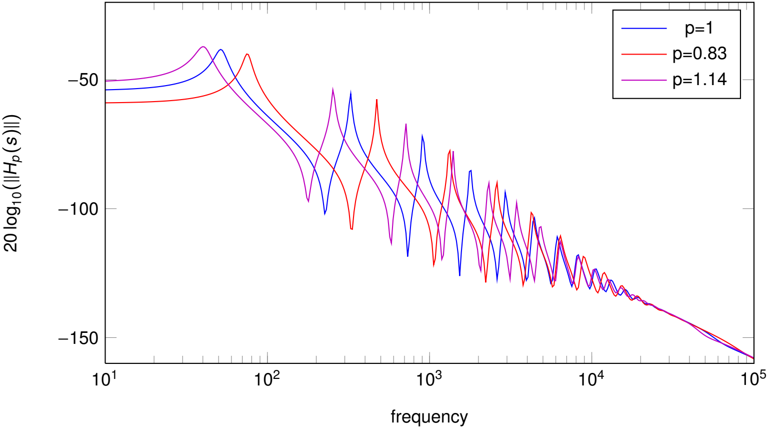
Parametric LTI system

Transfer function of a parametrized LTI system for different choices of *p* (elastic beam):



Parametric systems

Parametric model order reduction

- *Goal*: Fast computation of $\hat{A}(p), \hat{B}(p), \hat{C}(p) \forall p$
- *General ideas*:
  - Relax $\mathcal{H}_2$-optimality slightly
  - Apply well-established approximation methods
    ...such as radial basis function interpolation

- to be effective, *smoothness* is absolutely essential!

Approximation of parametric dependency

Candidates for approximation are

- $\hat{A}(p), \hat{B}(p), \hat{C}(p)$

Parametric systems

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Approximation of parametric dependency

Candidates for approximation are

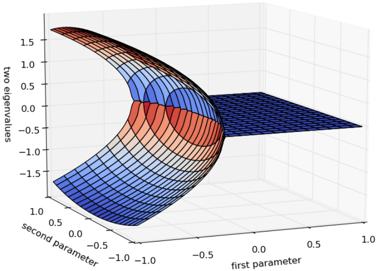
- $\hat{A}(p), \hat{B}(p), \hat{C}(p) \leadsto$ non-unique, matrix similarity!
- $\sigma_1(p), \ldots, \sigma_r(p)$

Approximation of parametric dependency

Candidates for approximation are

- $\hat{A}(p), \hat{B}(p), \hat{C}(p) \rightsquigarrow$ non-unique, matrix similarity!
- $\sigma_1(p), \ldots, \sigma_r(p) \rightsquigarrow$ eigenvalue crossings and splittings, non-smooth!

Imaginary parts of two eigenvalues of a matrix depending on two parameters:



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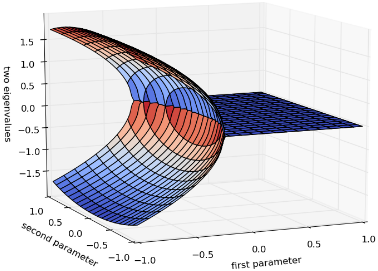

- Coefficients of the *characteristic polynomial* $\prod_{i=1}^{r}(s - \sigma_i(p))$ $\rightsquigarrow$ smooth enough?

Smoothness of the characteristic polynomial

Let

- π map a matrix to its characteristic polynomial
- Q map a polynomial to its coefficients
- λ map a matrix to its eigenvalues

Then

- $$\hat{A}(\cdot) \in C^\infty(\mathbb{R}^n;\mathbb{R}^{r\times r}) \;\Rightarrow\; Q(\pi(\hat{A}(\cdot))) \in C^\infty(\mathbb{R}^n;\mathbb{R}^{r+1})$$
- $$\hat{A}\text{ stable} \;\Rightarrow\; \begin{cases} Q(\pi(\hat{A}(p))) \geq 0 \\ \Re\lambda(\hat{A}(p)) \leq 0 \end{cases}$$

$$\forall P \in \mathbb{R}^{r\times r}, \det P \neq 0 : \begin{cases} \pi(\hat{A}(p)) = \pi(P\hat{A}(p)P^{-1}) \\ \lambda(\hat{A}(p)) = \lambda(P\hat{A}(p)P^{-1}) \end{cases}$$

Smoothness of the characteristic polynomial

Let

- ρ map a set of r roots to their polynomial
- Q map the resulting polynomial to its coefficients

Then

- Q is linear, hence Q^{-1}, too
- ρ^{-1} maps a polynomial to its roots
  - *closed form representations* for $r \leq 5$
  - computation unstable for $r > 5$

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Smoothness of the characteristic polynomial

Let $r \leq 5$. Assume IRKA converges

- locally
- to a local optimum
- returns $\Sigma(p) = (\sigma_1(p), ..., \sigma_r(p))$

Moreover, assume that *a perturbation of p* is small enough to not leave the region of

- convergence
- attraction to the local minimum

Then

- $f = Q \circ \rho \circ \Sigma(\cdot)$ is smooth
- standard *RBF interpolation* is applicable

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Smoothness of the characteristic polynomial

Assume IRKA converges as before, $r \leq 5$. Moreover, assume again that *a perturbation of p* is small enough to not leave the region of

- convergence
- attraction to the local minimum

Let

- $\tilde{f} \approx f = Q \circ \rho \circ \Sigma(\cdot)$
- $\tilde{\Sigma} = \rho^{-1} \circ Q^{-1} \circ \tilde{f}$

Then $\tilde{\Sigma}$

- approximates the *results of IRKA*
- can be computed stably

$\rightsquigarrow$ *find* those smooth regions!

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Smoothness of the characteristic polynomial

Let $f = Q \circ \rho \circ \Sigma(\cdot)$.

- We are looking for *discontinuities* of $f(p)$
- Simple *criterion* for k-means or spectral clustering (Ng et al.): tuple $(p, f(p))$

$\rightsquigarrow$ How to determine the *number of clusters*?

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Definition

Let

- $\Omega \subset \mathbb{R}^n$ a domain
- F a class of functions $f : \Omega \to \mathbb{C}$ that form a Hilbert space $\mathcal{H}$ with inner product $(\cdot, \cdot)$

The function $\kappa : \Omega \times \Omega \to \mathbb{C}$ is called *reproducing kernel* if

$$\begin{aligned} \forall y \in \Omega : &\quad \kappa(\cdot, y) \in F, \\ \forall f \in F, y \in \Omega : &\quad f(y) = (f(\cdot), \kappa(\cdot, y)) \quad \text{(reproducing property).} \end{aligned}$$

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Properties

Let $\xi_i \in \mathbb{C}, x_i, x, y, z \in \Omega, i, j = 1, .., N, N \in \mathbb{N}$ arbitrary

- *Positive definiteness*
$$\sum_{i,j} \xi_i \bar{\xi}_j \kappa(x_j, x_i) \geq 0$$
- $\kappa(y, z) = (\kappa(x, z), \kappa(x, y)), \; \kappa(x, y) = \overline{\kappa(y, x)}, \; \kappa(x, x) \geq 0, \ldots$

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Given: $\mathcal{H}(\Omega)$ with inner product $(\cdot,\cdot)$

Existence

Necessary and sufficient condition: A *continuous evaluation functional*

$$\delta_x : \mathcal{H} \to \mathbb{C},\ f \to f(x)$$

exists on $\mathcal{H}$

Uniqueness

- Assumption: A reproducing kernel κ exists for $\mathcal{H}$

Then the reproducing kernel κ of $\mathcal{H}$ is *unique* and, therefore, characterizes $\mathcal{H}$.

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Native space of κ

Given

- $\kappa : \Omega \times \Omega \to \mathcal{C}$, positive definite
- $F = \text{span}\,\{\kappa(\cdot, x) : \; x \in \Omega\}$

Moreover, define

$$(f, g)_\kappa \equiv \sum_{i,j} \alpha_i \bar{\beta}_j \kappa(x_j, x_i)$$

for arbitrary $f, g \in F$ with

- $f = \sum_i \alpha_i \kappa(\cdot, x_i)$
- $g = \sum_j \beta_j \kappa(\cdot, x_j)$

Then

- $\mathcal{H} = \text{cl}F$ with respect to $||f||_\kappa^2 \equiv (f, f)_\kappa$ has reproducing kernel κ
- $\mathcal{H}$ is called the *native space* of κ

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Examples

Let $x, y \in \Omega = \mathbb{R}^n$.

- *Positive definite functions*

$$\kappa(x, y) = \phi(x - y), \qquad \text{invariant to } \mathrm{T}(n)$$

- *Radial basic functions* (RBF)

$$\kappa(x, y) = \phi(\|x - y\|_2), \qquad \text{invariant to } \mathrm{SE}(n)$$

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RBF examples

Let $\epsilon > 0$, $\tau > n/2$. Denote by

- K_ν the modified Bessel function of 2^{nd} kind,
- $\mathcal{F}f$ the Fourier transform of f.

Popular RBF choices are

Sobolev splines

$$\phi(x) = \frac{K_{\tau-n/2}(\|x\|_2)\|x\|_2^{\tau-n/2}}{2^{\tau-1}\Gamma(\tau)}, \qquad \mathcal{H} = W_2^\tau(\mathbb{R}^n)$$

Gaussians

$$\phi(x) = e^{-\epsilon^2\|x\|_2^2}, \qquad \mathcal{H} = \left\{ f \in L_2(\mathbb{R}^n) \cap C^\infty(\mathbb{R}^n) : \; e^{\frac{\|\cdot\|_2^2}{8\epsilon^2}} \mathcal{F}f \in L^2(\mathbb{R}^n) \right\}$$

Reconstruction by symmetric interpolation

RBF interpolation

Given a function $f \in \mathcal{H}$, select

- sampling $X = \{x_1, \cdots, x_N\} \subset \Omega, N = |X| < \infty$
- *ansatz*

$$\tilde{f}(x) = \sum_{i=1}^{N} \xi_i \kappa(x, x_i).$$

Then $\tilde{f}$ is an *interpolant* to f on X if $(\xi_1, \cdots, \xi_N)$ is a solution of

$$\forall j = 1...N : \tilde{f}(x_j) = f(x_j). \quad (3)$$

$\rightsquigarrow$ *offline* phase (sampling, IRKA) $\leftrightarrow$ *online* phase (metamodel, reduced model)

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Reconstruction by symmetric interpolation

Given f, $\tilde{f}$, X as before.

Optimality of RBF interpolation

- $\forall \tilde{s} \in \{s \in \mathcal{H} \,:\, (3)\} \,:\, \|\tilde{f}\|_\kappa \leq \|\tilde{s}\|_\kappa$
- $\forall \tilde{s} \in \{\sum_i \xi_i \kappa(\cdot, x_i) \,:\, \xi_i \in \mathbb{C}\} \,:\, \|f - s\|_\kappa \leq \|f - \tilde{s}\|_\kappa$

Define the *fill-distance* of X as $h \equiv \sup_{y\in\Omega} \max_{x\in X} \|x - y\|_2$

Sampling inequalities

Let

- α a multi-index
- σ the sampling order

Then $\exists C_1 > 0 \,:\, \|D^\alpha f\|_{L_q(\Omega)} \leq C_1 \left(h^\sigma \|f\|_\kappa + h^{-|\alpha|} \|f(X)\|_{\ell_\infty(\mathbb{R}^{|X|})} \right)$

Error estimates

Assume a continuous embedding of $\mathcal{H}$ into $W_2^p, 0 < p < \infty$.

Then $\exists C > 0 \,:\, \|f - \tilde{f}\|_{L_q(\Omega)} \leq C h^{p-n\max\left(0, \frac{1}{2} - \frac{1}{q}\right)} \|f\|_\kappa$

Reconstruction by symmetric interpolation

Remarks

- Gaussians, multi-quadrics: *spectral* approximation orders
- *Sobolev* functions $\leftrightarrow$ ansatz with Gaussians: polynomial approximation orders
- *Conditionally* positive functions: polynomial detrending
- Native space *norm*: indicator for problems (e. g. discontinuities)

$\leadsto$ employ *Gaussians* (or multiquadrics)
$\leadsto$ use low-order polynomial *detrending*
$\leadsto$ determine *number of clusters* by norm of the native space

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Reconstruction by symmetric interpolation

Medium size model

- *Reuse results* from offline phase
- Galerkin projection for system matrices in *affine form* (medium size)
- Project *medium-size model* to $\tilde{\Sigma}$ in online phase

For details, see Sara Grundel's talks at MoRePas II, Nonlinear MOR Workshop, and Overton's "60th birthday" Workshop.

$\rightsquigarrow$ *speed-up* without additional cost

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Numerical results

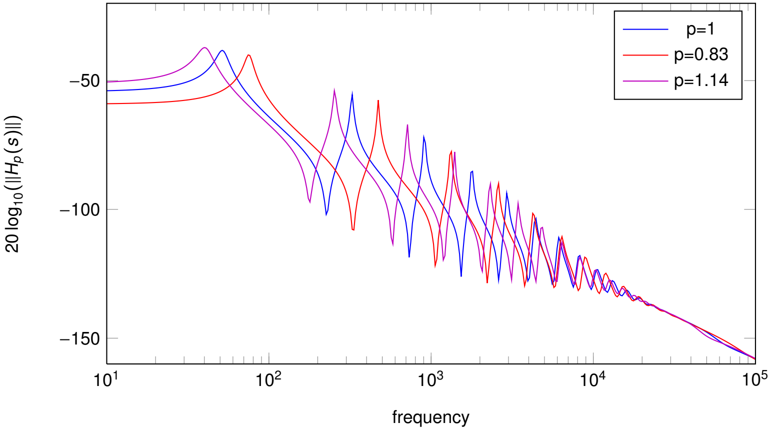
Examples

- Parametric beam model ($d = 240$)
- Anemometer ($d = 29,008$, $n = 1$ and $n = 3$)
- Synthetic model (to exhibit more challenging problems)

Numerical results

Timoshenko beam

Transfer function of a parametrized LTI system for different choices of p:



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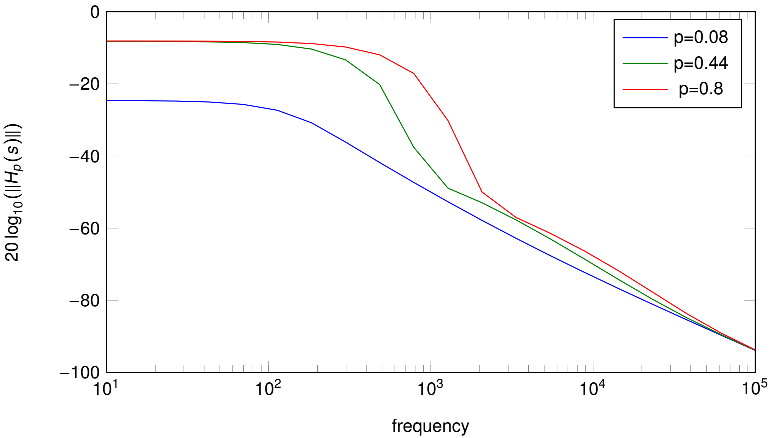
Numerical results

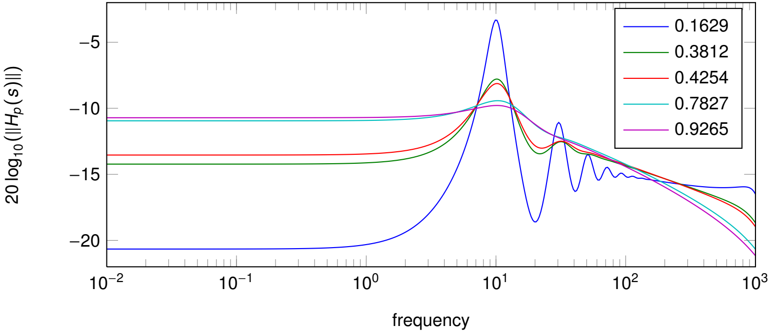
Anemometer (1D)

Transfer function of a parametrized LTI system for different choices of p:



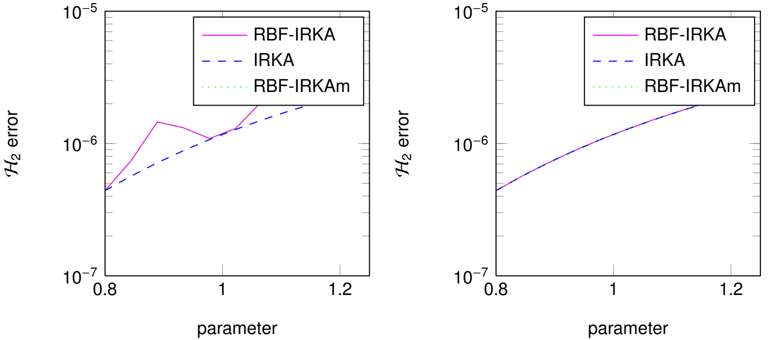
Synthetic example

Transfer function of a parametrized LTI system for different choices of p:



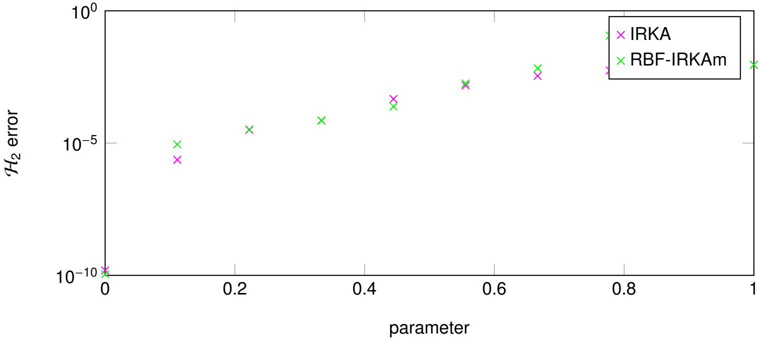
Error evaluation, Timoshenko beam

$\mathcal{H}_2$ error of the reduced parametrized system using IRKA (no interpolation), IRKA with RBF (intperolation), IRKA and medium-size model with RBF – three vs. five interpolation points:



Error evaluation, Anemometer (1D)

$\mathcal{H}_2$ error of the reduced parametrized system of size 4 using IRKA (no interpolation), IRKA and medium-size model with RBF – five interpolation points:



Numerical results

Error evaluation, Anemometer (3D)

$\mathcal{H}_2$ error of the reduced parametrized system using IRKA (no interpolation), IRKA and medium-size model with RBF – different reduced sized (r) and number of interpolation points (N):

	$r = 4, N = 5$	$r = 8, N = 5$	$r = 8, N = 10$
RBF-IRKAm	3.21×10^{-5}	1×10^{-6}	1×10^{-8}
IRKA	3.19×10^{-5}	3×10^{-8}	2×10^{-8}

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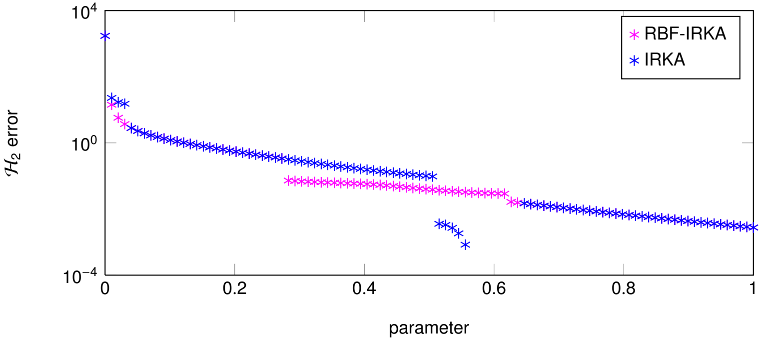
Error evaluation, synthetic example

$\mathcal{H}_2$ error of the reduced parametrized system using IRKA (no interpolation), IRKA with RBF – several p:



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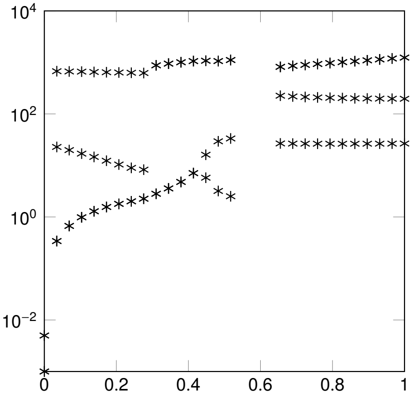
Numerical results

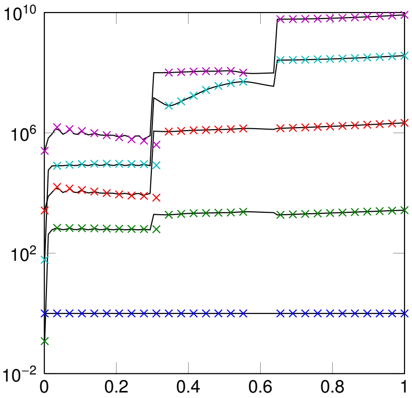
Clustering, synthetic example

Eigenvalues $\Sigma(p)$ of the reduced system matrix, for $r = 4$ and several p (dots):



Clustering, synthetic example

Coefficients $f(p)$ of the corresponding characteristic polynomial, for $r = 4$ and several p (colored dots), and approximation $\tilde{f}(p)$ (black line):



Summary

Parametric model order reduction

- Parametric linear time-invariant systems
- $\mathcal{H}_2$ optimal model order reduction (IRKA)
- *RBF interpolation* of $\Sigma(p)$ using coefficients of the characteristic polynomial
- *Clustering* guided by the norm of the reproducing kernel Hilbert space innate to a radial basis
- *Medium-size model* and projection to interpolated $\Sigma(p)$
- Numerical results (synthetic as well as simple practical test problems)

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Future work

Open problems

- Stable *root finding* (minimum polynomial?)
- Nonlinear systems (*bilinear* systems)
- Transfer RBF *error bounds* to reduced model

Thank you for your attention!