Structure-preserving interpolatory model reduction for linear and nonlinear dynamical systems

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Outline and Collaborators

- Optimal Rational Approximation for Linear Dynamical Systems
  - Thanos Antoulas (Rice Univ) and Chris Beattie (Virginia Tech)
  - Input-independent, optimal rational approximation by interpolation
- Structure-preserving Interpolation for Linear Dynamical Systems
  - Chris Beattie (Virginia Tech)
  - Reduced model preserves the internal structure
  - Not-necessarily a rational approximation
- DEIM and Structure-preserving MOR of nonlinear port-Hamiltonian systems
  - Chris Beattie (Virginia Tech), Saifon Chaturantabut (Thammasat Univ) and Zlatko Drmač (Univ. of Zagreb)
  - A new DEIM selection operator
  - Structure-preserving POD-DEIM
  - Enrich the POD subspace
- Dropped from slides: Optimal MOR of bilinear systems via interpolation
  - Garret Flagg (WesternGeco, Schlumberger)
  - Interpolating the Volterra series
  - Interpolation-based optimality conditions
  - See the related poster by Pawan Goyal

Generic Problem Setting

$$\begin{aligned}\mathbf{E}\dot{\mathbf{x}} &= \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t)\\ \mathbf{y}(t) &= \mathbf{C}\mathbf{x}(t)\end{aligned} \quad \overset{?}{\approx} \quad \begin{aligned}\mathbf{E}_r\dot{\mathbf{x}} &= \mathbf{A}_r\mathbf{x}_r(t) + \mathbf{B}_r\mathbf{u}(t)\\ \mathbf{y}_r(t) &= \mathbf{C}_r\mathbf{x}_r(t)\end{aligned}$$

(Original system) (Reduced system)

- $\mathbf{A}, \mathbf{E} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{n\times m}$, $\mathbf{C} \in \mathbb{R}^{p\times n}$
- $\mathbf{x}(t) \in \mathbb{R}^n$: states, $\mathbf{u}(t) \in \mathbb{R}^m$: Input, $\mathbf{y}(t) \in \mathbb{R}^p$: Output
- Pick $\mathbf{E}_r, \mathbf{A}_r \in \mathbb{R}^{r\times r}$, $\mathbf{B}_r \in \mathbb{R}^{r\times m}$, $\mathbf{C}_r : \mathbb{R}^{p\times r}$; so that $r \ll n$ and
  - $\|\mathbf{y} - \mathbf{y}_r\|$ is *small* in an appropriate norm
  - The procedure is *computationally efficient*.

Model Reduction via Projection

- Choose $\mathcal{V}_r = \text{Range}(\mathbf{V}_r)$: the r-dimensional *right modeling subspace* (the trial subspace) where $\mathbf{V}_r \in \mathbb{R}^{n\times r}$
- and $\mathcal{W}_r = \text{Range}(\mathbf{W}_r)$, the r-dimensional *left modeling subspace* (test subspace) where $\mathbf{W}_r \in \mathbb{R}^{n\times r}$
- Approximate $\underbrace{\mathbf{x}(t)}_{n\times 1} \approx \underbrace{\mathbf{V}_r}_{n\times r} \underbrace{\mathbf{x}_r(t)}_{r\times 1}$ by forcing $\mathbf{x}_r(t)$ to satisfy

$$\mathbf{W}_r{}^T \left(\mathbf{E}\mathbf{V}_r\dot{\mathbf{x}}_r - \mathbf{A}\mathbf{V}_r\mathbf{x}_r - \mathbf{B}\,\mathbf{u}\right) = \mathbf{0} \quad \text{(Petrov-Galerkin)}$$

- Leads to a reduced order model:

$$\mathbf{E}_r = \underbrace{\mathbf{W}_r{}^T\mathbf{E}\mathbf{V}_r}_{r\times r}, \quad \mathbf{A}_r = \underbrace{\mathbf{W}_r{}^T\mathbf{A}\mathbf{V}_r}_{r\times r}, \quad \mathbf{B}_r = \underbrace{\mathbf{W}_r{}^T\mathbf{B}}_{r\times m}, \quad \mathbf{C}_r = \underbrace{\mathbf{C}\mathbf{V}_r}_{p\times r}, \quad \mathbf{D}_r = \underbrace{\mathbf{D}}_{p\times m}$$

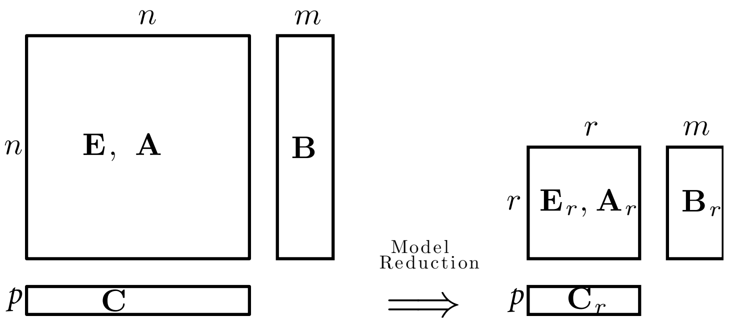


Figure: Projection-based Model Reduction

- Once $\mathcal{V}_r$ and $\mathcal{W}_r$ are selected, $\mathcal{S}_r$ is automatically determined.
- In other words: What matters are the $\mathrm{Ran}(\mathbf{V}_r)$ and $\mathrm{Ran}(\mathbf{W}_r)$.
- Antoulas, Beattie, Benner, Borggaard, Chaturantabut, Enns, Freund, Glover, Grimme, Haasdonk, Heinkenschloss, Hinze, Iliescu, Kunish, Mehrmann, Mullis, Roberts, Reis, Sorensen, Stykel, van Dooren, Volkwein, Willcox, and many many more

Frequecy Domain and Transfer Functions

- $\mathcal{S}: \quad \mathbf{u}(t) \mapsto \mathbf{y}(t) = (\mathcal{S}\mathbf{u})(t) = \int_{-\infty}^{t} h(t-\tau)\mathbf{u}(\tau)d\tau.$
- $\mathbf{H}(s) = (\mathcal{L}h)(s) = \mathbf{C}(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D}.$
- $\mathbf{H}(s)$: matrix-valued $(p \times m)$ rational function in $s \in \mathbb{C}$.
- Similarly: $\mathbf{H}_r(s) = \mathbf{C}_r(s\mathbf{E}_r - \mathbf{A}_r)^{-1}\mathbf{B}_r + \mathbf{D}_r$
- $\mathbf{H}(s) = \dfrac{\alpha_0 s^n + \alpha_1 s^{n-1} + \alpha_2 s^{n-2} + \cdots + \alpha_n}{s^n + \beta_1 s^{n-1} + \beta_2 s^{n-2} + \cdots + \beta_n}$ (Assuming SISO)
- $\mathbf{H}_r(s) = \dfrac{\gamma_0 s^r + \gamma_1 s^{r-1} + \gamma_2 s^{r-2} + \cdots + \gamma_r}{s^r + \eta_1 s^{r-1} + \eta_2 s^{r-2} + \cdots + \eta_r}$ (Assuming SISO)
- Model Reduction = Rational Approximation

A much more general problem setting

- Consider the following example from [Antoulas (2006)]:

$$\frac{\partial T}{\partial t}(z,t) = \frac{\partial^2 T}{\partial z^2}(z,t), \quad t \geq 0, \quad z \in [0,1]$$

$$\frac{\partial T}{\partial t}(0,t) = 0 \quad \text{and} \quad \frac{\partial T}{\partial z}(1,t) = u(t)$$

- $u(t)$ is the input function (supplied heat)
- $y(t) = T(0,t)$ is the output.
- Transfer function: $\mathcal{H}(s) = \dfrac{Y(s)}{U(s)} = \dfrac{1}{\sqrt{s}\sinh\sqrt{s}}$
- $\mathcal{H}(s) = \frac{1}{\sqrt{s}\sinh\sqrt{s}} \neq \mathbf{C}(s\mathbf{E}-\mathbf{A})^{-1}\mathbf{B}$

- Do not assume the generic first-order structure.
- For example:
  - $\mathcal{H}(s) = \mathbf{C}(s\mathbf{E} - \mathbf{A}_0 - e^{-\tau_1 s}\mathbf{A}_1 - e^{-\tau_2 s}\mathbf{A}_2)^{-1}\mathbf{B}$
  - $\mathcal{H}(s) = e^{-\sqrt{s}}$
  - $\mathcal{H}(s) = (s\mathbf{C}_1 + \mathbf{C}_0)(s^2\mathbf{M} + s\mathbf{D} + \mathbf{K})^{-1}\mathbf{B}$
  - $\mathcal{H}(s) = \frac{1}{\sqrt{s}\sinh\sqrt{s}}$
  - $\mathcal{H}(s) = \mathcal{C}(s)\mathcal{K}(s)^{-1}\mathbf{B}(s)$
- New goal: Given the ability to evaluate $\mathcal{H}(s)$:

$$\boxed{\mathcal{H}(s)} \overset{?}{\approx} \boxed{\begin{array}{c}\mathbf{E}_r\dot{\mathbf{x}} = \mathbf{A}_r\mathbf{x}_r(t) + \mathbf{B}_r\mathbf{u}(t) \\ \mathbf{y}_r(t) = \mathbf{C}_r\mathbf{x}_r(t)\end{array}}$$

- Realization independent and data-driven.

Model Reduction by Rational Interpolation

- For simplicity of notation, assume $m = p = 1$:

$$\mathbf{B} \rightarrow \mathbf{b} \in \mathbb{R}^n \quad \mathbf{C} \rightarrow \mathbf{c}^T \in \mathbb{R}^n$$

  For the MIMO case details, see [Antoulas/Beattie/G,11], [Beattie/G,15].

- Given a transfer function $\mathcal{H}(s)$ together with

  left driving frequencies: $\{\mu_i\}_{i=1}^r \subset \mathbb{C}$,

  right driving frequencies: $\{\sigma_i\}_{i=1}^r \subset \mathbb{C}$

  producing *left responses*: $\{\mathcal{H}(\mu_i)\}_{i=1}^r \subset \mathbb{C}$,

  producing *right responses*: $\{\mathcal{H}(\sigma_j)\}_{i=1}^r \subset \mathbb{C}$

- Find a reduced model $\mathcal{H}_r(s) = \mathbf{c}_r^T(s\mathbf{E}_r - \mathbf{A}_r)^{-1}\mathbf{b}_r$, that is a rational interpolant to $\mathcal{H}(s)$:

$$\mathcal{H}_r(\mu_i) = \mathcal{H}(\mu_i) \text{ for } i = 1, \cdots, r, \quad \text{and} \quad \mathcal{H}_r(\sigma_j) = \mathcal{H}(\sigma_j) \text{ for } j = 1, \cdots, r,$$

Interpolatory Model Reduction via Projection

- Given $\{\sigma_i\}_{i=1}^r$ and $\{\mu_j\}_{j=1}^r$, set

$$\mathbf{V}_r = \left[(\sigma_1\mathbf{E}-\mathbf{A})^{-1}\mathbf{b},\ \cdots,\ (\sigma_r\mathbf{E}-\mathbf{A})^{-1}\mathbf{b}\right] \in \mathbb{C}^{n\times r} \text{ and}$$
$$\mathbf{W}_r = \left[(\mu_1\mathbf{E}^T-\mathbf{A}^T)^{-1}\mathbf{c}^T\ \cdots\ (\mu_r\mathbf{E}^T-\mathbf{A}^T)^{-1}\mathbf{c}^T\ \right] \in \mathbb{C}^{n\times r}$$

- Obtain $\mathcal{H}_r(s)$ via projection as before

$$\mathbf{E}_r = \mathbf{W}_r{}^T\mathbf{E}\mathbf{V}_r \quad \mathbf{A}_r = \mathbf{W}_r{}^T\mathbf{A}\mathbf{V}_r, \quad \mathbf{b}_r = \mathbf{W}_r{}^T\mathbf{b}, \quad \mathbf{c}_r = \mathbf{V}_r{}^T\mathbf{c}, \quad \mathbf{D}_r = \mathbf{D}$$

- Then

$$\begin{aligned} \mathcal{H}(\sigma_i) &= \mathcal{H}_r(\sigma_i), && \text{for } i = 1,\cdots,r,\\ \mathcal{H}(\mu_j) &= \mathcal{H}_r(\mu_j), && \text{for } j = 1,\cdots,r,\\ \mathcal{H}'(\sigma_k) &= \mathcal{H}_r'(\sigma_k) && \text{if } \sigma_k = \mu_k \end{aligned}$$

- Hermite tangential interpolation *without explicit computations of the quantities to be matched*.
- [Skelton *et. al.*, 87], [Feldmann/Freund, 95], [Grimme, 97], [Gallivan *et. al.*, 05]

Rational Interpolation from Data [Mayo/Antoulas (2007)]

- Given $\{\sigma_i\}_{i=1}^r$ and $\{\mu_j\}_{j=1}^r$, evaluate or measure $\mathcal{H}(\sigma_i)$ and $\mathcal{H}(\mu_j)$
- Construct the *Loewner matrix*:

$$\mathbb{L}_{ij} = \frac{\mathcal{H}(\mu_i) - \mathcal{H}(\sigma_j)}{\mu_i - \sigma_j}, \quad i,j = 1,\ldots,r, \qquad (\mathcal{H}(s))$$

- Construct the *shifted Loewner matrix*:

$$\mathbb{M}_{ij} = \frac{\mu_i \mathcal{H}(\mu_i) - \mathcal{H}(\sigma_j)\sigma_j}{\mu_i - \sigma_j}, \quad i,j = 1,\ldots,r \qquad (s\mathcal{H}(s))$$

- In addition to $\mathbb{L}$ and $\mathbb{M}$, construct the following vectors from data:

$$\mathsf{z} = \begin{bmatrix} \mathcal{H}(\mu_1) \\ \vdots \\ \mathcal{H}(\mu_r) \end{bmatrix} \qquad \mathsf{y} = \begin{bmatrix} \mathcal{H}(\sigma_1) \\ \vdots \\ \mathcal{H}(\sigma_r) \end{bmatrix}$$

Data-Driven Interpolant

Theorem (Mayo/Antoulas,2007)

Assume that $\mu_i \neq \sigma_j$ *for all* $i, j = 1, \ldots, r$. *Suppose that* $\mathbb{M} - s\,\mathbb{L}$ *is invertible for all* $s \in \{\sigma_i\} \cup \{\mu_j\}$. *Then, with*

$$\mathbf{E}_r = -\mathbb{L}, \quad \mathbf{A}_r = -\mathbb{M}, \quad \mathbf{b}_r = \mathsf{z}, \quad \mathbf{c}_r = \mathsf{y},$$

the rational function (reduced model)

$$\mathcal{H}_r(s) = \mathbf{c}_r^T(s\mathbf{E}_r - \mathbf{A}_r)^{-1}\mathbf{b}_r = \mathsf{y}^T(\mathbb{M} - s\,\mathbb{L})^{-1}\mathsf{z}$$

interpolates the data and furthermore is a minimal realization.

- Once the data is collected, one directly writes down $\mathcal{H}_r(s)$.
- For Hermite interpolation, choose $\sigma_i = \mu_i$ and only modify

$$\mathbb{L}_{ii} = \mathcal{H}'(\sigma_i) \quad \text{and} \quad \mathbb{M}_{ii} = [s\mathcal{H}(s)]'_{s=\sigma_i}$$

A brief note on the DAEs

- $\mathcal{H}(s) = \mathcal{H}_{sp}(s) + \mathcal{P}(s)$.
- We want $\mathcal{H}_r(s) = \mathcal{H}_{r,sp}(s) + \mathcal{P}_r(s)$ with $\mathcal{P}_r(s) = \mathcal{P}(s)$,
- Problem reduces to: $\mathcal{H}_{r,sp}(s)$ interpolates $\mathcal{H}_{sp}(s)$.
- $\mathbf{P}_r$ = the spectral projector onto the right deflating subspace of $(\lambda\mathbf{E} - \mathbf{A})$ corresponding to the finite eigenvalues.
- $\mathbf{P}_l$: Defined similarly for the left deflating subspace.
- $\mathbf{W}_\infty$ and $\mathbf{V}_\infty$: Span, respectively, the right and left deflating subspaces of $(\lambda\mathbf{E} - \mathbf{A})$ corresponding to the infinite eigenvalues.

Theorem ([G./Stykel/Wyatt,12])

Given are $\mathcal{H}(s) = \mathbf{c}^T(s\mathbf{E} - \mathbf{A})^{-1}\mathbf{b} + \mathbf{D}$, *interpolation points* $\sigma \in \mathbb{C}$. *Define* $\mathbf{V}_f$ *and* $\mathbf{W}_f$ *such that*

$$\mathbf{V}_f = \left[(\sigma_1\mathbf{E} - \mathbf{A})^{-1}\mathbf{P}_l\mathbf{b}, \ \cdots, \ (\sigma_r\mathbf{E} - \mathbf{A})^{-1}\mathbf{P}_l\mathbf{b}\right] \in \mathbb{C}^{n\times r} \text{ and}$$
$$\mathbf{W}_f = \left[(\sigma_1\,\mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{P}_r^T\mathbf{c}^T \ \cdots \ (\sigma_r\,\mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{P}_r^T\mathbf{c}^T\ \right] \in \mathbb{C}^{n\times r}$$

Define $\mathbf{W}_r = [\,\mathbf{W}_f,\ \mathbf{W}_\infty\,]$ *and* $\mathbf{V}_r = [\,\mathbf{V}_f,\ \mathbf{V}_\infty\,]$, *and construct* $\mathcal{H}_r(s)$. *Then,*

1. $\mathcal{P}_r(s) = \mathcal{P}(s)$, *and*
2. $\mathcal{H}(\sigma_j) = \mathcal{H}_r(\sigma_j), \ \text{and}\ \mathcal{H}'(\sigma_j) = \mathcal{H}_r{}'(\sigma_j)$ *for* $j = 1, 2, \ldots, r.$

- Theorem requires explicit computation of $\mathbf{P}_l$ and $\mathbf{P}_r$ in general.
- [G./Stykel/Wyatt,12]: For index-1 and (Stokes-type) index-2 DAEs interpolation with polynomial matching achieves without explicit computation of $\mathbf{P}_l$ and $\mathbf{P}_r$.

Where to Interpolate: Performance Measures

- How to measure $\mathcal{H}(s) \approx \mathcal{H}_r(s)$

$$\|\mathcal{H} - \mathcal{H}_r\|_{\mathcal{H}_2} = \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \|\mathcal{H}(\imath\omega) - \mathcal{H}_r(\imath\omega)\|_F^2 \, d\omega \right)^{1/2}$$

- Make pointwise error $\max_{t>0} \|\mathbf{y}(t) - \mathbf{y}_r(t)\|_\infty$ small relative to input energy, $\left(\int_0^\infty \|\mathbf{u}(t)\|_2^2 \, dt\right)^{1/2}$

$$\max_{t>0} \|\mathbf{y}(t) - \mathbf{y}_r(t)\|_\infty \leq \|\mathcal{H} - \mathcal{H}_r\|_{\mathcal{H}_2} \cdot \left(\int_0^\infty \|\mathbf{u}(t)\|_2^2 \, dt \right)^{1/2}$$

- $2 - \infty$ induced norm if $m = 1$ and/or $p = 1$

$$\|\mathcal{H}\|_{\mathcal{H}_2} = \sup_{\mathbf{u} \neq 0} \frac{\|\mathbf{y}\|_\infty}{\|\mathbf{u}\|_2}$$

Interpolatory $\mathcal{H}_2$ optimality conditions

Theorem ([Meier /Luenberger,67], [G./Antoulas/Beattie,08])

Given $\mathcal{H}(s)$, let $\mathcal{H}_r(s)$ be the best stable r^{th} order rational approximation of $\mathcal{H}$ with respect to the $\mathcal{H}_2$ norm. Assume $\mathcal{H}_r$ has simple poles at $\hat{\lambda}_1, \hat{\lambda}_2, \ldots \hat{\lambda}_r$. Then

$$\mathcal{H}(-\hat{\lambda}_k) = \mathcal{H}_r(-\hat{\lambda}_k) \text{ and } \quad \mathcal{H}'(-\hat{\lambda}_k) = \mathcal{H}_r'(-\hat{\lambda}_k) \quad \text{for } k = 1, 2, \ldots, r.$$

- Hermite interpolation for $\mathcal{H}_2$ optimality
- $$\boxed{\text{Optimal interpolation points}: \ \sigma_i = -\hat{\lambda}_i}$$
- The MIMO conditions: [G./Antoulas/Beattie,08]
- Other MIMO works: [van Dooren et al..08], [Bunse-Gernster et al.,09]
- $\hat{\lambda}_i$ NOT known a priori $\Longrightarrow$ Need iterative steps

An Iterative Rational Krylov Algorithm (IRKA):

- If projection framework is preferred:

Algorithm (G./Antoulas/Beattie [2008])

1. *Choose* $\{\sigma_1, \ldots, \sigma_r\}$
2. $\mathbf{V}_r = \left[(\sigma_1 \mathbf{E} - \mathbf{A})^{-1}\mathbf{b}, \; \cdots, \; (\sigma_r \mathbf{E} - \mathbf{A})^{-1}\mathbf{b}\right]$
   $\mathbf{W}_r = \left[(\sigma_1 \mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{c}^T, \cdots, (\sigma_r \mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{c}^T\right]$.
3. *while (not converged)*
   1. $\mathbf{A}_r = \mathbf{W}_r{}^T \mathbf{A} \mathbf{V}_r$, $\mathbf{E}_r = \mathbf{W}_r^T \mathbf{E} \mathbf{V}_r$
   2. $\sigma_i \longleftarrow -\lambda_i(\mathbf{A}_r, \mathbf{E}_r)$.
   3. $\mathbf{V}_r = \left[(\sigma_1 \mathbf{E} - \mathbf{A})^{-1}\mathbf{b}, \; \cdots, \; (\sigma_r \mathbf{E} - \mathbf{A})^{-1}\mathbf{b}\right]$
   4. $\mathbf{W}_r = \left[(\sigma_1 \mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{c}^T, \cdots, (\sigma_r \mathbf{E}^T - \mathbf{A}^T)^{-1}\mathbf{c}^T\right]$
4. $\mathbf{A}_r = \mathbf{W}_r{}^T \mathbf{A} \mathbf{V}_r$, $\mathbf{E}_r = \mathbf{W}_r^T \mathbf{E} \mathbf{V}_r$, $\mathbf{b}_r = \mathbf{W}_r{}^T \mathbf{b}$, *and* $\mathbf{c}_r = \mathbf{V}_r{}^T \mathbf{c}$, $\mathbf{D}_r = \mathbf{D}$.

- Optimality conditions upon convergence

Realization Independent IRKA

- If $\mathcal{H}(s)$ is not rational or only $\mathcal{H}(s)$ is available

Algorithm (Realization Independent IRKA [Beattie/G., (2012)])

1. *Choose initial* $\{\sigma_i\}$ *for* $i = 1, \ldots, r$.
2. *while not converged*
   1. *Evaluate* $\mathcal{H}(\sigma_i)$ *and* $\mathcal{H}'(\sigma_i)$ *for* $i = 1, \ldots, r$.
   2. *Construct* $\mathbf{E}_r = -\mathbb{L}$, $\mathbf{A}_r = -\mathbb{M}$, $\mathbf{b}_r = \mathsf{z}$ *and* $\mathbf{c}_r = \mathsf{y}$
   3. *Construct* $\mathcal{H}_r(s) = \mathbf{c}_r^T(s\mathbf{E}_r - \mathbf{A}_r)^{-1}\mathbf{b}_r$
   4. $\sigma_i \longleftarrow -\lambda_i(\mathbf{A}_r, \mathbf{E}_r)$ *for* $i = 1, \ldots, r$
3. *Construct* $\mathcal{H}_r(s) = \mathbf{c}_r^T(s\mathbf{E}_r - \mathbf{A}_r)^{-1}\mathbf{b}_r = \mathsf{z}^T(\mathbb{M} - s\,\mathbb{L})^{-1}\mathsf{y}$

- Allows infinite order transfer functions !!
  e.g., $\mathcal{H}(s) = \mathbf{c}^T(s\mathbf{E} - \mathbf{A}_0 - e^{-\tau_1 s}\mathbf{A}_1 - e^{-\tau_2 s}\mathbf{A}_2)^{-1}\mathbf{b}$

- In its simplest form, IRKA is a fixed point iteration.
- IRKA is not a descent method and global convergence is not guaranteed *despite overwhelming numerical evidence.*
- Guaranteed convergence: State-space symmetric systems [Flagg/Beattie/G.,2012]
- Newton formulation is possible [G./Antoulas/Beattie,08]
- Globally convergent descent formulation: [Beattie/G.,09]
- Weighted-$\mathcal{H}_2$ IRKA: For minimizing $\|\mathbf{W}(s)\,(\mathcal{H}(s) - \mathcal{H}_r(s))\,\|_{\mathcal{H}_2}$: [Anic et al. 12], [Breiten/Beattie/G.,14], [Vuillemin et al., 15]
- IRKA for DAEs: [G./Stykel/Wyatt, 12]
- Extended to bilinear systems: B-IRKA by [Benner/Breiten, 12]. Analogous interpolation conditions for Volterra series [Flagg/G., 15].

Revisit: One-dimensional heat equation

- $\mathcal{H}(s) = \dfrac{1}{\sqrt{s}\sinh\sqrt{s}} = \dfrac{1}{s} + \displaystyle\sum_{k=1}^{\infty} \dfrac{2\,(-1)^k}{s+k^2\pi^2} = \dfrac{1}{s} + \mathcal{G}(s)$
- Apply Loewner-IRKA to $\mathcal{G}(s)$. Then $\mathcal{H}_r(s) = \mathcal{G}_r(s) + \frac{1}{s}$
- Optimal points upon convergence: $\sigma_1 = 20.9418,\ \sigma_2 = 10.8944.$
- $\mathcal{H}_r(s) = \frac{-0.9469s-37.84}{s^2+31.84s+228.1} + \frac{1}{s}.$
- $\|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_2} = 5.84\times 10^{-3}, \quad \|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_\infty} = 9.61\times 10^{-4}$
- $\mathcal{H}_r(s)$ exactly interpolates $\mathcal{H}(s)$
- Balanced truncation of the discretized model:
  - $n = 10$: $\|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_2} = 1.16\times 10^{-2}, \quad \|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_\infty} = 1.58\times 10^{-3}$
  - $n = 1000$: $\|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_2} = 5.91\times 10^{-3}, \quad \|\mathcal{H}-\mathcal{H}_r\|_{\mathcal{H}_\infty} = 1.01\times 10^{-3}$

Indoor-air environment in a conference room

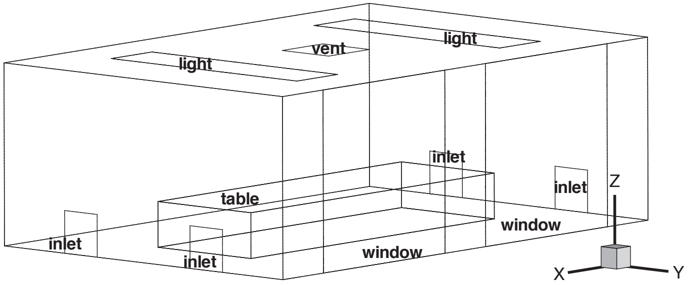


Figure: Geometry for our Indoor-air Simulation:
Example from [Borggaard/Cliff/G., 2011], research under EEBHUB

- Four inlets, one return vent
- Thermal loads: two windows, two overhead lights and occupants
- FLUENT to simulate the indoor-air velocity, temperature and moisture.

Finite Element Model of Convection/Diffusion

- A finite element model for thermal energy transfer with *frozen* velocity field $\overline{\mathbf{v}}$,

$$\frac{\partial T}{\partial t} + \overline{\mathbf{v}} \cdot \nabla T = \frac{1}{\mathrm{RePr}} \Delta T + Bu,$$

- leading to

$$\mathbf{E}\,\dot{\mathbf{x}}(t) = \mathbf{A}\,\mathbf{x}(t) + \mathbf{B}\,\mathbf{u}(t), \quad \mathbf{y}(t) = \mathbf{C}\,\mathbf{x}(t),$$

with $n = 202140$, $m = 2$ inputs
  1. the temperature of the inflow air at all four vents, and
  2. a disturbance caused by occupancy around the conference table,

and $p = 2$ outputs
  1. the temperature at a sensor location on the *max x* wall,
  2. the average temperature in an occupied volume around the table,

Conference Room: Reduction by IRKA

- Recall $n = 202140$, $m = 2$ and $p = 2$
- Reduced the order to $r = 30$ using IRKA.
- Relative errors in the subsystems by IRKA

	From Input [1]	From Input [2]
To Output [1]	6.62×10^{-3}	1.82×10^{-5}
To Output [2]	4.86×10^{-4}	5.40×10^{-7}

- Does IRKA pay off? How about some ad hoc selections:

	From Input [1]	From Input [2]
To Output [1]	9.19×10^{-2}	8.38×10^{-2}
To Output [2]	5.90×10^{-2}	2.22×10^{-2}

- One can keep trying different ad hoc selections but this is exactly what we want to avoid.

Structure-preserving model reduction

$$\mathbf{u}(t) \longrightarrow \boxed{\begin{array}{c} \mathbf{A}_0 \frac{d^\ell \mathbf{x}}{dt^\ell} + \mathbf{A}_1 \frac{d^{\ell-1}\mathbf{x}}{dt^{\ell-1}} + \ldots + \mathbf{A}_\ell \mathbf{x} = \mathbf{B}_0 \frac{d^k \mathbf{u}}{dt^k} + \ldots + \mathbf{B}_k \mathbf{u} \\ \mathbf{y}(t) = \mathbf{C}_0 \frac{d^q \mathbf{x}}{dt^q} + \ldots + \mathbf{C}_q \mathbf{x}(t) \end{array}} \longrightarrow \mathbf{y}(t)$$

- “Every linear ODE may be reduced to an equivalent first order system” Might not be the best approach ...
- For example

$$\mathbf{C}(s^2\mathbf{M} + s\mathbf{D} + \mathbf{K})^{-1}\mathbf{B} = \mathcal{C}(s\mathcal{E} - \mathcal{A})^{-1}\mathcal{B}$$

where

$$\mathcal{E} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{M} \end{bmatrix}, \ \mathcal{A} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{K} & -\mathbf{D} \end{bmatrix}, \ \mathcal{B} = \begin{bmatrix} \mathbf{0} \\ \mathbf{B} \end{bmatrix}, \ \mathcal{C} = \begin{bmatrix} \mathbf{C} & \mathbf{0} \end{bmatrix}$$

- Disadvantages???

- The "state space" is an aggregate of dynamic variables some of which may be internal and "locked" to other variables.

- *Refined goal*: Want to develop model reduction methods that can reduce selected state variables (i.e., on selected subspaces) while leaving other state variables untouched; maintain structural relationships among the variables.

  "Structure-preserving model reduction"

- For the second-order systems, see: [Craig Jr.,1981], [Chahlaoui et.al, 2005], [Bai,2002], [Su/Craig,(1991)], [Meyer/Srinivasan,1996], ...

- For $\mathcal{H}(s) = \mathbf{c}^T(s\mathbf{M} + \mathbf{D} + \mathbf{K}/s)^{-1}\mathbf{c}$: see [Freund, 2008]

- We will be investigating a much more general framework.

Example 1: Incompressible viscoelastic vibration

$$\partial_{tt}\mathbf{w}(x,t) - \eta\,\Delta\mathbf{w}(x,t) - \int_0^t \rho(t-\tau)\,\Delta\mathbf{w}(x,\tau)\,d\tau + \nabla\varpi(x,t) = \mathbf{b}(x)\cdot\mathbf{u}(t),$$

$\nabla\cdot\mathbf{w}(x,t) = 0$ which determines $\mathbf{y}(t) = [\varpi(x_1,t),\,\ldots,\,\varpi(x_p,t)]^T$

- [Leitman and Fisher, 1973]
- $\mathbf{w}(x,t)$ is the displacement field; $\varpi(x,t)$ is the pressure field; $\rho(\tau)$ is a “relaxation function”

$$\mathbf{M}\,\ddot{\mathbf{x}}(t) + \eta\,\mathbf{K}\,\mathbf{x}(t) + \int_0^t \rho(t-\tau)\,\mathbf{K}\,\mathbf{x}(\tau)\,d\tau + \mathbf{D}\,\boldsymbol{\varpi}(t) = \mathbf{B}\,\mathbf{u}(t),$$

$\mathbf{D}^T\,\mathbf{x}(t) = \mathbf{0},$ which determines $\mathbf{y}(t) = \mathbf{C}\,\boldsymbol{\varpi}(t)$

- $\mathbf{x} \in \mathbb{R}^{n_1}$ discretization of $\mathbf{w}$; $\boldsymbol{\varpi} \in \mathbb{R}^{n_2}$ discretization of ϖ.
- $\mathbf{M}$ and $\mathbf{K}$ are real, symmetric, positive-definite matrices, $\mathbf{B} \in \mathbb{R}^{n_1\times m}$, $\mathbf{C} \in \mathbb{R}^{p\times n_2}$, and $\mathbf{D} \in \mathbb{R}^{n_1\times n_2}$.

Example 1: Incompressible viscoelastic vibration

Transfer function (need not be a rational function !):

$$\mathcal{H}(s) = [\,\mathbf{0}\ \mathbf{C}\,] \begin{bmatrix} s^2\mathbf{M} + (\widehat{\rho}(s) + \eta)\,\mathbf{K} & \mathbf{D} \\ \mathbf{D}^T & \mathbf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix}$$

- Want a reduced order model that replicates input-output response with high fideliety yet retains “viscoelasticity”:

$$\mathbf{M}_r\,\ddot{\mathbf{x}}(t) + \eta\,\mathbf{K}_r\,\mathbf{x}_r(t) + \int_0^t \rho(t-\tau)\,\mathbf{K}_r\,\mathbf{x}_r(\tau)\,d\tau + \mathbf{D}_r\,\boldsymbol{\varpi}_r(t) = \mathbf{B}_r\,\mathbf{u}(t),$$

$$\mathbf{D}_r^T\,\mathbf{x}_r(t) = \mathbf{0}, \qquad \text{which determines} \quad \mathbf{y}_r(t) = \mathbf{C}_r\,\boldsymbol{\varpi}_r(t)$$

  with symmetric positive semidefinite $\mathbf{M}_r$, $\mathbf{K}_r \in \mathbb{R}^{r\times r}$, $\mathbf{B}_r \in \mathbb{R}^{r\times m}$, $\mathbf{C}_r \in \mathbb{R}^{p\times r}$, and $\mathbf{D}_r \in \mathbb{R}^{r\times r}$.

- Because of the memory term, both reduced and original systems have *infinite-order.*

Generalized Coprime Interpolation Setting

$$\mathbf{u}(t) \longrightarrow \boxed{\mathcal{H}(s) = \mathcal{C}(s)\mathcal{K}(s)^{-1}\mathcal{B}(s)} \longrightarrow \mathbf{y}(t)$$

- $\mathcal{C}(s) \in \mathbb{C}^{1\times n}$ and $\mathcal{B}(s) \in \mathbb{C}^{n\times 1}$ are analytic in the right half plane;
- $\mathcal{K}(s) \in \mathbb{C}^{n\times n}$ is analytic and full rank throughout the right half plane with $n \approx 10^5, 10^6$ or higher.
- "Internal state" $\mathbf{x}(t)$ is not itself important.
- How much state space detail is needed to replicate the map "$\mathbf{u} \mapsto \mathbf{y}$" ?

$$\boxed{\mathcal{H}(s) = \mathcal{C}(s)\mathcal{K}(s)^{-1}\mathcal{B}(s)} \longrightarrow \boxed{\mathcal{H}_r(s) = \mathcal{C}_r(s)\mathcal{K}_r(s)^{-1}\mathcal{B}_r(s)}$$

A General Projection Framework

- Select $\mathcal{V}_r \in \mathbb{R}^{n\times r}$ and $\mathcal{W}_r \in \mathbb{R}^{n\times r}$.
- The the reduced model $\mathcal{H}_r(s) = \mathcal{C}_r(s)\mathcal{K}_r(s)^{-1}\mathcal{B}_r(s)$ is

$$\mathcal{K}_r(s) = \mathcal{W}_r{}^T\mathcal{K}(s)\mathcal{V}_r, \quad \mathcal{B}_r(s) = \mathcal{W}_r{}^T\mathcal{B}(s), \quad \mathcal{C}_r(s) = \mathcal{C}(s)\mathcal{V}_r.$$

$$\mathbf{u}(t) \longrightarrow \boxed{\mathcal{H}_r(s) = \mathcal{C}_r(s)\mathcal{K}_r(s)^{-1}\mathcal{B}_r(s)} \longrightarrow \mathbf{y}_r(t) \approx \mathbf{y}(t)$$

- The generic case: $\mathcal{K}(s) = s\mathbf{E} - \mathbf{A}$, $\mathcal{B}(s) = \mathbf{B}$, $\mathcal{C}(s) = \mathbf{C}$,
- We choose $\mathcal{V}_r \in \mathbb{R}^{n\times r}$ and $\mathcal{W}_r \in \mathbb{R}^{n\times r}$ to enforce interpolation.

Model Reduction by Tangential Interpolation

- For selected points $\{\sigma_1, \sigma_2, ...\sigma_r\}$ in $\mathbb{C}$, find $\mathcal{H}_r(s)$ so that

$$\mathcal{H}(\sigma_i) = \mathcal{H}_r(\sigma_i), \quad \text{and} \quad \mathcal{H}'(\sigma_i) = \mathcal{H}_r'(\sigma_i) \ \text{ for } \ i = 1, 2, \ldots, r.$$

Theorem (Beattie/G,09)

Suppose that $\mathcal{B}(s)$, $\mathcal{C}(s)$, and $\mathcal{K}(s)$ are analytic at a point $\sigma \in \mathbb{C}$ and both $\mathcal{K}(\sigma)$ and $\mathcal{K}_r(\sigma) = \mathbf{W}_r^T \mathcal{K}(\sigma) \mathbf{V}_r$ have full rank.

- *If* $\mathcal{K}(\sigma)^{-1}\mathcal{B}(\sigma) \in Ran(\mathbf{V}_r)$, *then* $\mathcal{H}(\sigma) = \mathcal{H}_r(\sigma)$.
- *If* $\left(\mathcal{C}(\sigma)\mathcal{K}(\sigma)^{-1}\right)^T \in Ran(\mathbf{W}_r)$, *then* $\mathcal{H}(\sigma) = \mathcal{H}_r(\sigma)$
- *If* $\mathcal{K}(\sigma)^{-1}\mathcal{B}(\sigma) \in Ran(\mathbf{V}_r)$ *and* $\left(\mathcal{C}(\sigma)\mathcal{K}(\sigma)^{-1}\right)^T \in Ran(\mathbf{W}_r)$ *then* $\mathcal{H}'(\sigma) = \mathcal{H}_r'(\sigma)$

- Once again, Herminte interpolation via projection
- Flexibility of interpolation framework

Interpolatory projections in model reduction

- Given distinct (complex) frequencies $\{\sigma_1, \sigma_2, \ldots, \sigma_r\} \subset \mathbb{C}$,

$$\mathcal{V}_r = \left[\mathcal{K}(\sigma_1)^{-1}\mathcal{B}(\sigma_1), \cdots, \mathcal{K}(\sigma_r)^{-1}\mathcal{B}(\sigma_r)\right]$$

$$\mathcal{W}_r^T = \begin{bmatrix} \mathcal{C}(\sigma_1)\mathcal{K}(\sigma_1)^{-1} \\ \vdots \\ \mathcal{C}(\sigma_r)\mathcal{K}(\sigma_r)^{-1} \end{bmatrix}$$

- Guarantees that $\mathcal{H}(\sigma_j) = \mathcal{H}_r(\sigma_j)$ and $\mathcal{H}'(\sigma_j) = \mathcal{H}_r'(\sigma_j)$ for $j = 1, 2, \ldots, r$.
- Structure-preserving interpolation from data
  - [Schulze/Unger, 15]: Delay models
  - [Schulze/Unger/Beattie/G., 15]: Generalized coprime case

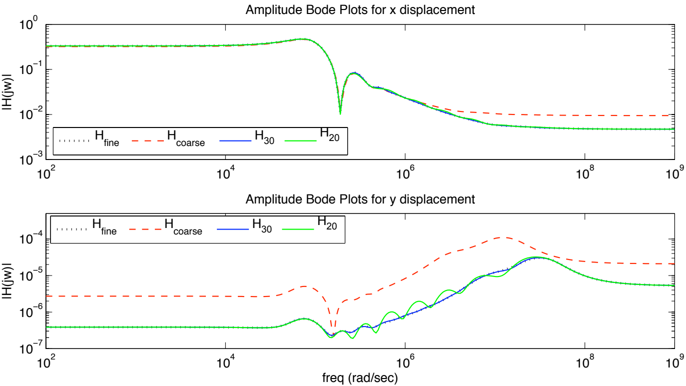
Viscoelastic Example

- A simple variation of the previous model:
- $\Omega = [0,1] \times [0,1]$: a volume filled with a viscoelastic material with boundary separated into a top edge ("lid"), $\partial\Omega_1$, and the complement, $\partial\Omega_0$ (bottom, left, and right edges).
- Excitation through shearing forces caused by transverse displacement of the lid, $u(t)$.
- Output: displacement $\mathbf{w}(\hat{x},t)$, at a fixed point $\hat{x} = (0.5, 0.5)$.

$$\partial_{tt}\mathbf{w}(x,t) - \eta_0\,\Delta\mathbf{w}(x,t) \; - \; \eta_1\partial_t \int_0^t \frac{\Delta\mathbf{w}(x,\tau)}{(t-\tau)^\alpha}\,d\tau \; + \; \nabla\varpi(x,t) = 0 \text{ for } x \in \Omega$$

$$\nabla \cdot \mathbf{w}(x,t) = 0 \text{ for } x \in \Omega,$$

$$\mathbf{w}(x,t) = 0 \text{ for } x \in \partial\Omega_0, \qquad \mathbf{w}(x,t) = u(t) \text{ for } x \in \partial\Omega_1$$



$\mathcal{H}_{\text{fine}}$: $n_x = 51,842$ and $n_p = 6,651$ $\mathcal{H}_{30}$: $n_x = n_p = 30$
$\mathcal{H}_{\text{coarse}}$: $n_x = 13,122$ $n_p = 1,681$ $\mathcal{H}_{20}$: $n_x = n_p = 20$

- $\mathcal{H}_{30}, \mathcal{H}_{20}$: reduced interpolatory viscoelastic models.
- $\mathcal{H}_{30}$ almost exactly replicates $\mathcal{H}_{\text{fine}}$ and outperforms $\mathcal{H}_{\text{coarse}}$
- Since input is a boundary *displacement* (as opposed to a boundary *force*), $\mathcal{B}(s) = s^2\,\mathbf{m} + \rho(s)\mathbf{k}$,

Delay Differential Equations

- Many physical processes exhibit some sort of delayed response in their input, output, or internal dynamics.

$$\mathbf{E}\dot{\mathbf{x}}(t) = \mathbf{A}_1\mathbf{x}(t) + \mathbf{A}_2\mathbf{x}(t-\tau) + \mathbf{B}\,\mathbf{u}(t), \qquad \mathbf{y}(t) = \mathbf{C}\mathbf{x}(t)$$

$$\mathcal{H}(s) = \underbrace{\mathbf{C}}_{\mathcal{C}(s)} \underbrace{(s\mathbf{E} - \mathbf{A}_1 - e^{-\tau s}\mathbf{A}_2)}_{\mathcal{K}(s)}{}^{-1} \underbrace{\mathbf{B}}_{\mathcal{B}(s)}.$$

- Delay systems are also infinite-order. The dynamic effects of even a small delay can be profound.
- Find a reduced order model retaining the same delay structure:

$$\mathbf{E}_r\dot{\mathbf{x}}_r(t) = \mathbf{A}_{1r}\mathbf{x}_r(t) + \mathbf{A}_{2r}\mathbf{x}_r(t-\tau) + \mathbf{B}_r\,\mathbf{u}(t), \qquad \mathbf{y}_r(t) = \mathbf{C}_r\mathbf{x}_r(t)$$

$$\mathcal{H}_r(s) = \underbrace{\mathbf{C}_r}_{\mathcal{C}_r(s)} \underbrace{(s\mathbf{E}_r - \mathbf{A}_{1r} - e^{-\tau s}\mathbf{A}_{2r})}_{\mathcal{K}_r(s)}{}^{-1} \underbrace{\mathbf{B}_r}_{\mathcal{B}_r(s)}.$$

- Construct $\mathcal{V}_r$ and $\mathcal{W}_r$ as in the Theorem. Then,

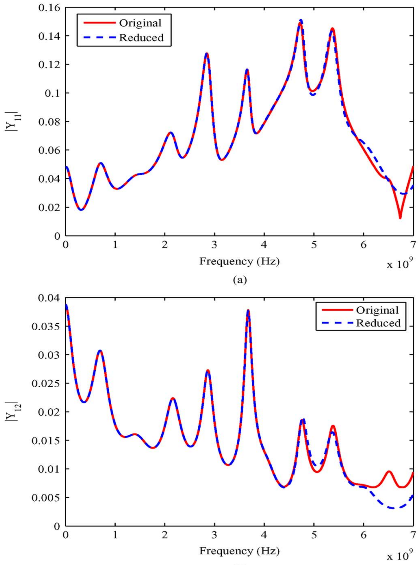
$$\mathcal{K}_r(s) = \mathcal{W}_r^T \mathcal{K} \mathcal{V}_r = s\,\mathcal{W}_r^T \mathbf{E} \mathcal{V}_r - \mathcal{W}_r^T \mathbf{A}_1 \mathcal{V}_r - \mathcal{W}_r^T \mathbf{A}_2 \mathcal{V}_r\, e^{-\tau s}$$

$$\mathbf{B}_r = \mathcal{W}_r^T \mathbf{B} \qquad \text{and} \qquad \mathbf{C}_r = \mathbf{C} \mathcal{V}_r$$

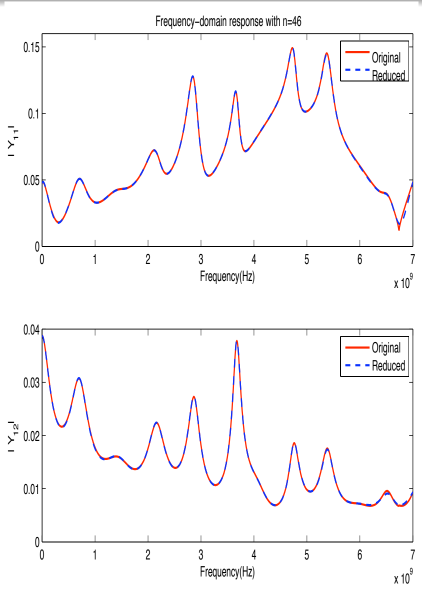
- $\mathcal{H}_r(s)$ has exactly the same delay structure
- $\mathcal{H}_r(s)$ exactly interpolates $\mathcal{H}(s)$. This will not be the case if $e^{-\tau s}$ is approximated by a rational function.
- Moreover, the rational approximation of $e^{-\tau s}$ increases the order drastically.
- Multiple state-delays, delays in the input/output mappings are welcome.

A two-port newtork with internal delay

- Example from [Tseng *et al.*, 07].
- $n = 2390$: 2097 lumped components and 120 sets of lossless two-conductor TLs.
- Method of [Tseng*et al.*, 07]: 4^{th}-order Taylor series expansion of $e^{-\tau s}$ to obtain $\mathcal{V}_r$ and $\mathcal{W}_r$; but the reduction is performed on the original delay system.
  - Dimension grows to $N = 5 \times 2390$
  - Delay structure and passivity are preserved but no interpolation.
- Compare with our approach where delay structure and passivity are preserved and interpolation is guaranteed.



From [Tseng*et al.*, 07]. with $r = 60$



Our approach with $r = 46$

Interpolatory Model Reduction for Parametric Systems

- $\mathcal{H}(s,\mathsf{p}) = \mathbf{C}(\mathsf{p})\left(s\mathbf{E}(\mathsf{p}) - \mathbf{A}(\mathsf{p})\right)^{-1}\mathbf{B}(\mathsf{p})$
- $\mathbf{E}_r(\mathsf{p}) = \mathbf{W}_r^T\mathbf{E}(\mathsf{p})\mathbf{V}_r, \quad \mathbf{A}_r(\mathsf{p}) = \mathbf{W}_r^T\mathbf{A}(\mathsf{p})\mathbf{V}_r,$
  $\mathbf{B}_r(\mathsf{p}) = \mathbf{W}_r^T\mathbf{B}(\mathsf{p}), \quad \mathbf{C}_r(\mathsf{p}) = \mathbf{C}(\mathsf{p})\mathbf{V}_r$

Theorem ([Baur/Beattie/Benner/G.,11])

Suppose $\sigma\mathbf{E}(\mathsf{p}) - \mathbf{A}(\mathsf{p})$, $\mathbf{B}(\mathsf{p})$, *and* $\mathbf{C}(\mathsf{p})$ *are continuously differentiable with respect to* p *in a neighborhood of* π. *If*

$$\left(\sigma\mathbf{E}(\boldsymbol{\pi}) - \mathbf{A}(\boldsymbol{\pi})\right)^{-1}\mathbf{B}(\boldsymbol{\pi}) \in \mathrm{Ran}(\mathbf{V}_r) \text{ and } \left(\sigma\mathbf{E}(\boldsymbol{\pi}) - \mathbf{A}(\boldsymbol{\pi})\right)^{-T}\mathbf{C}(\boldsymbol{\pi})^T \in \mathrm{Ran}(\mathbf{W}_r),$$

then

$$\mathcal{H}(\sigma,\boldsymbol{\pi}) = \mathcal{H}_r(\sigma,\boldsymbol{\pi}), \qquad \mathcal{H}'(\sigma,\boldsymbol{\pi}) = \mathcal{H}_r'(\sigma,\boldsymbol{\pi}),$$
$$\text{and } \nabla_{\mathsf{p}}\mathcal{H}(\sigma,\boldsymbol{\pi}) = \nabla_{\mathsf{p}}\mathcal{H}_r(\sigma,\boldsymbol{\pi}).$$

- Two-sided interpolation matches parameter gradients.
- Nonlinear Inversion in Diffuse Optical Tomography ([G. et al, 2015])
- [Daniel *et al.*, 2004], [Gunupudi *et al.*, 2004], [Weile *et al.*, 1999]

Model Reduction for Nonlinear Systems

- Consider the nonlinear case:

$$\mathbf{E}\,\dot{\mathbf{x}}(t) = \mathbf{A}\,\mathbf{x}(t)+\mathbf{f}(\mathbf{x}(t))+\mathbf{B}\,\mathbf{g}(t) \Rightarrow \mathbf{E}_r\,\dot{\mathbf{x}}_r(t) = \mathbf{A}_r\,\mathbf{x}(t)+\mathbf{f}_r(x(t))+\mathbf{B}_r\,\mathbf{g}(t),$$

- Approximate: $\mathbf{x}(t) \approx \mathbf{V}\mathbf{x}_r(t)$ and enforce the Galerkin condition

$$\Big(\mathbf{E}\mathbf{V}\dot{\mathbf{x}}_r(t) - \mathbf{A}\mathbf{V}\mathbf{x}_r(t) - \mathbf{f}\big(\mathbf{V}\mathbf{x}_r(t)\big) - \mathbf{B}\mathbf{g}(t)\Big) \perp \mathcal{V}_r \qquad \text{to obtain}$$

$$\mathbf{E}_r = \mathbf{V}^T\mathbf{E}\mathbf{V},\ \mathbf{A}_r = \mathbf{V}^T\mathbf{A}\mathbf{V},\ \mathbf{B}_r = \mathbf{V}^T\mathbf{B}, \quad \text{and} \quad \mathbf{f}_r(\mathbf{x}_r(t)) = \mathbf{V}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r(t)).$$

- For *general* nonlinear systems, we use POD: Construct

$$\mathbb{X} = [\,\mathbf{x}(t_0),\mathbf{x}(t_1),\mathbf{x}(t_2),\ldots,\mathbf{x}(t_{N-1})] = \mathbf{Z}\,\mathbf{\Sigma}\mathbf{Y}^T$$

- Choose $\mathbf{V} = \mathbf{Z}(:,1:r)$. See: [Hinze/Volkwein, 2005], [Kunish/Volkwein, 2002]
- $\mathbf{f}_r(\mathbf{x}_r(t)) = \mathbf{V}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r(t))$: Lifting bottleneck

How to resolve the lifting bottleneck

- [Astrid et al., 2008], [Barrult et al., 2004] , [Carlberg et al., 2013].
- Discrete Empirical Interpolation Method: [Chaturantabut/Sorensen, 2010]
- Given are: $\mathbf{f}: \mathbb{R}^n \longrightarrow \mathbb{R}^n$ and a basis matrix $\mathsf{U} \in \mathbb{R}^{n \times m}$
- The goal is: $\mathbf{f}(t) \approx \mathsf{U}\,\mathbf{c}(t)$ where $\mathbf{c}(t) \in \mathbb{R}^m$

  DEIM approximation is $\widehat{\mathbf{f}}(t) = \mathsf{U}(\mathbb{S}^T\mathsf{U})^{-1}\mathbb{S}^T\mathbf{f}(t)$,

  where $\mathbb{S}$ is $n \times m$ matrix obtained by selecting columns of $\mathbb{I}$.
- Note that $\mathbb{S}^T\mathbf{f}(t) = \mathbb{S}^T\widehat{\mathbf{f}}(t)$, i.e., interpolation at the selected rows.

$$\mathbf{f}_r(\mathbf{x}_r) = \underbrace{\mathbf{V}^T}_{r\times n}\underbrace{\mathbf{f}(\mathbf{V}\mathbf{x}_r(t))}_{n\times 1} \approx \underbrace{\mathbf{V}^T\mathsf{U}(\mathbb{S}^T\mathsf{U})^{-1}}_{\text{precomp }: r\times m}\underbrace{\mathbb{S}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r)}_{m\times 1} := \hat{\mathbf{f}}_r(\mathbf{x}_r)$$

- $\mathbf{f}_r(\mathbf{x}_r) \approx \mathbf{V}^T \mathsf{U}(\mathbb{S}^T\mathsf{U})^{-1}\mathbb{S}^T\mathbf{f}(\mathbf{V}\mathbf{x}_r)$

- $\mathbb{S}^T$ *"extracts m rows"* $\wp_1, \ldots, \wp_m$. $\wp := [\wp_1, \ldots, \wp_m]$

- $\mathbb{S}^T\mathsf{U} = \mathsf{U}(\wp, :)$ $\mathbb{S} = [\mathbf{e}_{\wp_1}, \ldots, \mathbf{e}_{\wp_m}],$, $\mathbf{e}_{\wp_i}$ = $\wp_i$-th column of $\mathbf{I}_n$

- U is the POD basis for $[\mathbf{f}(t_1)\ \mathbf{f}(t_2), \ldots, \mathbf{f}(t_N)]$. How to pick $\mathbb{S}$?

- Discrete Empirical Interpolation Method (DEIM): [Chaturantabut/Sorensen, 2010]: A greedy selection strategy to pick the interpolation indices.

- DEIM is LU with partial pivoting without replacement: [Sorensen, 2010]

- Discrete variation of the EIM algorithm (Barrault, Maday, Nguyen, Patera; 2004)

Lemma (Chaturantabut/Sorensen, 2010)

Let $\mathsf{U} \in \mathbb{R}^{n \times m}$ *be orthonormal* ($\mathsf{U}^*\mathsf{U} = \mathbb{I}_m$, $m < n$) *and let*

$$\widehat{f} = \mathsf{U}(\mathbb{S}^T\mathsf{U})^{-1}\mathbb{S}^T f \qquad (1)$$

be the DEIM projection $f \in \mathbb{R}^n$, *with* $\mathbb{S}$ *computed by DEIM. Then*

$$\|f - \widehat{f}\|_2 \leq \mathbf{c}\|(\mathbb{I} - \mathsf{U}\mathsf{U}^*)f\|_2, \quad \mathbf{c} = \|(\mathbb{S}^T\mathsf{U})^{-1}\|_2, \qquad (2)$$

where

$$\mathbf{c} \leq \frac{(1+\sqrt{2n})^{m-1}}{\|u_1\|_\infty} \leq \sqrt{n}(1+\sqrt{2n})^{m-1}.$$

- If $\mathcal{R}(\mathsf{U})$ captures the behavior of $\mathbf{f}$ well, and if $\mathbb{S}$ results in a moderate $\mathbf{c}$, the DEIM approximation will succeed.
- More on this upper bound later (a recent improved version)

Towards a different selection operator $\mathbb{S}$

- The error bound is rather pessimistic and DEIM performs drastically better than the bound predicts.
- $\mathbb{S}$ computed by DEIM depends on a particular basis for $\mathcal{U}$.
- The complexity of DEIM is $O(m^2n) + O(m^3)$
- Questions of interests:
  - Can the upper bound be improved and what selection operator $\mathbb{S}$ will have sharper a priori error bound?
  - Can we devise a selection operator $\mathbb{S}$ independent of the choice of an orthonormal basis U of $\mathcal{U}$?
  - Can we reduce the contribution of the factor n without substantial loss in the quality of the computed selection operator?

A new DEIM framework

Theorem (Drmač/G.,2015)

Let $\mathsf{U} \in \mathbb{C}^{n\times m}$, $\mathsf{U}^*\mathsf{U} = \mathbb{I}_m$, $m < n$. *Then :*

- *There exists an algorithm to compute* $\mathbb{S}$ *with complexity* $O(nm^2)$ *s.t.*

$$\|(\mathbb{S}^T\mathsf{U})^{-1}\|_2 \leq \sqrt{n-m+1}\ \frac{\sqrt{4^m+6m-1}}{3}, \tag{3}$$

  and for any $f \in \mathbb{C}^n$

$$\|f - \mathsf{U}(\mathbb{S}^T\mathsf{U})^{-1}\mathbb{S}^T f\|_2 \leq \sqrt{n}\, O(2^m)\, \|f - \mathsf{U}\mathsf{U}^* f\|_2. \tag{4}$$

- *There exists a selection operator* $\mathbb{S}_\star$ *such that*

$$\|f - \mathsf{U}(\mathbb{S}_\star^T\mathsf{U})^{-1}\mathbb{S}_\star^T f\|_2 \leq \sqrt{1+m(n-m)}\, \|f - \mathsf{U}\mathsf{U}^* f\|_2. \tag{5}$$

- *The selection operators* $\mathbb{S}$, $\mathbb{S}_\star$ *do not change if* U *is changed to* $\mathsf{U}\Omega$ *where* Ω *is arbitrary* $m \times m$ *unitary matrix.*

- Proof is constructive and uses the ideas from [Drmač,2009], arising in the analysis of block Jacobi algorithm for diagonalization of Hermitian matrices.
- Selection strategy $\mathbb{S}$ simply amounts to the pivot selection in QR factorization with column pivoting of U^* !!! Let

$$\mathsf{U}^*\Pi = \mathsf{W}\Pi = \begin{pmatrix} \widehat{\mathsf{W}}_1 & \widehat{\mathsf{W}}_2 \end{pmatrix} = Q\mathsf{R} = \left(\begin{array}{ccc|cccc} \divideontimes & * & * & * & * & * & * \\ 0 & * & * & * & * & * & * \\ 0 & 0 & \star & * & * & * & * \end{array}\right)$$

be pivoted QR. Consider the Businger–Golub pivoting:

$$\begin{array}{c} \\ i \\ \\ m \end{array}\overset{\begin{array}{ccccccc} & i & & p_i & & & n \end{array}}{\begin{pmatrix} \star & \star & \star & \star & \star & \star & \star \\ 0 & * & * & \circledast & * & * & * \\ 0 & * & * & \circledast & * & * & * \\ 0 & * & * & \circledast & * & * & * \end{pmatrix}} \xrightarrow{swap(i,p_i)} \begin{array}{c} \\ i \\ \\ m \end{array}\overset{\begin{array}{ccccccc} & i & & & & & n \end{array}}{\begin{pmatrix} \star & \star & \star & \star & \star & \star & \star \\ 0 & \circledast & * & * & * & * & * \\ 0 & \circledast & * & * & * & * & * \\ 0 & \circledast & * & * & * & * & * \end{pmatrix}}.$$

- $\mathbb{S}$: selection operator that collects the columns of W to build $\widehat{\mathsf{W}}_1$;

- The existence of $\mathbb{S}_\star$ is due to [Goreinov et al., 1997]) and uses the concept of matrix volume (the absolute value of the determinant).
- $\mathbb{S}_\star$ is defined to be the one that maximizes the volume of $\mathbb{S}_\star^T$U over all $\binom{n}{m} = \frac{n!}{m!(n-m)!}$ $m \times m$ submatrices of U.
- Either $\mathbb{S}$ or $\mathbb{S}_\star$ does not change by a unitary transformation
- Computing $\mathbb{S}_\star$ is difficult and $\mathbb{S}$ behaves very well in practice
- The volume of the submatrix selected by $\mathbb{S}$ equals the volume $\prod_{i=1}^m |\mathrm{T}_{ii}|$ of the upper triangular T.
- Following a similar analysis, [Sorensen/Embree, 15] very recently improved the original DEIM upper bound to: $\mathbf{c} \leq \sqrt{\frac{nm}{3}2^m}$
- [Bos et al., 2009]: Approximate Feketa points and pivoted QR.

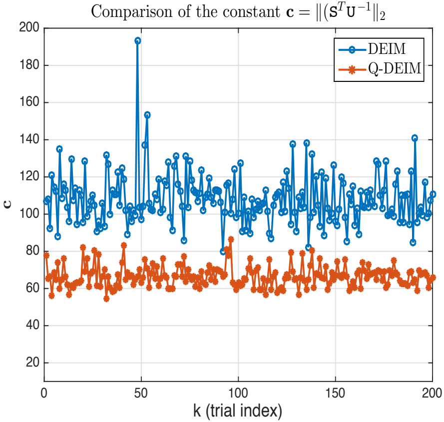
Numerical Implementation

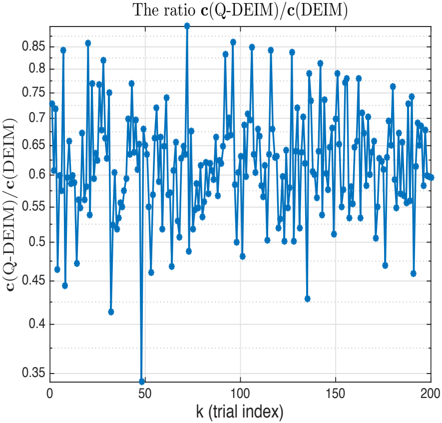
- The new selection is called `Q-DEIM`
- It is still an interpolatory `DEIM` process, but with a different $\mathbb{S}$

```
function [ S, M ] = q_dime( U ) ;
% Input  : U n-by-m with orthonormal columns
% Output : S selection of m row indices with guaranteed upper bound
%          norm(inv(U(S,:))) <= sqrt(n-m+1) * O(2^m).
%        : M the matrix U*inv(U(S,:)); the DEIM projection of
%          n-by-1 f is M*f(S).
% Coded by Zlatko Drmac, April 2015.
[n,m] = size(U) ;
if nargout == 1
[~,~,P] = qr(U','vector') ; S = P(1:m)   ;
else
[Q,R,P] = qr(U','vector') ; S = P(1:m)   ;
M = [eye(m) ; (R(:,1:m)\R(:,m+1:n))']    ;
Pinverse(P) = 1 : n ; M = M(Pinverse,:) ;
end
end
```

Example 1

- Computed DEIM and Q-DEIM using 200 randomly generated orthonormal matrices of size 10000×100.
- Compare $\mathbf{c}(\texttt{DEIM})$ and $\mathbf{c}(\texttt{Q-DEIM})$





Example 2: The FitzHugh-Naguma (F–N) System

- Model and parameters from [Chaturantabut/Sorensen,2010]
- Arises in modeling the activation and deactivation dynamics of a spiking neuron.
- Let v and w denote, respectively, the voltage and recovery of voltage. Also, let $x \in [0, L]$ and $t \geq 0$.

$$\begin{aligned} \varepsilon v_t(x,t) &= \varepsilon^2 v_{xx}(x,t) + f(v(x,t)) - w(x,t) + c \\ w_t(x,t) &= bv(x,t) - \gamma w(x,t) + c \end{aligned}$$

where $f(v) = v(v - 0.1)(1 - v)$ and

$$\begin{array}{ccc} v(x,0) = 0, & w(x,0) = 0, & x \in [0,L], \\ v_x(0,t) = -i_0(t), & v_x(L,t) = 0, & t \geq 0, \end{array}$$

- $L = 1$, $\varepsilon = 0.015$, $b = 0.5$, $\gamma = 2$, $c = 0.05$ and $i_0(t) = 50000t^3e^{-15t}$.
- A finite difference discretization leads to $n = 2048$.
- Simulation $t = [0, 8]$ leads to $N = 100$ snapshots.

- As before, compare $\mathbf{c}(\texttt{DEIM})$ and $\mathbf{c}(\texttt{Q-DEIM})$

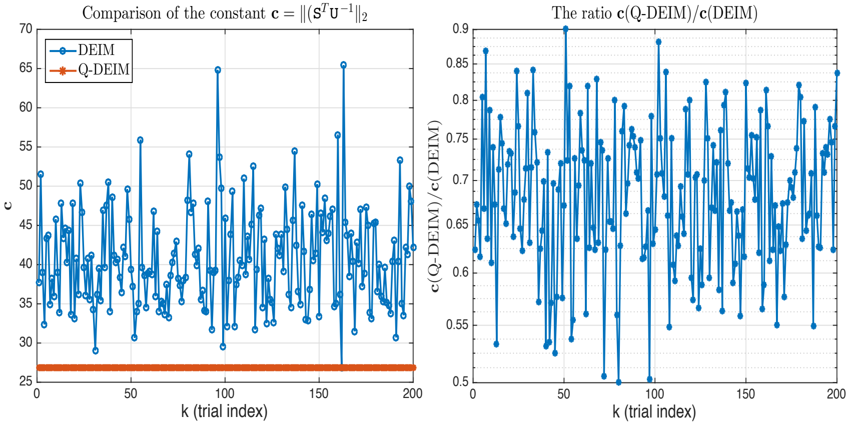


Figure: 200 random changes of a DEIM orthonormal basis U of size 2048×100 via post-multiplication by random 100×100 orthogonal matrices

Using restricted/randomized basis information

- If n is gargantuan, it will be necessary to reduce the $O(m^2 n)$ factor
- We only need to ensure that $\mathsf{T} = \mathsf{R}(1:m, 1:m)$ has small inverse where T is the pivoted QR triangular factor of columns of W.
- Use only a small selection of the columns of W (the rows of U):
- Randomly pick $k \geq m$ columns and store them in L:

$$\begin{array}{ccccccccccccccccccc} \Uparrow & \uparrow & & & \uparrow & & \uparrow & & \uparrow & \Uparrow & & & \Uparrow & & \uparrow & & \uparrow & & \Uparrow \end{array}$$

$$\begin{pmatrix} \star & * & . & . & * & . & * & . & * & \star & . & . & \star & . & * & . & * & . & \star \\ \star & * & . & . & * & . & * & . & * & \star & . & . & \star & . & * & . & * & . & \star \\ \star & * & . & . & * & . & * & . & * & \star & . & . & \star & . & * & . & * & . & \star \\ \star & * & . & . & * & . & * & . & * & \star & . & . & \star & . & * & . & * & . & \star \end{pmatrix} \mapsto \overbrace{\begin{pmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \end{pmatrix}}^{\mathsf{L}}$$

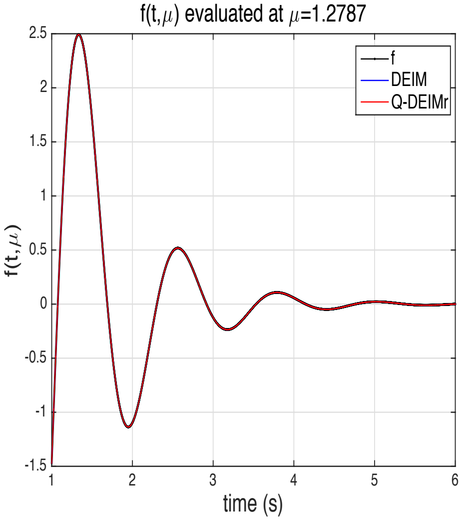
- Apply QR with column pivoting on L with a built-in Incremental Condition Estimator (ICE) that estimates $\|\mathsf{L}(1:j, 1:j)^{-1}\|$
- Define a threshold for the inverse.

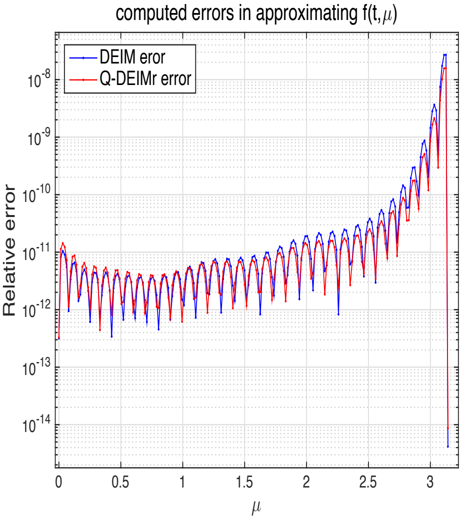
$$\begin{pmatrix} * & * & \times & \times & \times & \times \\ 0 & * & \times & \times & \times & \times \\ 0 & 0 & \circledast & \odot & \odot & \odot \\ 0 & 0 & 0 & \odot & \odot & \odot \end{pmatrix} \rightsquigarrow \begin{pmatrix} * & * & \star & \star & \star & \star \\ 0 & * & \star & \star & \star & \star \\ 0 & 0 & \star & \star & \star & \star \\ 0 & 0 & \star & \star & \star & \star \end{pmatrix} \rightsquigarrow \begin{pmatrix} * & * & * & \star & \star & \star \\ 0 & * & * & \star & \star & \star \\ 0 & 0 & * & \star & \star & \star \\ 0 & 0 & 0 & \star & \star & \star \end{pmatrix}$$

- If $\|\mathsf{L}(1:j,1:j)^{-1}\|$ is below threshold, continue.
- If not, the (j,j)th position $\circledast$ is too small, and, due to pivoting, that all entries in the active submatrix of L ($\odot$ are also small. ($\circledast$)
- The columns j to k in L are useless; discard them
- Draw new $k-j+1$ columns from the active columns of W ($\Uparrow \atop \star$).
- At any point, only k columns are processed.
- Algorithm is called `Q-DEIMr`.

Example 3

- $\mathbf{f}(t;\mu) = 10e^{-\mu t}(\cos(4\mu t) + \sin(4\mu t))$, $1 \le t \le 6$, $0 \le \mu \le \pi$.
- Take 40 uniformly μ sample and compute the snapshots over the discretized t–domain at $n = 10000$ uniformly spaced nodes.
- The best low rank approximation returned U with $m = 34$ columns.
- Let $k = m$ columns in the work array L, and set the upper bound for $\mathbf{c}$ at $\sqrt{m}\sqrt{n-m+1}$.
- Column index drawing is "random".
- After processing 113 rows of U (out of 10000), `Q-DEIMr` selected a submatrix with $\mathbf{c} \approx 181.45$;
- `DEIM` processed the whole matrix U and returned $\mathbf{c} \approx 79.13$.


f(t,μ) evaluated at μ=1.2787
f
DEIM
Q-DEIMr
f(t,μ)
time (s)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
1
2
3
4
5
6


computed errors in approximating f(t,μ)
DEIM eror
Q-DEIMr error
Relative error
μ
10^-8
10^-9
10^-10
10^-11
10^-12
10^-13
10^-14
0
0.5
1
1.5
2
2.5
3

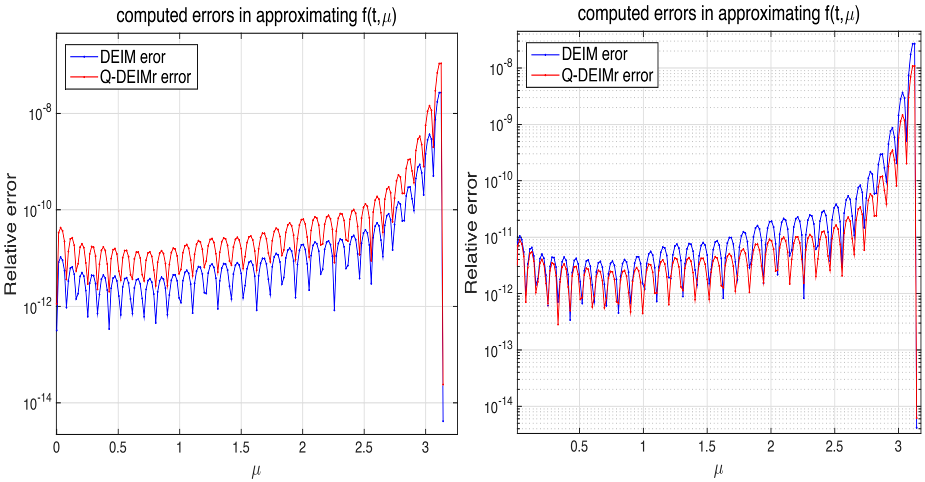


Figure: Left figure: Upper bound in `Q-DEIMr` set to $m\sqrt{n-m+1}$; it used 53 rows with $\mathbf{c} \approx 2532.9$. Right figure: Upper bound in `Q-DEIMr` set to $\sqrt{m}\sqrt{n-m+1}/5$; it used 220 rows with $\mathbf{c} \approx 103.1$.

Nonlinear Port-Hamiltonian (NPH) systems

Full-order system (dim n):

$$\begin{aligned} \dot{\mathbf{x}} &= (\mathbf{J}-\mathbf{R})\nabla_{\mathbf{x}} H(\mathbf{x}) + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y} &= \mathbf{B}^T \nabla_{\mathbf{x}} H(\mathbf{x}), \end{aligned}$$

- $\mathbf{x} \in \mathbb{R}^n$: State variable; $\mathbf{u} \in \mathbb{R}^{n_{in}}$: Input; $\mathbf{y} \in \mathbb{R}^{n_{out}}$: Output
- H: Hamiltonian - total energy in the system. $H : \mathbb{R}^n \to [0, \infty)$
- $\mathbf{J}$: Structure matrix (interconnection of energy storage components)
- $\mathbf{R}$: Dissipation matrix (describing internal energy losses)

- Structure: $\mathbf{J} = -\mathbf{J}^T$, $\mathbf{R} = \mathbf{R}^T \geq 0$. $H : \mathbb{R}^n \to [0, \infty)$

- Passive system: $H(\mathbf{x}(t_1)) - H(\mathbf{x}(t_0)) \leq \int_{t_0}^{t_1} \mathbf{y}(t)^T \mathbf{u}(t) dt.$
- Generalizes classical Hamiltonian systems: $\dot{\mathbf{x}} = \mathbf{J}\nabla_{\mathbf{x}} H(\mathbf{x})$.
- [van der Schaft, 2006], [Zwart/Jacob, 2009]
- **Applications:** Circuit, Network/interconnect structure, Mechanics (Euler-Lagrange eqn), e.g. Toda Lattice, Ladder Network

Model Reduction

Full-order system (dim n):

$$\dot{\mathbf{x}} = (\mathbf{J} - \mathbf{R})\nabla_{\mathbf{x}} H(\mathbf{x}) + \mathbf{B}\mathbf{u}(t), \quad \mathbf{y} = \mathbf{B}^T \nabla_{\mathbf{x}} H(\mathbf{x}),$$

GOAL: Reduced system (dim $r \ll n$):

$$\dot{\mathbf{x}}_r = (\mathbf{J}_r - \mathbf{R}_r)\nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r) + \mathbf{B}_r\mathbf{u}(t), \quad \mathbf{y}_r = \mathbf{B}_r^T \nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r),$$

- $\mathbf{J} = -\mathbf{J}^T$, $\mathbf{R} = \mathbf{R}^T \geq 0$. Hamiltonian: $H : \mathbb{R}^n \to [0, \infty)$, $H(\mathbf{x}) > 0$, $H(\mathbf{0}) = 0$

  " Preserve Structure, Stability & Passivity"

- $\mathbf{J}_r = -\mathbf{J}_r^T$, $\mathbf{R}_r = \mathbf{R}_r^T \geq 0$. Hamiltonian: $H_r : \mathbb{R}^r \to [0, \infty)$, $H_r(\mathbf{x}_r) > 0$, $H_r(\mathbf{0}) = 0$
- $H_r(\mathbf{x}_r(t_1)) - H_r(\mathbf{x}_r(t_0)) \leq \int_{t_0}^{t_1} \mathbf{y}_r(t)^T \mathbf{u}(t) dt.$

Model Reduction via Petrov-Galerkin Projection

Choose basis matrices $\mathbf{V}_r \in \mathbb{R}^{n\times r}$ and $\mathbf{W}_r \in \mathbb{R}^{n\times r}$ so that

- $\mathbf{x} \approx \mathbf{V}_r\mathbf{x}_r$ ($\mathbf{x}(t)$ approximately lives in an r-dimensional subspace)
- $\mathrm{Span}\{\mathbf{W}_\mathrm{r}\}$ is orthogonal to the residual:

$$\mathbf{W}_r^T \quad [\mathbf{V}_r\dot{\mathbf{x}}_r(t) - (\mathbf{J}-\mathbf{R})\,\nabla_\mathbf{x} H(\mathbf{V}_r\mathbf{x}_r) - \mathbf{B}\mathbf{u}(t)] = \mathbf{0}$$
$$\mathbf{y}_r(t) = \mathbf{B}^T\nabla_\mathbf{x} H(\mathbf{V}_r\mathbf{x}_r).$$

- and with $\mathbf{W}_r^T\mathbf{V}_r = \mathbf{I}$ (change of basis)

$$\dot{\mathbf{x}}_r = \mathbf{W}_r^T\,(\mathbf{J}-\mathbf{R})\,\nabla_\mathbf{x} H(\mathbf{V}_r\mathbf{x}_r) + \mathbf{W}_r^T\mathbf{B}\mathbf{u}(t)$$
$$\mathbf{y}_r = \mathbf{B}^T\nabla_\mathbf{x} H(\mathbf{V}_r\mathbf{x}_r),$$

Main Issues:

- Port-Hamiltonian structure is not preserved $\Longrightarrow$ Stability and passivity of the reduced model are not guaranteed.
- The complexity is not reduced – complexity of nonlinear term $\sim \mathcal{O}(n)$

MOR for Nonlinear PH Systems [Beattie & G. (2011)]

- [Fujimoto, H. Kajiura (2007], [Scherpen, van der Schaft (2008)]
- Find $\mathbf{V}_r$ such that $\mathbf{x}(t) \approx \mathbf{V}_r \mathbf{x}_r(t)$
- Find $\mathbf{W}_r$ such that
  $\nabla_{\mathbf{x}} H(\mathbf{x}(t)) \approx \mathbf{W}_r \, \mathbf{c}(t) \qquad \text{for} \quad \text{some} \qquad \mathbf{c}(\mathrm{t}) \in \mathbb{R}^{\mathrm{r}}$

$$\nabla_{\mathbf{x}} H(\mathbf{V}_r \mathbf{x}_r(t)) \;\approx\; \nabla_{\mathbf{x}} H(\mathbf{x}(t)) \;\approx\; \mathbf{W}_r \, \mathbf{c}(t)$$

- $\mathbf{V}_r^T \mathbf{W}_r = \mathbf{I}$,

$$\Longrightarrow \mathbf{c}(t) = \mathbf{V}_r^T \nabla_{\mathbf{x}} H(\mathbf{V}_r \mathbf{x}_r(t)) \quad = \nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r(t))$$

Reduced-order Hamiltonian:

$$H_r(\mathbf{x}_r(t)) := H(\mathbf{V}_r \mathbf{x}_r(t))$$

- Substitute $\mathbf{x} \longrightarrow \mathbf{V}_r\mathbf{x}_r$, and $\nabla_{\mathbf{x}} H(\mathbf{V}_r\mathbf{x}_r(t)) \longrightarrow \mathbf{W}_r \nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r(t))$ with

$$\mathbf{W}_r{}^T \left[\mathbf{V}_r\dot{\mathbf{x}}_r - (\mathbf{J}-\mathbf{R})\mathbf{W}_r\mathbf{V}_r^T\nabla_{\mathbf{x}} H(\mathbf{V}_r\mathbf{x}_r) + \mathbf{B}\mathbf{u}(t) = 0\right], \qquad \mathbf{W}_r^T\mathbf{V}_r = \mathbf{I}.$$

Reduced system:

$$\dot{\mathbf{x}}_r = (\mathbf{J}_r - \mathbf{R}_r)\nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r) + \mathbf{B}_r\mathbf{u}(t), \qquad \mathbf{y}_r = \mathbf{B}_r^T\nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r),$$

where $\mathbf{J}_r = \mathbf{W}_r^T\mathbf{J}\mathbf{W}_r$, $\mathbf{R}_r = \mathbf{W}_r^T\mathbf{R}\mathbf{W}_r$, $\mathbf{B}_r = \mathbf{W}_r^T\mathbf{B}$,
$\nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r) = \mathbf{V}_r^T\nabla_{\mathbf{x}} H(\mathbf{V}_r\mathbf{x}_r)$.

POD for port-Hamiltonian systems (POD-PH)

Algorithm (POD-based MOR for pH systems [Beattie, G. (2011)])

1. *Generate trajectory* $\mathbf{x}(t)$*, and collect snapshots:*

$$\mathbb{X} = [\mathbf{x}(t_0), \mathbf{x}(t_1), \mathbf{x}(t_2), \ldots, \mathbf{x}(t_N)] \,.$$

2. *Truncate SVD of snapshot matrix,* $\mathbb{X}$*, to get POD basis,* $\widetilde{\mathbf{V}}_r$*.*
3. *Collect associated force snapshots:*

$$\mathbb{F} = [\nabla_{\mathbf{x}} H(\mathbf{x}(t_0)), \nabla_{\mathbf{x}} H(\mathbf{x}(t_1)), \ldots, \nabla_{\mathbf{x}} H(\mathbf{x}(t_N))] \,.$$

4. *Truncate SVD of* $\mathbb{F}$ *to get a second POD basis,* $\widetilde{\mathbf{W}}_r$*.*

The POD-PH reduced system is

$$\dot{\mathbf{x}}_r = (\mathbf{J}_r - \mathbf{R}_r)\nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r) + \mathbf{B}_r \mathbf{u}(t), \qquad \mathbf{y}_r(t) = \mathbf{B}_r^T \nabla_{\mathbf{x}_r} H_r(\mathbf{x}_r)$$

with $\mathbf{J}_r = \mathbf{W}_r^T \mathbf{J} \mathbf{W}_r$, $\mathbf{R}_r = \mathbf{W}_r^T \mathbf{R} \mathbf{W}_r$, $\mathbf{B}_r = \mathbf{W}_r^T \mathbf{B}$, and $H_r(\mathbf{x}_r) = H(\mathbf{V}_r \mathbf{x}_r)$.

A-Priori Error for NPH from structure preserving MOR

Error bounds **[Chaturantaut, Beattie & G. (2013)]:**

Basis matrices $\mathbf{V}_r, \mathbf{W}_r$ with $\mathbf{W}_r^T \mathbf{V}_r = \mathbf{V}_r^T \mathbf{W} = \mathbf{I}$ and $\mathbf{V}_r^T \mathbf{V}_r = \mathbf{I}$,

$$\int_0^T \|\mathbf{x}(t) - \mathbf{V}_r \mathbf{x}_r(t)\|^2 dt \;\leq\; C_{\mathbf{x}} \sum_{\ell=r+1}^{n_t} \lambda_\ell + C_{\mathbf{f}} \sum_{\ell=r+1}^{n_t} \varrho_\ell$$

and

$$\int_0^T \|\mathbf{y}(t) - \mathbf{y}_r(t)\|^2 dt \;\leq\; \widehat{C}_{\mathbf{x}} \sum_{\ell=r+1}^{n_t} \lambda_\ell + \widehat{C}_F \sum_{\ell=r+1}^{n_t} \varrho_\ell$$

$\Longrightarrow$ *Error bounds are proportional to the least-squares errors ($\mathcal{L}_2$-norm) of snapshots* $\mathbf{x}(t)$ *and* $\mathbf{F}(t) = \nabla_{\mathbf{x}} H(\mathbf{x}(t))$.

An Alternative Approach

- POD provides one set of choices for $\mathbf{V}_r$ and $\mathbf{W}_r$. Consider others
- Find a choice of subspaces that is *asymptotically optimal* for small $\mathbf{u}$ (hence for small $\mathbf{x}$).
- $\nabla_{\mathbf{x}} H(\mathbf{x}) \approx \mathbf{Q}\mathbf{x}$ for a symmetric positive semidefinite $\mathbf{Q} \in \mathbb{R}^{n\times n}$.
- Leads to consideration of *Linear Port-Hamiltonian Systems*

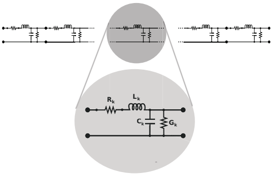
$$\begin{aligned} \dot{\mathbf{x}} &= (\mathbf{J}-\mathbf{R})\mathbf{Q}\mathbf{x} + \mathbf{B}\mathbf{u}(t) \\ \mathbf{y}(t) &= \mathbf{B}^T\mathbf{Q}\mathbf{x} \end{aligned} \quad \longrightarrow \quad \begin{aligned} \dot{\mathbf{x}}_r &= (\mathbf{J}_r-\mathbf{R}_r)\mathbf{Q}_r\mathbf{x}_r + \mathbf{B}_r\mathbf{u}(t) \\ \mathbf{y}_r(t) &= \mathbf{B}_r^T\mathbf{Q}_r\mathbf{x}_r \end{aligned}$$

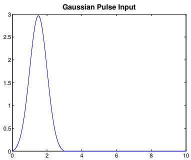
(Original system) (Reduced system)

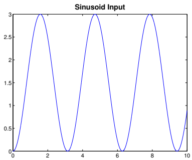
- $\mathbf{G}(s) = \mathbf{B}^T\mathbf{Q}(s\mathbf{I}-(\mathbf{J}-\mathbf{R})\mathbf{Q})^{-1}\mathbf{B} \longrightarrow \mathbf{G}_r(s) = \mathbf{B}_r^T\mathbf{Q}_r(s\mathbf{I}-(\mathbf{J}_r-\mathbf{R}_r)\mathbf{Q}_r)^{-1}\mathbf{B}_r$
- Find $\mathbf{V}_r$ and $\mathbf{W}_r$ that are optimal reduction spaces for $\|\mathbf{G}-\mathbf{G}_r\|_{\mathcal{H}_2}$, use them to reduce the original nonlinear system
- We use Quasi-$\mathcal{H}_2$ optimal subspaces using PH-IRKA method of [G./Polyuga/Beatie/van der Schaft/09]

N-stage Nonlinear Ladder Network

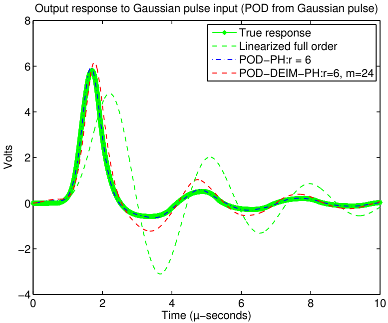
- Magnetic fluxes: $\{\phi_k(t)\}_{k=1}^N$; Charges: $\{Q_k\}_{k=1}^N$. $C_k(V) = \frac{C_0 V_0}{V_0+V}$
- Total energy in stage k: $H^{[k]}(\phi_k, Q_k) = C_0 V_0^2 \left[\exp\left(\frac{Q_k}{C_0 V_0}\right) - 1\right] - Q_k V_0 + \frac{1}{2\,L_0}\phi_k^2.$
- State variable: $\mathbf{x} = [Q_1, \ldots, Q_N, \phi_1, \ldots, \phi_N]^T$.
- Hamiltonian: $H(\mathbf{x}) = \sum_{k=1}^N H^{[k]}(\phi_k, Q_k).$
- *Gaussian pulse*-generated POD basis.
- Testing: *Sinusoid input*; $R_0 = 1\Omega$ $G_0 = 10\mu℧$, $L_0 = 2\mu$H, $C_0 = 100$pF $V_0 = 1$V.

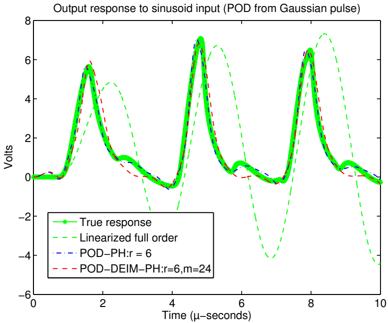






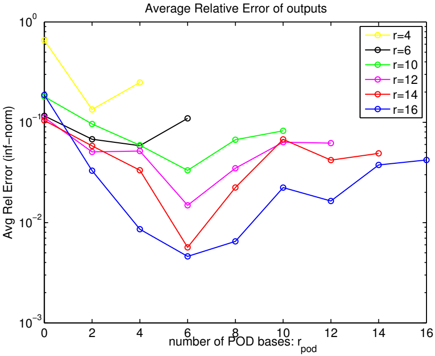
- Testing: *Sinusoid input*; $R_0 = 1\Omega$ $G_0 = 10\mu\mho$, $L_0 = 2\mu$H, $C_0 = 100$pF $V_0 = 1$V.





Combining POD and *Quasi-optimal* $\mathcal{H}_2$ bases.

- POD is very accurate for the choice of specific inputs
- Enrich this POD basis by including components that are optimal for (small) variations from an equilibrium point, i.e. optimal subspaces from linear approximations



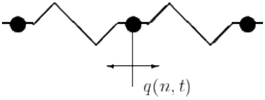
$\Longrightarrow$ Much more accurate than only POD or only quasi-optimal $\mathcal{H}_2$

Toda Lattice

- 1-D motion of N-particle chain with nearest neighbor exponential interactions, e.g., crystal model in solid state physics.

$$\dot{\mathbf{x}} = (\mathbf{J}-\mathbf{R})\nabla_{\mathbf{x}}H(\mathbf{x}) + \mathbf{B}\mathbf{u}(t), \qquad \mathbf{y} = \mathbf{B}^T\nabla_{\mathbf{x}}H(\mathbf{x}).$$

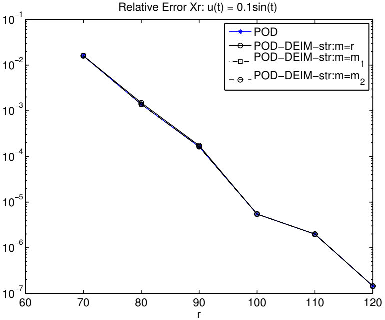
$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix} \mathbf{R} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathrm{diag}(\gamma_1,\ldots,\gamma_N) \end{bmatrix} \in \mathbb{R}^{n\times n}, \mathbf{B} = \begin{bmatrix} \mathbf{0} \\ \mathbf{e}_1 \end{bmatrix} \in \mathbb{R}^{n\times n}.$$



- State variable: $\mathbf{x} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix}$; q_j =displacement; p_j =momentum.
- Hamiltonian: $H = \sum_{k=1}^{N} \frac{1}{2}p_k^2 + \sum_{k=1}^{N-1} \exp(q_k - q_{k+1}) + \exp(q_N) - q_1.$
- $Q := \nabla^2\mathbf{H}(0)$, $N = 1000$; Full dim $n = 2N = 2000$.
- $\gamma_j = 0.1, j = 1,\ldots,N$

Input: $\mathbf{u}(t) = 0.1\sin(t)$

- POD basis dimension r
- DEIM dim.: $m = r, m_1, m_2,\quad m_1 = r + \texttt{ceil}(r/3),\quad m_2 = r + \texttt{ceil}(2r/3).$



Conclusions

- Interpolation is good for you.
- Optimal rational approximation for linear dynamical
  - Hermite interpolation at mirror images
  - Input-independent approximations via IRKA
- Structure-preserving interpolation for generalized coprime setting
  - Rational interpolation naturally extends
  - Reduced models preserve the internal structure
  - Approximants are not necessarily rational
- DEIM and MOR of nonlinear port-Hamiltonian systems
  - A new DEIM selection operator: Q-DEIM
  - Structure-preserving POD-DEIM for port-Hamiltonian systems
- Some open problems
  - Structure-preserving optimal interpolation
  - Input-independent model reduction for nonlinear systems
  - Effect of structure-preservation in nonlinear model reduction

Related Papers:

1. S. Gugercin, A.C. Antoulas, and C.A. Beattie, $\mathcal{H}_2$ *model reduction for large-scale linear dynamical systems*, SIMAX, 2008.
2. C.A. Beattie and S. Gugercin, *Interpolatory Projection Methods for Structure-preserving Model Reduction*, Systems and Control Letters, 2009.
3. C.A. Beattie and S. Gugercin, *A Trust Region Method for Optimal* $\mathcal{H}_2$ *Model Reduction*, Proceedings of the 48th IEEE Conference on Decision and Control, 2009.
4. A.C. Antoulas, C.A. Beattie and S. Gugercin, *Interpolatory Model Reduction of Large-scale Dynamical Systems*, Efficient Modeling and Control of Large-Scale System, 2011.
5. C.A. Beattie, and S. Gugercin. *Realization-independent* $\mathcal{H}_2$*-approximation*. Proceedings of the 51st IEEE Conference on Decision and Control, 2012.
6. S. Gugercin, T. Stykel, and S. Wyatt. *Model Reduction of Descriptor Systems by Interpolatory Projections Methods.* SIAM Journal on Scientific Computing, 2013.
7. C.A. Beattie and S. Gugercin, *Model Reduction by Rational Interpolation*, Model Reduction and Approximation for Complex Systems, 2015.
8. Z. Drmac and S. Gugercin, *A New Selection Operator for the Discrete Empirical Interpolation Method – improved a priori error bound and extensions.*, 2015.
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