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Model Reduction of Complex Dynamical Systems

An a posteriori output error bound for linear parametric systems

Peter Benner, Lihong Feng

Computational Methods in Systems and Control Theory
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

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Projection based PMOR

Original model	Reduced model
$E(\mathbf{p})\frac{d\mathbf{x}}{dt} = A(\mathbf{p})\mathbf{x} + Bu(t),$	$\hat{E}(\mathbf{p})\frac{d\mathbf{z}}{dt} = \hat{A}(\mathbf{p})\mathbf{z} + \hat{B}u(t),$
$y(t) = C\mathbf{x}.$	$y(t) = CV\mathbf{z}.$

Here, $\mathbf{p} = (p_1, \ldots, p_m)^T$ is a vector of parameters $p_1, \ldots, p_m$.
$\hat{E} = W^T E(\mathbf{p}) V$, $\hat{A} = W^T A(\mathbf{p}) V$, $\hat{B} = W^T B$.

Different choices of W, V lead to different PMOR methods.

Review

For the dynamical parametric system,

$$\begin{aligned} E(\mathbf{p})\frac{d\mathbf{x}}{dt} &= A(\mathbf{p})\mathbf{x} + Bu(t), \\ y(t) &= C\mathbf{x}, \end{aligned}$$

or

$$\begin{aligned} M(\mathbf{p})\frac{d^2\mathbf{x}}{dt^2} + K(\mathbf{p})\frac{d\mathbf{x}}{dt} + A(\mathbf{p})\mathbf{x} &= Bu(t), \\ y(t) &= C\mathbf{x}. \end{aligned}$$

Using Laplace transform to get the parametric system in the frequency domain (free from time t),

$$\begin{aligned} sE(\mathbf{p})\mathbf{x} &= A(\mathbf{p})\mathbf{x} + B\bar{u}(s), \\ y(\mu) &= C\mathbf{x}, \end{aligned}$$

or

$$\begin{aligned} s^2M(\mathbf{p})\mathbf{x} + sK(\mathbf{p})\mathbf{x} + A(\mathbf{p})\mathbf{x} &= B\bar{u}(s), \\ y(\mu) &= C\mathbf{x}. \end{aligned}$$

Review

Either of the above equations can be generally written as

$$\begin{aligned} G(\mu)\mathbf{x} &= B\bar{u}(\mu), \\ y(\mu) &= C\mathbf{x}, \end{aligned}$$

where $\mu = (\mathbf{p}, s)^T$.

Transfer function $H(\mu) = y(\mu)/\bar{u}(\mu) = C\mathbf{x}/\bar{u}(\mu) = C[G(\mu)]^{-1}B$.

$$\text{If } \bar{u}(\mu) = 1,\ H(\mu) = y(\mu) = C\mathbf{x}.$$

Analogously, the transfer function of the reduced model is $\hat{H}(\mu) = \hat{C}[\hat{G}(\mu)]^{-1}\hat{B}$. Where $\hat{C} = CV$, $\hat{G} = W^T G(\mu)V$, $\hat{B} = W^T B$.

$$||H(\mu) - \hat{H}(\mu)|| \leq ?$$

Derivation of $\Delta(\mu)$

Define

the primal system

$$\begin{aligned} G(\mu)\mathbf{x} &= B, \\ y^{pr}(\mu) &= C\mathbf{x}. \end{aligned}$$

the dual system

$$\begin{aligned} G^*(\mu)\mathbf{x}^{du} &= -C^*, \\ y^{du}(\mu) &= B^*\mathbf{x}^{du}. \end{aligned}$$

reduced primal system

$$\begin{aligned} W^TG(\mu)V\mathbf{z} = W^TB, \\ \hat{y}^{pr}(\mu) = CV\mathbf{z}. \end{aligned}$$

reduced dual system

$$\begin{aligned} (W^{du})^TG^*(\mu)V^{du}\mathbf{x}^{du} = -(W^{du})^TC^*, \\ \hat{y}^{du}(\mu) = B^*V^{du}\mathbf{z}^{du}. \end{aligned}$$

Then $\mathbf{x} \approx \hat{\mathbf{x}} = V\mathbf{z}$. $\quad \mathbf{x}^{du} \approx \hat{\mathbf{x}}^{du} = V^{du}\mathbf{z}^{du}$.

$\mathbf{r}^{pr}(\mu) = B - G(\mu)\hat{\mathbf{x}}$. $\quad \mathbf{r}^{du}(\mu) = -C^* - G^*(\mu)\hat{\mathbf{x}}^{du}$.

Observe:

$y^{pr}(\mu) = C\mathbf{x} = C[G(\mu)]^{-1}B = H(\mu)$,

$\hat{y}^{pr}(\mu) = C\hat{\mathbf{x}} = CV[W^TG(\mu)V]^{-1}W^TB = \hat{C}[\hat{G}(\mu)]^{-1}\hat{B} = \hat{H}(\mu)$.

Derivation of $\Delta(\mu)$

Assume[1],

$$\inf_{\substack{\mathbf{w}\in\mathbb{C}^n\\ \mathbf{w}\neq\mathbf{0}}} \sup_{\substack{\mathbf{v}\in\mathbb{C}^n\\ \mathbf{v}\neq\mathbf{0}}} \frac{\mathbf{w}^* G(\mu)\mathbf{v}}{||\mathbf{v}||_2||\mathbf{w}||_2} = \beta(\mu) > 0. \tag{1}$$

Theorem

For a single-input single-output system, if $G(\mu)$ satisfies (1), then $|y^{pr}(\mu) - \tilde{y}^{pr}(\mu)| \leq \tilde{\Delta}(\mu) := \frac{||\mathbf{r}^{du}(\mu)||_2||\mathbf{r}^{pr}(\mu)||_2}{\beta(\mu)}$. *As a result,* $|H(\mu) - \hat{H}(\mu)| = |y^{pr}(\mu) - \hat{y}^{pr}(\mu)| \leq \tilde{\Delta}(\mu) + |e(\mu)| =: \Delta(\mu).$

Here, $\tilde{y}^{pr}(\mu) = \hat{y}^{pr}(\mu) - e(\mu)$, $e(\mu) = (\hat{\mathbf{x}}^{du})^*\mathbf{r}^{pr}(\mu)$. Notice that when $W^{du} = V$, $V^{du} = W$, $e(\mu) = 0$.

Error bound for a **multiple-input multiple-output** system:
$||H(\mu) - \hat{H}(\mu)||_{\max} = \max_{ij} |H_{ij}(\mu) - \hat{H}_{ij}(\mu)| \leq \max_{ij} \Delta_{ij}(\mu) =: \Delta(\mu).$

[1] Sébastien Boyabal, Mathematical modelling and numerical simulation in materials science, PhD thesis, Université Paris Est, 2009.

Computation of $\Delta(\mu)$

Recall,

$$\inf_{\substack{\mathbf{w}\in\mathbb{C}^n\\ \mathbf{w}\neq\mathbf{0}}} \sup_{\substack{\mathbf{v}\in\mathbb{C}^n\\ \mathbf{v}\neq\mathbf{0}}} \frac{\mathbf{w}^* G(\mu)\mathbf{v}}{||\mathbf{v}||_2||\mathbf{w}||_2} = \beta(\mu) > 0.$$

Since

$$\inf_{\substack{\mathbf{w}\in\mathbb{C}^n\\ \mathbf{w}\neq\mathbf{0}}} \sup_{\substack{\mathbf{v}\in\mathbb{C}^n\\ \mathbf{v}\neq\mathbf{0}}} \frac{\mathbf{w}^* G^*(\mu)\mathbf{v}}{||\mathbf{w}||_2||\mathbf{v}||_2} = \inf_{\substack{\mathbf{w}\in\mathbb{C}^n\\ \mathbf{w}\neq\mathbf{0}}} \frac{||G^*(\mu)\mathbf{w}||_2}{||\mathbf{w}||_2},$$

and,

$$\min_{\substack{\mathbf{w}\in\mathbb{C}^n\\ \mathbf{w}\neq\mathbf{0}}} \frac{\mathbf{w}^* G(\mu)G^*(\mu)\mathbf{w}}{\mathbf{w}^*\mathbf{w}} = \lambda_{min}(G(\mu)G^*(\mu)).$$

Therefore $\beta(\mu) = \sqrt{\lambda_{min}(G(\mu)G^*(\mu))}$.

Computation of $\Delta(\mu)$

Estimation of $\beta(\mu)$

Instead of solving the big eigenvalue problem

$$\beta(\mu) = \sqrt{\lambda_{min}(G(\mu)G^*(\mu))},$$

one can solve the projected eigenvalue problem

$$\beta(\mu) \approx \hat{\beta}(\mu) = \sqrt{\lambda_{min}(\hat{G}(\mu)\hat{G}^*(\mu))},$$

where $\hat{G}(\mu) = W^T G(\mu) V$.

The estimated error bound is $\hat{\Delta}(\mu) = \frac{||\mathbf{r}^{du}(\mu)||_2 ||\mathbf{r}^{pr}(\mu)||_2}{\hat{\beta}(\mu)} + |e(\mu)|$

$$|\Delta(\mu) - \hat{\Delta}(\mu)| \leq ?$$

Krylov subspace based PMOR—multi-moment matching

System in the frequency domain

$$\begin{aligned} G(\mu)\mathbf{x} &= B\bar{u}(\mu), \\ y(\mu) &= C\mathbf{x}. \end{aligned}$$

For simplicity, we assume that $G(\mu)$ has an affine structure,

$$G(\mu) = G_0 + \mu_1 G_1 + \ldots + \mu_m G_m.$$

Consider the solution $\mathbf{x}$ in the frequency domain,

$$\mathbf{x} = [G(\mu)]^{-1} B\bar{u}(\mu).$$

Krylov subspace based PMOR—multi-moment matching

$\mathbf{x}$ can be expanded into power series at an expansion point[2] $\mu^0 = (\mu_1^0, \ldots, \mu_m^0)$,

$$
\begin{aligned}
\mathbf{x} &= (G_0 + \mu_1 G_1 + \ldots + \mu_m G_m)^{-1} B\bar{u} \\
&= [I - (\sigma_1 M_1 + \ldots + \sigma_m M_p)]^{-1} B_M \bar{u} \\
&= \sum_{i=0}^{\infty} (\sigma_1 M_1 + \ldots + \sigma_m M_m)^i B_M \bar{u} \\
&\approx \sum_{i=0}^{q} (\sigma_1 M_1 + \ldots + \sigma_m M_m)^i B_M \bar{u},
\end{aligned}
$$

where $\sigma_i = \mu_i - \mu_i^0, i = 1, 2, \ldots, p$,
$M_i = -[G(\mu^0)]^{-1} G_i, i = 1, \ldots, m,\ B_M = [G(\mu^0)]^{-1} B$.

[2] [Daniel et al.' 04]

Krylov subspace based PMOR—multi-moment matching

Since

$$\mathbf{x} \approx \sum_{i=0}^{q}(\sigma_1 M_1 + \ldots + \sigma_m M_m)^i B_M \bar{u},$$

$\mathbf{x} \approx \hat{\mathbf{x}} \in \mathrm{span}\{B_M, R_1, \ldots, R_q\}$.

$$\begin{aligned} R_1 &= (M_1, \ldots, M_m)B_M \quad (i = 1), \\ &\vdots \\ R_q &= (M_1, \ldots, M_m)R_{q-1} \quad (i = q). \end{aligned}$$

$B_M, R_i, i = 1, \ldots, q$ are free from the parameters $\sigma_j, j = 1, \ldots, m$. The orthonormal matrix V for PMOR can be computed as[3]

$$\mathrm{range}(V) = \mathrm{span}\{B_M, R_1, \ldots, R_q\}.$$

[3] [Feng, Benner'07]

Krylov subspace based PMOR—multi-moment matching

The reduced model is obtained by Galerkin projection, e.g.

$$\begin{aligned} V^T E(\mathbf{p}) V \frac{d\mathbf{z}}{dt} &= V^T A V(\mathbf{p})\mathbf{z} + V^T B u(t), \\ y(t) &= C V \mathbf{z}. \end{aligned}$$

- The multi-moments $CB_M, CR_i, i = 1, \ldots, q$ (coefficients in the series expansion) of the transfer function $H(\mu)$ are equal to those of the transfer function $\hat{H}(s)$: multi-moment matching.
- If there are more than three parameters, multiple-point expansion is needed.

Krylov subspace based PMOR—multi-moment matching

Multiple-point expansion: given $\mu^i, i = 1, \ldots, exp$

- For each expansion point μ^i, we can compute a matrix $\mathrm{range}(V_i) = \mathrm{span}\{B_M, R_1, \ldots, R_{\tilde{q}}\}_{\mu^i}, \ \tilde{q} \ll q$.
- Finally $V = \mathrm{orth}\{V_1, \ldots, V_{exp}\}$.

How to choose μ^i?

$\Delta(\mu)$: $||H(\mu) - \hat{H}(\mu)||_{\max} \leq \Delta(\mu)$ can guide the selection of μ^i.

Selecting μ^i with the guidance of $\Delta(\mu)$

Selection of the expansion points μ^i

$V = []$; $\epsilon = 1$;
Initial expansion point: $\hat{\mu}$; $i = -1$;
Ξ_{train}: a large set of the samples of μ
WHILE $\epsilon > \epsilon_{tol}$
  i=i+1;
  $\mu^i = \hat{\mu}$;
  $V_i = span\{R_0, \ldots, R_{\tilde{q}}\}_{\mu^i}$;
  $V = [V, V_i]$;
  $\hat{\mu} = arg \max_{\mu \in \Xi_{train}} \Delta(\mu)(\text{or} \hat{\Delta}(\mu))$;
  $\epsilon = \Delta(\hat{\mu})$;
END WHILE.

[4]

[4] Resemble the greedy algorithm for the reduced basis methods [Patera, Rozza'06]

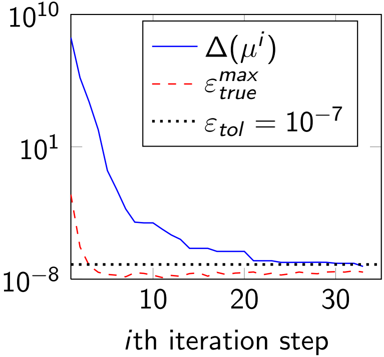
Simulation results

Example 1: A MEMS model with 4 parameters (benchmark available at `http://modlereduction.org`),

$$\begin{aligned} M(d)\ddot{x} + D(\theta,\alpha,\beta,d)\dot{x} + T(d)x &= Bu(t), \\ y &= Cx. \end{aligned}$$

Here, $M(d) = (M_1 + dM_2)$, $T(d) = (T_1 + \frac{1}{d}T_2 + dT_3)$, $D(\theta,\alpha,\beta,d) = \theta(D_1 + dD_2) + \alpha M(d) + \beta T(d) \in R^{n\times n}$, n=17,913. Parameters, d, θ, α, β.

- $\theta \in [10^{-7}, 10^{-5}]$, $s \in 2\pi\sqrt{-1} \times [0.05, 0.25]$, $d \in [1, 2]$.
- Ξ_{train}: 3 random θ, 10 random s, 5 random d, $\alpha = 0$, $\beta = 0$ [Salimbahrami et al.' 06]. Totally 150 samples of μ.



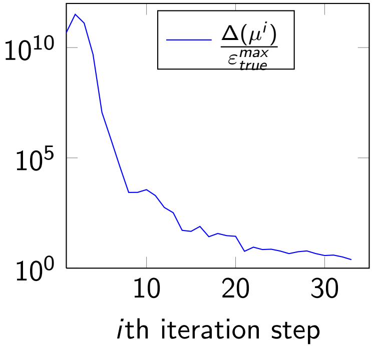


Figure : $V_{\mu^i} = span\{B_M, R_1, R_2\}_{\mu^i}$, $i = 1, \ldots, 33$. $\epsilon_{tol} = 10^{-7}$, $\varepsilon_{true}^{max} = \max_{\mu \in \Xi_{train}} |H(\mu) - \hat{H}(\mu)|$, ROM size=804.

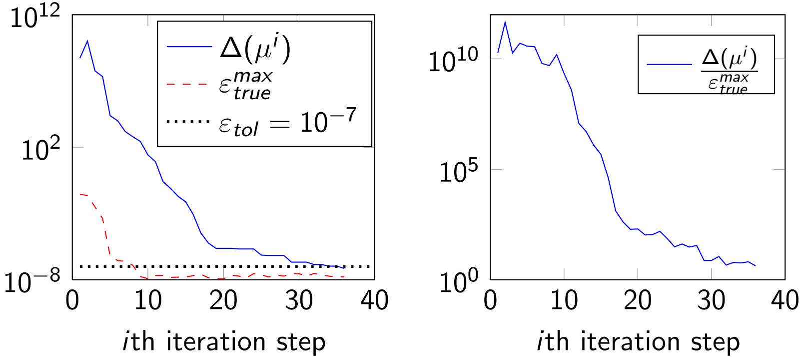


Figure : $V_{\mu^i} = span\{B_M, R_1\}_{\mu^i}$, $i = 1, \ldots, 36$. $\epsilon_{tol} = 10^{-7}$, ROM size=210.

- When $V_{\mu^i} = span\{B_M\}_{\mu^i}$, it is reduced basis method. Because $B_M(\mu^i) = [G(\mu^i)]^{-1}B = \mathbf{x}(\mu^i)$.

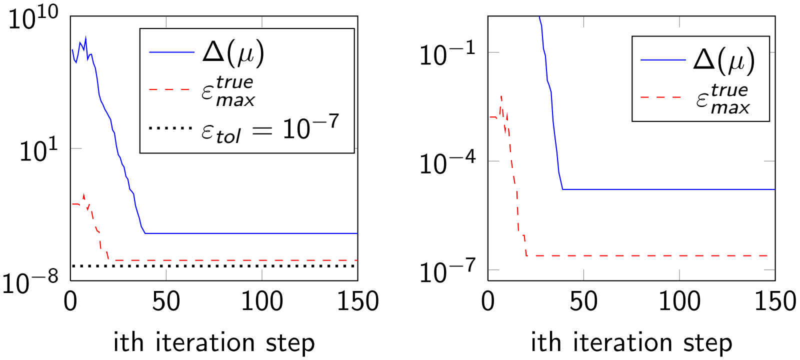


Figure : $V_{\mu^i} = span\{B_M\}_{\mu^i}$, $i = 1, \ldots, 150$. $\epsilon_{tol} = 10^{-7}$, failed.

- Case 1: $V_{\mu^i} = span\{B_M, R_1, R_2\}_{\mu^i}$.
- Case 2: $V_{\mu^i} = span\{B_M, R_1\}_{\mu^i}$.
- Case 3: $V_{\mu^i} = span\{B_M\}_{\mu^i} = span\{\mathbf{x}(\mu^i)\}$, failed.

- Ξ_{ver}: 10 random samples for d, 50 random samples for s, 5 random samples for θ. Totally 2500 samples of μ.
- $\epsilon_{true}^{max} = \max\limits_{\mu \in \Xi_{ver}} |H(\mu) - \hat{H}(\mu)|$.

Table : Verification of the final ROM on a finer sample space Ξ_{ver}.

Cases	$\Delta(\mu^{final})$	ϵ_{true}^{max}	iterations	ROM size	time
Case 1	7.4×10^{-8}	1.77×10^{-9}	33	804	1295s
Case 2	7.1×10^{-8}	1.4×10^{-9}	36	210	29s

- Ξ_{train}: the same as above. $\hat{\Delta}(\mu)$ is used instead.

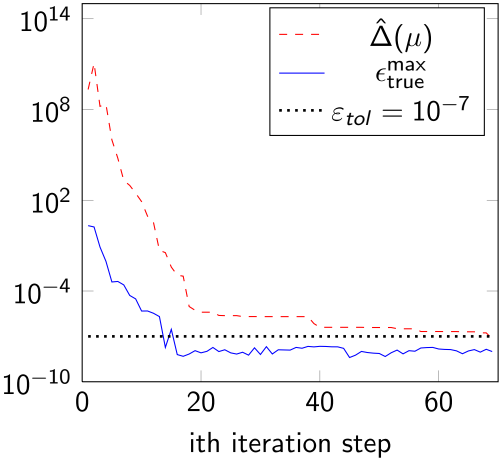


Figure : $V_{\mu^i} = span\{B_M, R_1\}_{\mu^i}$, $i = 1, \ldots, 150$. $\epsilon_{tol} = 10^{-7}$, r=243.

Example 2: a silicon nitride membrane

$$\begin{aligned}(E_0 + \rho c_p E_1) dx/dt + (K_0 + \kappa K_1 + h K_2)x &= bu(t) \\ y &= Cx.\end{aligned}$$

Here, the parameters $\rho \in [3000, 3200]$, $c_p \in [400, 750]$, $\kappa \in [2.5, 4]$, $h \in [10, 12]$, $f \in [0, 25] Hz$

Ξ_{train}: 2250 random samples have been taken for the four parameters and the frequency.

$\varepsilon^{re}_{true} = \max_{\mu \in \Xi_{train}} |H(\mu) - \hat{H}(\mu)|/|H(\mu)|$, $\hat{\Delta}^{re}(\mu) = \hat{\Delta}(\mu)/|\hat{H}(\mu)|$

Table : $V_{\mu^i = \mathrm{span}\{B_M, R_1\}}$, $\epsilon^{re}_{tol} = 10^{-2}$, $n = 60,020$, $r = 8$,

iteration	ε^{re}_{true}	$\hat{\Delta}^{re}(\mu^i)$
1	1×10^{-3}	3.44
2	1×10^{-4}	4.59×10^{-2}
3	2.80×10^{-5}	4.07×10^{-2}
4	2.58×10^{-6}	2.62×10^{-5}

- Ξ_{train}: 3 samples for κ, 10 samples for the frequency.
- Ξ_{var}: 16 samples for κ, 51 samples for the frequency.

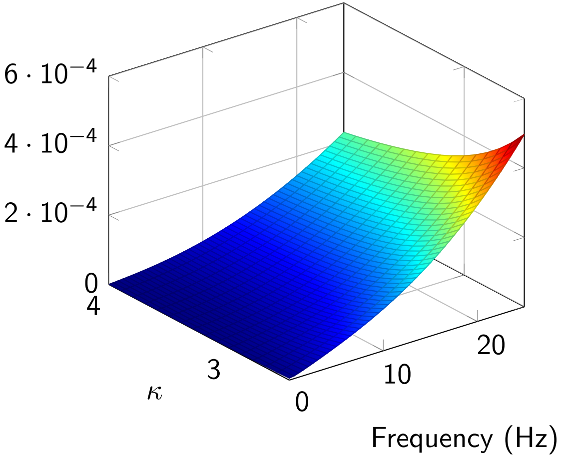


Figure : Relative error of the final ROM over Ξ_{var}.

Conclusions and future work

- An a posteriori output error bound for linear parametric systems in state space is proposed, which is free from the discretization method employed.
- The error bound enables adaptive selection of the expansion points, and in turn, automatic implementation of multi-moment-matching PMOR.
- Theoretical analysis for the approximate error bound $\hat{\Delta}(\mu)$?

Thank you for your attention!