Realification and PCC-Krylov Subspaces for Projection-Based Model Reduction

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Thanks in Advance to Pizza Seminar Attendees!

Unreduced Model

Input-Output system represented as a system of Differential Algebraic Equations (DAEs)

$$
\begin{array}{ccc}
u_1(t) \longrightarrow & & \longrightarrow y_1(t) \\
u_2(t) \longrightarrow & \boxed{\begin{aligned} Ex' &= Ax + Bu \\ y &= B^T x, \end{aligned}} & \longrightarrow y_2(t) \\
\vdots & & \vdots \\
u_p(t) \longrightarrow & & \longrightarrow y_p(t)
\end{array}
$$

where $A, E \in \mathbb{R}^{N \times N}$ are sparse (possibly singular), $B \in \mathbb{R}^{N \times p}$.

- $N \gg p$ typically large, e.g. $N = \mathcal{O}\left(10^9\right)$
- $x(t) \in \mathbb{R}^N$ represents internal state.

Reduced Order Model (ROM) via Projection

System of DAEs of the same form

$$
\begin{array}{ccccc}
u_1(t) & \longrightarrow & & \longrightarrow & y_1(t) \\
u_2(t) & \longrightarrow & \boxed{\begin{aligned} \widetilde{E}x' &= \widetilde{A}x + \widetilde{B}u \\ y &= \widetilde{B}^T x \end{aligned}} & \longrightarrow & y_2(t) \\
\vdots & & & & \vdots \\
u_p(t) & \longrightarrow & & \longrightarrow & y_p(t)
\end{array}
$$

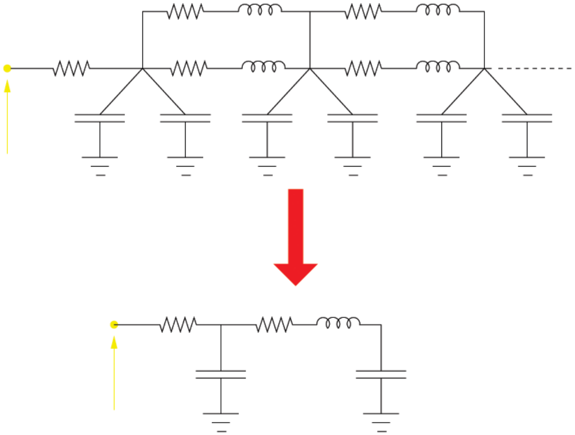
$$\widetilde{A} := V^T A V, \quad \widetilde{E} := V^T E V \quad \in \mathbb{R}^{n \times n}$$

$$\widetilde{B} := V^T \widetilde{B} \in \mathbb{R}^{n \times p},$$

with state-space dimension $n \ll N$ and $V \in \mathbb{R}^{N \times n}$ is basis for some ideal space.

Reduced Model Must Preserve Original Structure

Example: RCL circuit



Transfer Function

Relates Output directly to Input in Frequency Domain

Original system:

$$\begin{aligned} Ex' &= Ax + Bu \\ y &= B^T x. \end{aligned}$$

Applying the Laplace transform,

$$\begin{aligned} sEX &= AX(s) + BU(s) \\ Y(s) &= B^T X(s). \end{aligned}$$

In the frequency domain,

$$Y(s) = B^T (sE - A)^{-1} BU(s) \equiv H(s)U(s).$$

Transfer Function

Input $\rightarrow$ Output Map in Frequency Domain

In the frequency domain, $Y(s) = H(s)U(s)$ with transfer function

$$H(s) = B^T(sE - A)^{-1}B \quad \in \quad (\mathbb{C} \cup \infty)^{p \times p}$$

For the reduced model,

$$\widetilde{H}(s) = \widetilde{B}^T(s\widetilde{E} - \widetilde{A})^{-1}\widetilde{B} \quad \in \quad (\mathbb{C} \cup \infty)^{p \times p}$$

$\widetilde{H}(s) \approx H(s) \quad \Longleftrightarrow \quad$ 'Good' Reduced Order Model

Moment Matching

Expressed as Taylor series expansion about $s_0 \in \mathbb{C}$:

$$\text{Original:} \quad H(s) = \sum_{j=0}^{\infty} (s - s_0)^j M_j$$

$$\text{ROM:} \quad \widetilde{H}(s) = \sum_{j=0}^{\infty} (s - s_0)^j \widetilde{M}_j$$

ROM matches n moments about σ if $\widetilde{M}_j = M_j$ for $j = 1, 2, \ldots, n$.

- Padè-Type Approximant

$$\widetilde{H}(s) = H(s) + \mathcal{O}\left((s - s_0)^n\right)$$

Transfer function
Single-matrix formulation

Choose expansion point $s_0 \in \mathbb{C}$, re-write $H(s)$ as

$$\begin{aligned} H(s) &= B^T(sE - A)^{-1}B \\ &= B^T\left[(s - s_0)E + s_0E - A\right]^{-1}B \\ &= B^T\left(I - (s - s_0)H\right)^{-1}R \end{aligned}$$

(*Single matrix formulation*), where

$$H := -(s_0E - A)^{-1}E \quad \text{and} \quad R := (s_0E - A)^{-1}B.$$

We're interested in the *block-Krylov sequence*

$$R, HR, H^2R, \ldots$$

Moments of the transfer function about s_0

Via Neumann (geometric series) expansion,

$$\begin{aligned} H(s) &= B^T \left(I - (s - s_0)H\right)^{-1} R \\ &= B^T \left(\sum_{j=0}^{\infty} (s - s_0)^j H^j \right) R \\ &= \sum_{j=0}^{\infty} (s - s_0)^j B^T H^j R \end{aligned}$$

- This the Taylor series expansion of $H(s)$ about s_0.
- Block-Krylov sequence

$$R, HR, H^2R, \ldots H^jR, \ldots$$

Moment matching

...suggests n-th Block-Krylov subspace

$$\mathcal{K}_n(H,R) := \text{span}\left\{R, HR, H^2R, \ldots, H^{n-1}R\right\}.$$

For $V \in \mathbb{R}^{N\times n}$ such that

$$\mathcal{K}_n(H,R) \subseteq \text{range}\, V,$$

ROM via projection on to V matches n moments about s_0.

$$\widetilde{B}^T\widetilde{H}^j\widetilde{R} = B^T H^j R \quad \text{for} \quad j = 0, 1, 2, \ldots, n-1$$

- because $\widetilde{B}^T\widetilde{H}^j\widetilde{R} = B^T V\widetilde{H}^j\widetilde{R} = B^T H^j R$

Progressive Discovery of Krylov Space

For general $s_0 \in \mathbb{C}$,

$$H := -(s_0E - A)^{-1}E \quad \text{and} \quad R := (s_0E - A)^{-1}B$$

$$\mathcal{K}_n(H,R) := \text{span } \left\{R, HR, H^2R, \ldots, H^{n-1}R\right\} \subset \mathbb{C}^N$$

$H : \mathcal{K}_j(H,R) \to \mathcal{K}_{j+1}(H,R)$ *advances* the Krylov subspace.

- Not Real!
- We need $V \in \mathbb{R}^{N\times n}$ for which

$$\mathcal{K}_n(H,R) \subseteq \text{range}\, V.$$

Non-Real Expansion Point?

For $s_0 \in \mathbb{C}$, $H = H(s_0)$ and $R = R(s_0)$

Grimme (1997) suggested:

- Construct complex basis $V \in \mathbb{C}^{N\times\eta}$ for $\mathcal{K}_n(H,R)$
- Split V into (separate Re and Im parts)

$$V^* := \begin{bmatrix} v_1^{\mathbf{r}} & v_1^{\mathbf{i}} & v_2^{\mathbf{r}} & v_2^{\mathbf{i}} & \cdots & v_\eta^{\mathbf{r}} & v_\eta^{\mathbf{i}} \end{bmatrix} \in \mathbb{R}^{N\times 2\eta}$$

- Then,

$$\begin{aligned} \text{span}\, V^* &= \text{span}\, \mathcal{K}_n(H,R) \cup \mathcal{K}_n(\overline{H},\overline{R}) \\ &= \text{span}\, \mathcal{K}_n(H(s_0),R(s_0)) \cup \mathcal{K}_n(H(\overline{s_0}),R(\overline{s_0})) \end{aligned}$$

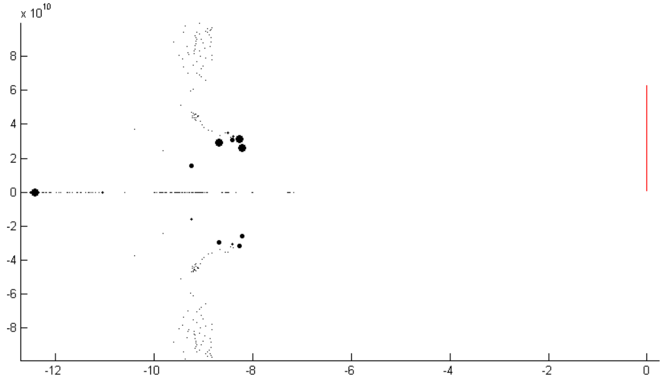
Match n moments about points s_0 and $\overline{s_0}$ simultaneously .

- $s_0 \notin \mathbb{R} \Rightarrow 2\times$ model size, $4\times$ computational cost
- Re-orthogonalize 2η vectors $v^* \in \mathbb{R}^N$? AIEEE!

Motivation for Complex Expansion Point(s)

Example Pole Distribution

Poles of transfer function $H(s) = B^T(sE - A)^{-1}B$ correspond with eigenvalues of operator H.



We want eigen-information associated with dominant poles.

Complex Split

For a set of vectors $V \in \mathbb{C}^n$, the *split* of V is

$$V^* := V^{\mathbf{r}} \cup V^{\mathbf{i}} = \{ \operatorname{Re} v \cup \operatorname{Im} v \mid v \in V \} \subset \mathbb{R}^N.$$

Similarly for a vector space $S = \operatorname{span} V$,

$$\begin{aligned} S^* &:= \operatorname{span} V^* \\ &= \operatorname{span} V^{\mathbf{r}} \cup V^{\mathbf{i}} \\ &= \operatorname{span} V \cup \overline{V} \end{aligned}$$

(spans over $\mathbb{C}$).

PCC-Krylov Subspace

Definition

Paired Complex Conjugate (PCC)-Krylov subspace induced by $H \in \mathbb{C}^{N\times N}$ and $R \in \mathbb{C}^{N}$.

$$\begin{aligned}\mathcal{K}_n(H,R)^* &= \text{span}\,\mathcal{K}_n(H,R)\ \cup\ \mathcal{K}_n(\overline{H},\overline{R})\\ &= \text{span}\ \left\{ R, \overline{R}, HR, \overline{HR}, H^2R, \overline{H^2R}, \ldots, H^{n-1}R, \overline{H^{n-1}R} \right\}\end{aligned}$$

Equivalent Real Formulation

Definition

Realification functor on $\mathbb{C}^N$ (Arnol'd,1992).

$$^{\mathbb{R}}\mathbb{C}^N = \mathbb{R}^{2N}$$

$$x + iy \in \mathbb{C}^N \quad \longleftrightarrow \quad \begin{bmatrix} x \\ y \end{bmatrix} \in \mathbb{R}^{2N}$$

For general $\{v_1, v_2, \ldots, v_n\}$,

$$^{\mathbb{R}}\left\{ \sum a_j v_j \,\middle|\, a_j \in \mathbb{C} \right\} = \left\{ \sum a_j v_j \,\middle|\, a_j \in \mathbb{R} \right\}.$$

- Similarly, *complexification* $^{\mathbb{C}}(^{\mathbb{R}}\mathbb{C}^N) = \mathbb{C}^N$

Equivalent Real Formulation

For operator matrix $H \in \mathbb{C}^{N\times N}$ and vector(s) $v \in \mathbb{C}^N$,

$$\widehat{H} = \begin{bmatrix} H^{\mathbf{r}} & -H^{\mathbf{i}} \\ H^{\mathbf{i}} & H^{\mathbf{r}} \end{bmatrix} \in \mathbb{R}^{2N\times 2N} \quad \text{and} \quad \hat{v} = \begin{bmatrix} v^{\mathbf{r}} \\ v^{\mathbf{i}} \end{bmatrix} \in \mathbb{R}^{2N}.$$

$w = \begin{bmatrix} w^{\mathbf{t}} \\ w^{\mathbf{b}} \end{bmatrix} \in {}^{\mathbb{R}}\mathbb{C}^N$ has *top* and *bottom* parts in $\mathbb{R}^N$.

Define the split of $W \subseteq {}^{\mathbb{R}}\mathbb{C}^N$ as

$$W^* := W^{\mathbf{t}} \cup W^{\mathbf{b}} = \left\{ w^{\mathbf{t}} \cup w^{\mathbf{b}} \;\middle|\; w \in W \right\} \subset \mathbb{R}^N.$$

Recall the Krylov subspace (over $\mathbb{C}$)

$$\mathcal{K}_n(H,R) := \text{span}\,\{R, HR, H^2R, \ldots, H^{n-1}R\} \subset \mathbb{C}^N.$$

Operator $\widehat{H}$, initial vector block $\widehat{R}$ yield (over $\mathbb{R}$)

$$\mathcal{K}_n(\widehat{H},\widehat{R}) := \text{span}\,\left\{\widehat{R}, \widehat{H}\widehat{R}, \widehat{H}^2\widehat{R}, \ldots, \widehat{H}^{n-1}\widehat{R}\right\} \subset \mathbb{R}^{2N}.$$

Computing basis $\widehat{V}$ for $\mathcal{K}_n(\widehat{H},\widehat{R})$ cuts cost in half.

- Why? Inner product in $\mathbb{R}^{2N}$ vs. $\mathbb{C}^N$

Non-Equivalent Bases Yield The Same Split

Bases V and $\widehat{V}$ of these isomorphic Krylov subspaces

$$\operatorname{span} V = \mathcal{K}_n(H, R) \subset \mathbb{C}^N$$
$$\operatorname{span} \widehat{V} = \mathcal{K}_n(\widehat{H}, \widehat{R}) \subset {}^{\mathbb{R}}\mathbb{C}^N$$

are not equivalent: ${}^{\mathbb{R}}V \neq \widehat{V}$ in general, but their splits

$$\operatorname{span} V^* = \operatorname{span} \widehat{V}^* = \mathcal{K}_n(H, R)^* \subset \mathbb{R}^N$$

both span the same PCC-Krylov subspace.

- This follows from

$$^{\mathbb{R}}(\cdot) : H^j R \leftrightarrow \widehat{H}^j \widehat{R}.$$

Concluding Remarks

- PCC-Krylov subspace is a complex space containing two complex conjugate Krylov subspaces and admits a real basis.
- Realified Krylov subspaces are cheaper to work with and ideal for methods implementing the general complex expansion point.