Krylov Subspaces and Their Application to Model Order Reduction

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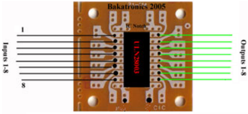


Basic Linear Algebra

Take $H \in \mathbb{C}^{N \times N}$ and $r \in \mathbb{C}^N$. The matrix-vector product

$$Hr \in \mathbb{C}^N$$

is a vector.
Example in $\mathbb{R}^3$:

$$\underbrace{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 7 & 3 \end{bmatrix}}_{H} \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}}_{r} = \begin{bmatrix} 6 \\ 15 \\ 12 \end{bmatrix}$$

Basic Linear Algebra

Take $H \in \mathbb{C}^{N \times N}$ and *block* $R \in \mathbb{C}^{N \times p}$. The product

$$HR \in \mathbb{C}^{N \times p}$$

is an $N \times p$ block.
Example in $\mathbb{R}^3$:

$$\underbrace{\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 7 & 3 \end{bmatrix}}_{H} \underbrace{\begin{bmatrix} 1 & 3 \\ 1 & 2 \\ 1 & 1 \end{bmatrix}}_{R} = \begin{bmatrix} 6 & 10 \\ 15 & 28 \\ 12 & 23 \end{bmatrix}$$

Krylov Sequence

Successive applications of operator H to a start vector r

$$r, Hr, HHr, HHHr, \ldots$$

result in the *Krylov sequence*

$$r, Hr, H^2 r, H^3 r, \ldots$$

Krylov Sequence

Example:

- $$\underbrace{\begin{bmatrix}1 & 2 & 3\\ 4 & 5 & 6\\ 2 & 7 & 3\end{bmatrix}}_{H}\underbrace{\begin{bmatrix}1\\ 1\\ 1\end{bmatrix}}_{r} = \begin{bmatrix}6\\ 15\\ 12\end{bmatrix}$$
- $$H^2 r = \begin{bmatrix}1 & 2 & 3\\ 4 & 5 & 6\\ 2 & 7 & 3\end{bmatrix}\begin{bmatrix}6\\ 15\\ 12\end{bmatrix} = \begin{bmatrix}72\\ 171\\ 153\end{bmatrix}$$
- $$H^3 r = \begin{bmatrix}1 & 2 & 3\\ 4 & 5 & 6\\ 2 & 7 & 3\end{bmatrix}\begin{bmatrix}72\\ 171\\ 153\end{bmatrix} = \begin{bmatrix}873\\ 2061\\ 1800\end{bmatrix}$$

Krylov Sequence

The Krylov sequence induced by H and r is

$$\underbrace{\begin{bmatrix}1\\1\\1\end{bmatrix}}_{r}, \underbrace{\begin{bmatrix}6\\15\\12\end{bmatrix}}_{Hr}, \underbrace{\begin{bmatrix}72\\171\\153\end{bmatrix}}_{H^2 r}, \underbrace{\begin{bmatrix}873\\2061\\1800\end{bmatrix}}_{H^3 r}, \underbrace{\begin{bmatrix}10395\\24597\\21573\end{bmatrix}}_{H^4 r}, \ldots \in \mathbb{R}^3$$

Krylov Subspace
Example

The 3rd *Krylov subspace* induced by H and r:

$$\mathcal{K}_3(H, r) = \text{span}\left\{r, Hr, H^2 r\right\}$$

All of the following are in $\mathcal{K}_3(H, r)$

- r
- $H^2 r + 2Hr$
- $r + 3Hr + 5H^2 r$

In fact,

$$c_0 r + c_1 Hr + c_2 H^2 r \quad \text{for any} \quad c_0, c_1, c_2 \in \mathbb{C}$$

Krylov Subspace

For $H \in \mathbb{C}^{N\times N}$ and $r \in \mathbb{C}^N$,

- Biggest possible Krylov subspace is N-th

$$\mathcal{K}_N(H,r) = \text{span}\left\{r, Hr, H^2r, \ldots, H^{N-1}r\right\} \subseteq \mathbb{C}^N$$

Example: Recall in $\mathbb{R}^3$

$$H = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 7 & 3 \end{bmatrix}, \quad r = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Krylov sequence is

$$\underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}}_{r}, \underbrace{\begin{bmatrix} 6 \\ 15 \\ 12 \end{bmatrix}}_{Hr}, \underbrace{\begin{bmatrix} 72 \\ 171 \\ 153 \end{bmatrix}}_{H^2r}, \underbrace{\begin{bmatrix} 873 \\ 2061 \\ 1800 \end{bmatrix}}_{H^3r}, \ldots$$

$$H = \begin{bmatrix} -4.8 & 10.6 & -3.8 \\ -5.8 & 11.6 & -3.8 \\ -6.7 & 12.4 & -3.7 \end{bmatrix}, \quad z = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Multiply:

$$\begin{bmatrix} -4.8 & 10.6 & -3.8 \\ -5.8 & 11.6 & -3.8 \\ -6.7 & 12.4 & -3.7 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 2 \end{bmatrix}$$

- $Hz = 2z$
- $(2, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix})$ is an eigen-pair of H.

Krylov sequence induced by H and z is

$$\underbrace{\begin{bmatrix}1\\1\\1\end{bmatrix}}_{z}, \underbrace{\begin{bmatrix}2\\2\\2\end{bmatrix}}_{2z}, \underbrace{\begin{bmatrix}4\\4\\4\end{bmatrix}}_{4z}, \underbrace{\begin{bmatrix}8\\8\\8\end{bmatrix}}_{8z}, \ldots, \underbrace{\begin{bmatrix}2^j\\2^j\\2^j\end{bmatrix}}_{2^j z}, \ldots$$

- $\mathcal{K}_n(H, z) = \text{span}\{z\} = \text{span}\left\{\begin{bmatrix}1\\1\\1\end{bmatrix}\right\}$ for any n.
- *Invariant Subspace* with respect to H
- Eigenspace

$$\left(\frac{1}{2}, \begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix}\right) \quad \text{is another eigen-pair of } H$$

$$\begin{bmatrix} -4.8 & 10.6 & -3.8 \\ -5.8 & 11.6 & -3.8 \\ -6.7 & 12.4 & -3.7 \end{bmatrix} \begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1.5 \end{bmatrix}$$

Krylov sequence:

$$\begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \\ 0.75 \end{bmatrix}, \begin{bmatrix} 0.25 \\ 0.25 \\ 0.375 \end{bmatrix}, \ldots, \begin{bmatrix} 2 \cdot 2^{-j} \\ 2 \cdot 2^{-j} \\ 3 \cdot 2^{-j} \end{bmatrix}, \ldots$$

Invariance
Example

$$H = \begin{bmatrix} -4.8 & 10.6 & -3.8 \\ -5.8 & 11.6 & -3.8 \\ -6.7 & 12.4 & -3.7 \end{bmatrix}$$

- Eigenvalues of H are 2, $\frac{1}{2}$, (and 1)
- 2 is the *dominant eigenvalue*, with eigenvector $z_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$

Krylov Sequence Convergence

Sequence usually converges to the dominant eigenvector

- 2 is the *dominant eigenvalue* of H, with eigenvector $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$
- Generate a Krylov sequence with H and *almost* any start vector r. Say,

$$r = \begin{bmatrix} 0 \\ -1 \\ -4 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}}_{z_1} \underbrace{- 2 \begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix}}_{2z_2} + \underbrace{\begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}}_{z_3}$$

Krylov Sequence Convergence

Sequence usually converges to the dominant eigenvector

- 2 is the *dominant eigenvalue* of H, with eigenvector $\begin{bmatrix}1\\1\\1\end{bmatrix}$
- Generate a Krylov sequence with H and *almost* any start vector r.

$$Hr = H\begin{bmatrix}0\\-1\\-4\end{bmatrix} = \underbrace{H\begin{bmatrix}1\\1\\1\end{bmatrix}}_{Hz_1} - \underbrace{2H\begin{bmatrix}2\\2\\3\end{bmatrix}}_{2Hz_2} + \underbrace{H\begin{bmatrix}3\\2\\1\end{bmatrix}}_{Hz_3}$$

Krylov Sequence Convergence

Sequence usually converges to the dominant eigenvector

- 2 is the *dominant eigenvalue* of H, with eigenvector $\begin{bmatrix}1\\1\\1\end{bmatrix}$
- Generate a Krylov sequence with H and *almost* any start vector r.

$$Hr = \begin{bmatrix}3\\2\\0\end{bmatrix} = \underbrace{\begin{bmatrix}2\\2\\2\end{bmatrix}}_{2z_1} - \underbrace{\begin{bmatrix}2\\2\\3\end{bmatrix}}_{2\cdot\frac{1}{2}z_2} + \underbrace{\begin{bmatrix}3\\2\\1\end{bmatrix}}_{z_3}$$

Krylov Sequence Convergence

Compute $r, Hr, H^2r, H^3r, \ldots$:

$$\begin{bmatrix} 0 \\ -1 \\ -4 \end{bmatrix}, \begin{bmatrix} 3 \\ 2 \\ 0 \end{bmatrix}, \begin{bmatrix} 6 \\ 5 \\ 3.5 \end{bmatrix}, \ldots, \underbrace{\begin{bmatrix} 1027 \\ 1026 \\ 1025 \end{bmatrix}}_{H^{10}r}, \ldots$$

Converges to a multiple of $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ (dominant eigenvector) quickly.

Krylov Sequence Convergence

Actually, power iterations compute

$$v_1 = \frac{r}{\|r\|}, \quad v_2 = \frac{Hv_1}{\|Hv_1\|} = \frac{H^2 r}{\|H^2 r\|}, \quad v_3 = \frac{Hv_2}{\|Hv_2\|} = \frac{H^3 r}{\|H^3 r\|}, \quad \ldots$$

$$\underbrace{\begin{bmatrix} 0 \\ -0.2425 \\ -0.9701 \end{bmatrix}}_{v_1}, \underbrace{\begin{bmatrix} 0.8321 \\ 0.5547 \\ 0 \end{bmatrix}}_{v_2}, \underbrace{\begin{bmatrix} 0.701 \\ 0.5842 \\ 0.4089 \end{bmatrix}}_{v_3}, \ldots, \underbrace{\begin{bmatrix} 0.5779 \\ 0.5774 \\ 0.5768 \end{bmatrix}}_{v_{10}}, \ldots$$

Krylov Sequence Convergence

Using Power Iterations:

Computing basis for

$$\mathcal{K}_n(H, r) = \text{span}\{r, Hr, H^2r, \ldots, H^{n-1}r\}$$

using finite precision arithmetic

- We quickly get stuck at the dominant eigenvector after a few iterations!
- (Useful for eigenvalue computation though)

Krylov Sequence Convergence

In general, for $H \in \mathbb{C}^{N \times N}$ with

- N eigenvalues $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_N|$
- eigenvectors $z_1, z_2, \ldots, z_N$,

For any start vector $r \in \mathbb{C}^N$

$$\begin{aligned} H^k r &= H^k \left(a_1 z_1 + a_2 z_2 + \cdots + a_k z_k\right) \\ &= a_1 \lambda_1^k \left(z_1 + \sum \frac{a_j}{a_1} \left(\frac{\lambda_j}{\lambda_1} \right)^k z_j \right) \end{aligned}$$

Basis for $\mathcal{K}_n(H, r)$

Assuming we don't get stuck in an invariant subspace, Krylov vectors

$$\{r, Hr, H^2 r, H^3 r, \ldots, H^{n-1} r\}$$

- Are linearly independent, and span $\mathcal{K}_n(H, r)$
- Form a bad basis for $\mathcal{K}_n(H, r)$

Arnoldi process computes orthogonal basis matrix $V_n = [v_1\, v_2 \ldots v_n]$ for Krylov subspace $\mathcal{K}_n(H, r)$:

- $v_1 = r/\|r\|$
- $v_2 = (Hv_1$ orthogonalized against $v_1)$

  $\vdots$
- $v_n = (Hv_{n-1}$ orthogonalized against $\{v_1, v_2, \ldots, v_{n-1}\})$

Arnoldi Process

Computationally expensive for large N

The n-th iteration of Arnoldi

$$\begin{aligned} v_{n+1} &\approx (Hv_n \text{ orthogonalized against } \{v_1, v_2, \ldots, v_n\}) \\ &= Hv_n - \alpha_1 v_1 - \alpha_2 v_2 - \cdots - \alpha_n v_n \end{aligned}$$

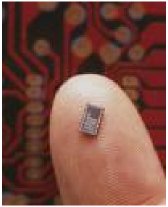
where

$$\alpha_j = \frac{v_j^H v_n}{\|v_j\|}$$

For large N ($\approx 10^6$)

- computing each α_j requires $\approx 2N$ scalar multiplications & additions.
- Computing $v_n \in \mathbb{C}^N$ grinds to a halt with increasing n !

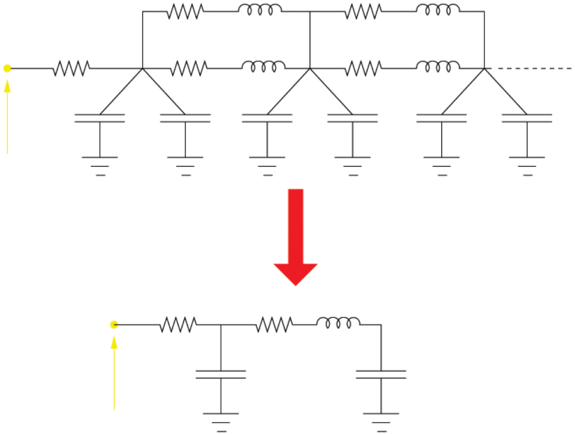
Application: RCL Circuit Simulation



- Why simulate a circuit?

VLSI Circuit Model Reduction

Example: RCL circuit



Circuit Equations

(You Don't Need To Understand This!!)

Equations determining any circuit determined via

- Kirchhoff's current and voltage laws (KCLs, KVLs)
- Branch Constitutive Relations (BCRs)

KCLs, KVLs of the circuit can be stated as

$$\mathcal{A} i_\varepsilon = 0 \quad \text{and} \quad \mathcal{A}^T v = v_\varepsilon$$

with *incidence matrix*

$$\mathcal{A} = \begin{bmatrix} \mathcal{A}_r & \mathcal{A}_c & \mathcal{A}_l & \mathcal{A}_v & \mathcal{A}_i \end{bmatrix},$$

and *current, voltage* vectors

$$i_\varepsilon = \begin{bmatrix} i_r \\ i_c \\ i_l \\ i_v \\ i_i \end{bmatrix}, v_\varepsilon = \begin{bmatrix} v_r \\ v_c \\ v_l \\ v_v \\ v_i \end{bmatrix}.$$

Circuit Equations

(You Don't Need To Understand This!!)

Equations determining any circuit determined via

- Kirchhoff's current and voltage laws (KCLs, KVLs)
- Branch Constitutive Relations (BCRs)

BCRs of the circuit can be stated as

$$v_r(t) = Ri_r(t), \quad i_c(t) = C\frac{d}{dt}v_c(t), \quad v_l(t) = L\frac{d}{dt}i_l(t)$$

- R, C, and L are diagonal matrices containing resistances, capacitances, inductances of components

Then we formulate *Realization* of the circuit:

Block matrices

$$A = \begin{bmatrix} A_{11} & -\mathcal{A}_l & -\mathcal{A}_v \\ \mathcal{A}_l^T & 0 & 0 \\ A_v^T & 0 & 0 \end{bmatrix}, \quad E = \begin{bmatrix} E_{11} & 0 & 0 \\ 0 & L & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} \mathcal{A}_i & 0 \\ 0 & 0 \\ 0 & -I \end{bmatrix},$$

where

$$A_{11} = -\mathcal{A}_r R^{-1} \mathcal{A}_r^T \quad \text{and} \quad E_{11} = \mathcal{A}_c C \mathcal{A}_c^T.$$

- $A, E \in \mathbb{R}^{N \times N}$ and $B \in \mathbb{R}^{N \times p}$ sparse, large ($N > 10^6$).
- Any A, E, B having this structure determine a RCL circuit.

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

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

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

- $u(t), y(t) \in \mathbb{R}^p$ input,output vectors
- $x(t) \in \mathbb{R}^N$ represents internal state space (to be reduced).
- *Behavior* of model: $y(t) = F(u(t))$

Reduced Order Model (ROM) via Projection

System of DAEs of the same form

$$
\begin{array}{lcc|c|cc}
u_1(t) & \longrightarrow & & & \longrightarrow & y_1(t) \\
u_2(t) & \longrightarrow & & E_n x' = A_n x + B_n u & \longrightarrow & y_2(t) \\
\vdots & & & y = B_n^T x & & \vdots \\
u_p(t) & \longrightarrow & & & \longrightarrow & y_p(t)
\end{array}
$$

$$A_n := V_n^T A V_n, \quad E_n := V_n^T E V_n \quad \in \mathbb{R}^{n \times n}$$

$$B_n := V_n^T B_n \in \mathbb{R}^{n \times p},$$

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

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,

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

In the frequency domain,

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

Transfer Function

Relates Output directly to Input

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

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

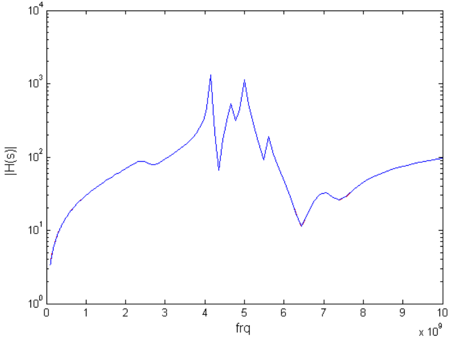
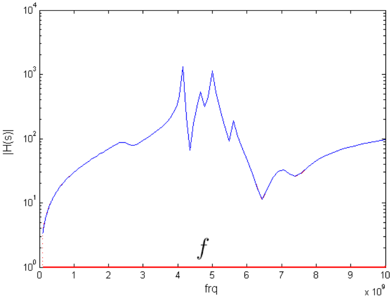
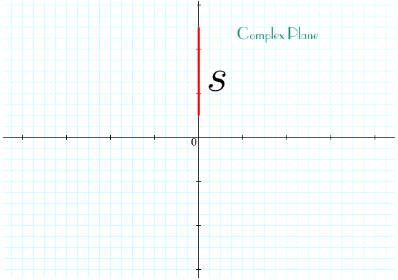


Figure: $\|H(s)\|$ vs. frequency for $N = 1841$ test model

We consider $H(s)$ over $s \in S$.

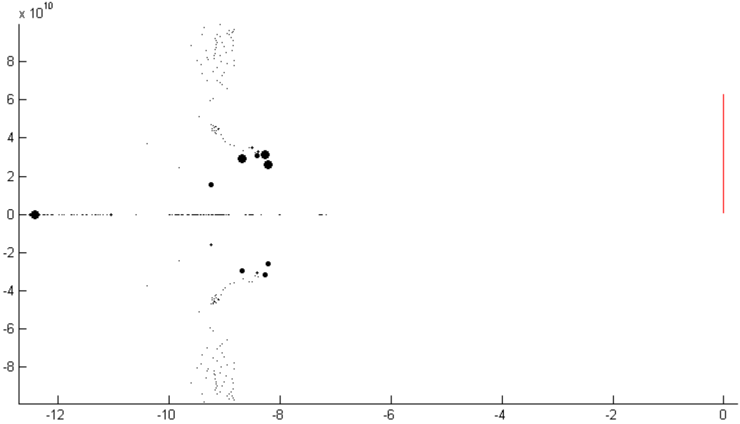
$$S = 2\pi i f, \quad f \in [f_{\min}, f_{\max}]$$





Pole decomposition of model

Example: poles of a size $N = 1841$ test model



$\log_{10}$ scale on Re axis. Dot size indicates dominance.

Transfer Function

Input → 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,

$$H_n(s) = B_n^T(sE_n - A_n)^{-1}B_n \quad \in \quad (\mathbb{C} \cup \infty)^{p \times p}$$

$H_n(s) \approx H(s) \quad \Longleftrightarrow \quad$ 'Good' Reduced Order Model

Local Convergence of ROM

Reduced order transfer function

$$H_n(s) = B_n^T(sE_n - A_n)^{-1}B_n$$

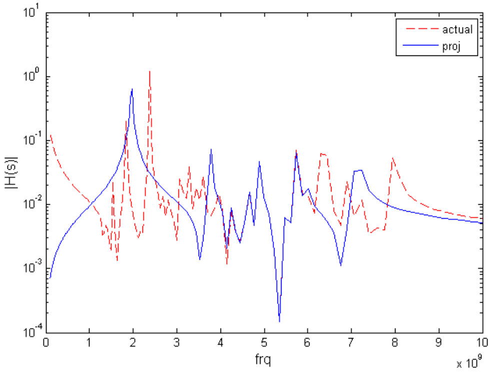


Figure: $\|H_{15}(s)\|$ converges near placement of s_0

Moment Matching

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

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

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

ROM matches n moments about s_0 if $\widetilde{M}_j = M_j$ for $j = 0, 1, \ldots, n-1$.

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

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

(*Single matrix formulation*), where

$$H := -(s_0 E - A)^{-1} E \quad \text{and} \quad R := (s_0 E - A)^{-1} B.$$

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.
- Recall Block-Krylov sequence

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

Moment matching

...suggests n-th Block-Krylov subspace

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

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.

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

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

Reduced Order Model (ROM) via Projection

System of DAEs of the form

$$\begin{array}{ccccc} u_1(t) & \longrightarrow & & \longrightarrow & y_1(t) \\ u_2(t) & \longrightarrow & E_n x' = A_n x + B_n u & \longrightarrow & y_2(t) \\ \vdots & & y = B_n^T x & & \vdots \\ u_p(t) & \longrightarrow & & \longrightarrow & y_p(t) \end{array}$$

$$A_n := V_n^T A V_n, \quad E_n := V_n^T E V_n \quad \in \mathbb{R}^{n \times n}$$

$$B_n := V_n^T B_n \in \mathbb{R}^{n \times p},$$

with $n \ll N$ and $V_n \in \mathbb{R}^{N \times \eta}$ such that

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

How Much Reduction Possible?

Experimentally, on the order of $2\aleph_0$

- But this can be improved. (current ongoing research)

The End

Thanks a lot SJSU Math!

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UNIVERSITY