MODEL REDUCTION BY A CROSS-GRAMIAN APPROACH FOR DATA-SPARSE SYSTEMS

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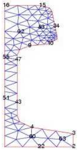
Outline

Balancing-related model reduction
by a data-sparse cross-Gramian approach

- Large-scale systems
- Model reduction - cross-Gramian approach
- The sign function method
- $\mathcal{H}$-matrix implementation
- Numerical results

$$\begin{aligned} \frac{d}{dt}x(t) &= Ax(t) + Bu(t), \quad x(0) = x_0, \\ y(t) &= Cx(t), \end{aligned}$$



where $x(t) \in \mathbb{R}^n, u(t) \in \mathbb{R}^m, y(t) \in \mathbb{R}^p$.

Assumptions on $(A, B, C, D) \in \mathbb{R}^{n \times n} \times \mathbb{R}^{n \times m} \times \mathbb{R}^{p \times n} \times \mathbb{R}^{p \times p}$:

- A asymptotically stable, i.e. $\lambda(A) \subset \mathbb{C}^-$
- large-scale, e.g. $n = \mathcal{O}(10^5)$, and $n \gg m, p$
- controllable and observable

We consider large-scale systems arising from control problems for instationary PDEs semi-discretized by FEM, FDM or BEM.

Model reduction - main issues

Find a reduced-order model of order $r \ll n$

$$\begin{aligned} \frac{d}{dt}\hat{x}(t) &= \hat{A}\hat{x}(t) + \hat{B}u(t), \quad \hat{x}(0) = \hat{x}_0 \\ \hat{y}(t) &= \hat{C}\hat{x}(t) + Du(t), \quad t \geq 0 \end{aligned}$$

- $(\hat{A}, \hat{B}, \hat{C}, D) \in \mathbb{R}^{r \times r} \times \mathbb{R}^{r \times m} \times \mathbb{R}^{p \times r} \times \mathbb{R}^{p \times p}$
- $\hat{A}$ is asymptotically stable
- small error $\|G - \hat{G}\|_\infty$,

$$\|y - \hat{y}\|_2 \leq \|G - \hat{G}\|_\infty \|u\|_2,$$

where

$$\begin{aligned} G(s) &= C(sI_n - A)^{-1}B + D, \\ \hat{G}(s) &= \hat{C}(sI_r - \hat{A})^{-1}\hat{B} + D. \end{aligned}$$

Balanced truncation computes reduced order system

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

where $V,\, W \in \mathbb{R}^{n \times r}$ are computed from T which diagonalizes controllability Gramian $\mathcal{P}$ and observability Gramian $\mathcal{Q}$:

$$T\mathcal{P}T^T = T^{-T}\mathcal{Q}T^{-1} = \mathrm{diag}(\sigma_1, \cdots, \sigma_n), \quad \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$$

$V,\, W$ can be computed by $\quad w_k^T (\mathcal{P}\mathcal{Q})\, v_k = \sigma_k^2, \quad k = 1, \ldots, r$

1. $\lambda(\hat{A}) \subset \mathbb{C}^-$
2. $\|y - \hat{y}\|_2 \leq \|G - \hat{G}\|_\infty \|u\|_2 \leq 2 \sum_{k=r+1}^{n} \sigma_k \, \|u\|_2$

System Gramians

Controllability Gramian $\mathcal{P}$ and observability Gramian $\mathcal{Q}$ defined by

$$\mathcal{P} = \int_0^\infty e^{At} BB^T e^{A^T t} dt, \quad \mathcal{Q} = \int_0^\infty e^{A^T t} CC^T e^{At} dt.$$

Gramians equivalently given by solutions of Lyapunov equations

$$A\mathcal{P} + \mathcal{P}A^T + BB^T = 0, \qquad A^T\mathcal{Q} + \mathcal{Q}A + C^T C = 0$$

Thus, main computational task in balanced truncation:

Compute solutions of large-scale matrix equations!

Model reduction - cross-Gramian approach

Define the cross-Gramian X for square systems ($m = p$) by

$$AX + XA + BC = 0$$

and project the system onto the dominant invariant subspace of X corresponding to r largest eigenvalues.

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If

- system is SISO $(p = m = 1)$ [*Fernando/Nicholson 83*] or
- symmetric MIMO [*Laub/Silverman/Verma 83, Fernando/Nicholson 84*].

then

$$X^2 = \mathcal{P}\mathcal{Q} \text{ and } \sigma_k = |\lambda_k(X)|.$$

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Model order reduction with cross-Gramian:

Aldhaheri 91, Antoulas/Sorensen 00

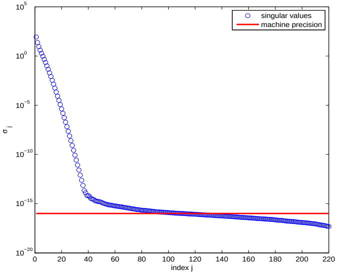
Sylvester equation $AX + XA + BC = 0$

In many situations: $\mathrm{rank}(X, \tau) = n_\tau \ll n$,
e.g. $n_\tau = \mathcal{O}(\log(1/\tau)\log(n))$ [*Grasedyck 04*].

Compute low-rank factors of X:

$$X \approx YZ, \quad Y \in \mathbb{R}^{n \times n_\tau}, \quad Z \in \mathbb{R}^{n_\tau \times n}.$$

- low-rank ADI [*Benner 05*] analogous to [*Penzl 00, Li/White 02*]
- implicitly restarted method [*Antoulas/Sorensen 00*]
- multigrid method [*Grasedyck/Hackbusch 04*]
- sign function method [*Benner 04, B. 05*]



Sign function method in factored form

Newton iteration for the solution $X \approx YZ$ of $AX + XA + BC = 0$:

$$
\begin{array}{llrcllr}
(1) & A_0 = A & A_{k+1} & = & \frac{1}{2}(A_k + A_k^{-1}) & \rightarrow & -I_n \\
(2) & B_0 = B & B_{k+1} & = & \frac{1}{\sqrt{2}}\left[\, B_k,\ A_k^{-1}B_k \,\right] & \rightarrow & \sqrt{2}Y \\
(3) & C_0 = C & C_{k+1} & = & \frac{1}{\sqrt{2}}\left[\begin{array}{c} C_k \\ C_k A_k^{-1} \end{array}\right] & \rightarrow & \sqrt{2}Z
\end{array}
$$

Complexity:

(1): $\mathcal{O}(n^3)$ $\Rightarrow$ hierarchical matrices

Storage:

$(1): \quad A_k \in \mathbb{R}^{n\times n}$ $\Rightarrow$ *hierarchical matrices*

$(2)+(3): \quad B_k \in \mathbb{R}^{n\times 2^k p}, \ C_k \in \mathbb{R}^{2^k m\times n}$ $\Rightarrow$ *row compression*

Sign function method - row compression

In each Newton step compute:

1. Compute RRQR $\begin{bmatrix} C_k \\ C_k A_k^{-1} \end{bmatrix} = U \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} \pi_C$

   $R_{11} \in \mathbb{R}^{s \times s}$, $s = \mathrm{rank}(C_{k+1}, \tau)$

2. Compute RRLQ $\begin{bmatrix} B_k, & A_k^{-1} B_k \end{bmatrix} U = \pi_B \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} V$

   $L_{11} \in \mathbb{R}^{t \times t}$, $t = \mathrm{rank}(B_{k+1}, \tau)$

3. Partition V: $V_{11} \in \mathbb{R}^{t \times s}$

4. If $(t < s)$

   $B_{j+1} \leftarrow \frac{1}{\sqrt{2}} \pi_B \begin{bmatrix} L_{11} \\ L_{21} \end{bmatrix}$, $C_{j+1} \leftarrow \frac{1}{\sqrt{2}} V_{11} [R_{11} \;\; R_{12}] \pi_C$

   else $B_{j+1} \leftarrow \frac{1}{\sqrt{2}} \pi_B \begin{bmatrix} L_{11} \\ L_{21} \end{bmatrix} V_{11}$, $C_{j+1} \leftarrow \frac{1}{\sqrt{2}} [R_{11} \;\; R_{12}] \pi_C$

$$\frac{1}{\sqrt{2}} B_k \rightarrow Y \in \mathbb{R}^{n \times n_\tau} \qquad \frac{1}{\sqrt{2}} C_k \rightarrow Z \in \mathbb{R}^{n_\tau \times n}$$

$\mathcal{H}$-matrices [Hackbusch 98]

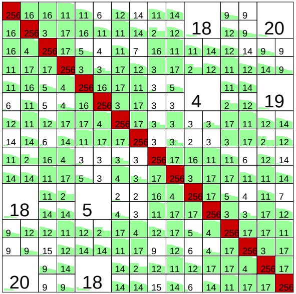
$\mathcal{H}$-matrices provide data-sparse representation for certain densely populated matrices (FEM^{-1}, BEM, ...).

- hierarchy of blocks, approximation by matrices of rank $k(\epsilon)$
- approximation error:

$$\frac{\|A - A_{\mathcal{H}}\|_2}{\|A\|_2} \leq \epsilon$$

- storage for $A_{\mathcal{H}} \in \mathbb{R}^{n \times n}$: $\mathcal{O}(n \log_2(n)\, k(\epsilon))$
- formatted arithmetic with complexity:

$$\begin{aligned} Ax \quad &: \quad \mathcal{O}(n \log_2(n)\, k(\epsilon)) \\ \oplus \quad &: \quad \mathcal{O}(n \log_2^2(n)\, k(\epsilon)) \\ \odot, \mathrm{Inv}_{\mathcal{H}} \quad &: \quad \mathcal{O}(n \log_2^2(n)\, k(\epsilon)^2) \end{aligned}$$



Blockwise SVD of $A_{\mathcal{H}}$, $n = 4096$, $\epsilon = 10^{-4}$.

Newton iteration for the solution $X \approx YZ$ of $AX + XA + BC = 0$:

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\begin{array}{llllll}
(1) & A_0 = A_{\mathcal{H}} & A_{k+1} & = & \frac{1}{2}(A_k \oplus \mathrm{Inv}_{\mathcal{H}}(A_k)) & \rightarrow & -I_n \\
(2) & B_0 = B & B_{k+1} & = & \frac{1}{\sqrt{2}}\,[\,B_k,\ \mathrm{Inv}_{\mathcal{H}}(A_k)B_k\,] & \rightarrow & \sqrt{2}Y \\
(3) & C_0 = C & C_{k+1} & = & \frac{1}{\sqrt{2}}\left[\begin{array}{c} C_k \\ C_k\mathrm{Inv}_{\mathcal{H}}(A_k) \end{array}\right] & \rightarrow & \sqrt{2}Z
\end{array}
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Complexity:

(1): $\mathcal{O}(n\,\log_2^2(n)\,k(\epsilon)^2)$ $\Rightarrow$ hierarchical matrices

Storage:

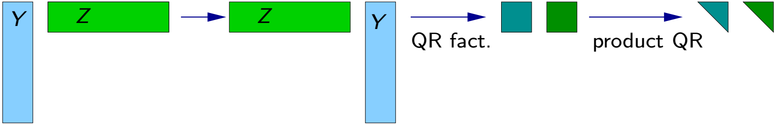
$$
\begin{array}{rll}
(1): & A_k : \mathcal{O}(n\,\log_2(n)\,k(\epsilon)) & \Rightarrow \ \textit{hierarchical matrices} \\
(2)+(3): & B_k \in \mathbb{R}^{n\times n_\tau},\ C_k \in \mathbb{R}^{n_\tau \times n} & \Rightarrow \ \textit{row compression}
\end{array}
$$

Model order reduction with cross-Gramian

Compute basis of dominant invariant subspace of $X \approx YZ$

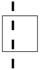
$$W^T X V = T \quad \text{with } \lambda(T) = \{\sigma_1, \cdots, \sigma_r\}$$

1. Compute basis $\tilde{V}$ of right invariant subspace of ZY



$\Rightarrow$ basis of right dominant invariant subspace of YZ:

$$V = Y\tilde{V}(:, 1:r)$$



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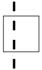
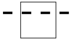


2. Compute basis $\tilde{W}$ of left invariant subspace of ZY
   $\Rightarrow$ basis of left dominant invariant subspace of YZ:

$$W^T = \tilde{W}^T(1:r, :)Z$$



3. Orthogonalize W and V: $\quad W^T V = I_r$

Model order reduction with cross-Gramian

Compute basis of dominant invariant subspace of $X \approx YZ$

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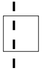
1. Compute basis $\tilde{V}$ of right invariant subspace of ZY
   $\Rightarrow$ basis of right dominant invariant subspace of YZ:

$$V = Y\tilde{V}(:, 1:r)$$



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   $\Rightarrow$ basis of left dominant invariant subspace of YZ:

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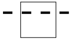


3. Orthogonalize W and V: $\quad W^T V = I_r$

Reduced system of order r: $\quad \hat{A} = W^T AV, \; \hat{B} = W^T B, \; \hat{C} = CV$

$\mathcal{H}$-matrix - accuracy of reduced model

Recall: balanced truncation error bound

$$\|y - \hat{y}\|_2 \leq \|G - \hat{G}\|_\infty \|u\|_2 \quad \textit{with} \ \|G - \hat{G}\|_\infty \leq 2 \sum_{k=r+1}^{n} \sigma_k \leq \mathrm{tol}$$

Recall: balanced truncation error bound

$$\|y - \hat{y}\|_2 \leq \|G - \hat{G}\|_\infty \|u\|_2 \quad \textit{with} \ \|G - \hat{G}\|_\infty \leq 2 \sum_{k=r+1}^{n} \sigma_k \leq \mathrm{tol}$$

Theorem [B./Benner 06]

For symmetric A, $A_{\mathcal{H}}$ with eigenvalues $\lambda_n \leq \cdots \leq \lambda_1 < 0$ and

$$\|A - A_{\mathcal{H}}\|_2 \leq c\epsilon$$

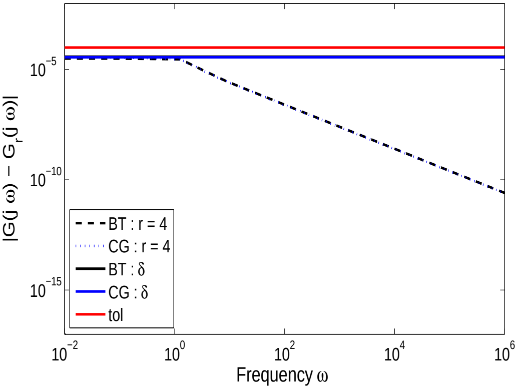
we have

$$\begin{aligned}\|G - \hat{G}\|_\infty &\leq \|G - G_{\mathcal{H}}\|_\infty + \|G_{\mathcal{H}} - \hat{G}\|_\infty \\ &\leq c\,\epsilon\,\frac{1}{\lambda_1^2}\,\|C\|_2\,\|B\|_2 + 2\sum_{k=r+1}^{n}\sigma_k\,.\end{aligned}$$

Numerical results - 2d heat equation

$$\frac{\partial x}{\partial t}(t,\xi) - a\,\Delta x(t,\xi) = b(\xi)u(t), \qquad \xi \in [0,1]^2,\ t \in (0,\infty)$$

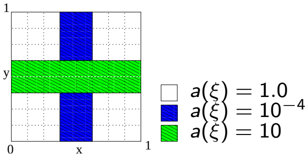
- $y(t) = x(t,\xi)_{|\Omega_o}$
- $n = 16,384$
- diffusion: $a = 1$
- HLib 1.3 [Börm/Grasedyck/Hackbusch]
- $\tau = \epsilon = 10^{-4}$
- rel. residual of X: 2.5×10^{-8}
- tol$=10^{-4} \Rightarrow r = 4$

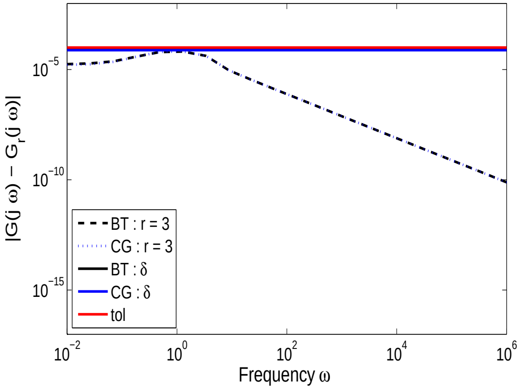


Numerical results - 2d heat equation

$$\frac{\partial x}{\partial t}(t,\xi) - a(\xi)\,\Delta x(t,\xi) = b(\xi)u(t), \qquad \xi \in [0,1]^2,\ \ t \in (0,\infty)$$

varying diffusion $a(\xi)$:



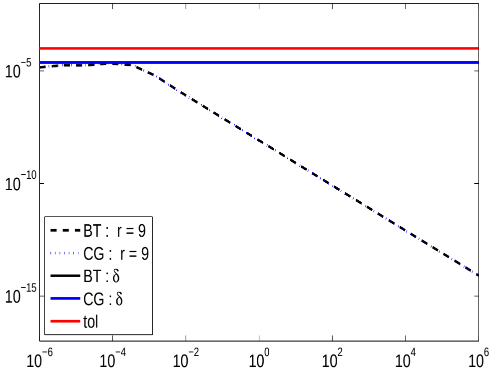


- $n = 16{,}384$
- $\tau = \epsilon = 10^{-4}$
- tol$= 10^{-4} \Rightarrow r = 3$

Numerical results - convection-diffusion equation

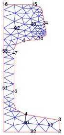
$$\frac{\partial x}{\partial t}(t,\xi) - a\,\Delta x(t,\xi) - c\cdot\nabla x(t,\xi) = b(\xi)u(t),\ \ \xi\in[0,1]^2,\ \ t\in(0,\infty)$$

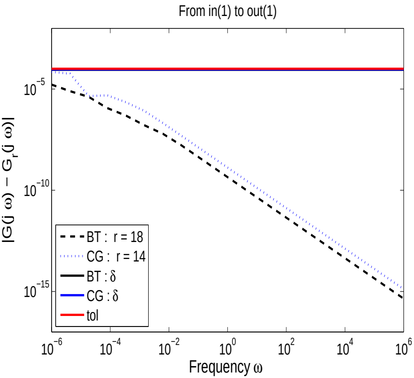
- $n = 16,384$
- convection: $c = (0,1)^T$
- diffusion: $a = 10^{-4}$
- $\tau = \epsilon = 10^{-6}$
- tol$= 10^{-4} \Rightarrow r = 9$

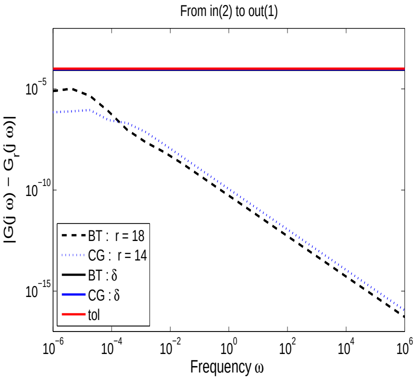


Numerical results - MIMO example

optimal cooling of steel profiles [Benner/Saak 05]
nonsymmetric MIMO system with $n = 5177$ $m = p = 6$
$\tau = \epsilon = 10^{-4}$, tol$= 10^{-4}$







- With $\mathcal{H}$-matrix arithmetic we can solve large-scale Sylvester equations

n	# iter.	$n_\mathcal{T}$		time[sec]		rel. residual		rel. error
		$\mathcal{H}$	full	$\mathcal{H}$	full	$\mathcal{H}$	full	
1024	11	12	12	16	40	1.26e-07	1.62e-09	2.43e-05
4096	12	14	14	196	2434	5.79e-08	2.48e-10	3.81e-05
16,384	13	15	-	1776	-	2.55e-08	-	-
65,536	14	16	-	13,176	-	1.46e-08	-	-
262,144	15	17	-	116,225	-	-	-	-

- $\mathcal{H}$-matrix based sign function solver well suited for the solution of large-scale Sylvester equations arising from FEM/BEM discretizations of elliptic partial differential operators.
- With $\mathcal{H}$-matrix based Sylvester solver we obtain efficient new implementation of model reduction method based on cross-Gramian.

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4096	12	14	14	196	2434	5.79e-08	2.48e-10	3.81e-05
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Thank you for your attention !