BALANCING-RELATED MODEL REDUCTION FOR DATA-SPARSE SYSTEMS

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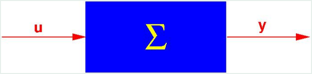
Overview

Model Reduction Introduction

Original System

$$\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t), \\ y(t) = Cx(t) + Du(t), \end{cases}$$

- states $x(t) \in \mathbb{R}^n$,
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t) \in \mathbb{R}^p$.



Reduced-Order System

$$\hat{\Sigma} : \begin{cases} \dot{\hat{x}}(t) = \hat{A}\hat{x}(t) + \hat{B}u(t), \\ \hat{y}(t) = \hat{C}\hat{x}(t) + \hat{D}u(t). \end{cases}$$

- states $\hat{x}(t) \in \mathbb{R}^r$, $r \ll n$,
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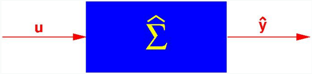

Goal:

$\|y - \hat{y}\| < \text{tolerance} \cdot \|u\|$ for all admissible input signals.

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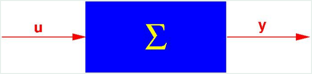

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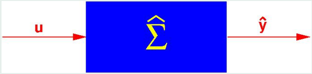

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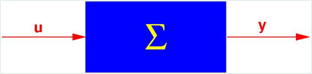

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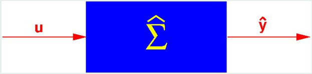

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Linear Systems in Frequency Domain

Application of Laplace transformation ($x(t) \mapsto x(s)$, $\dot{x}(t) \mapsto sx(s)$) to linear system with $x(0) = 0$:

$$sx(s) = Ax(s) + Bu(s), \quad y(s) = Bx(s) + Du(s),$$

yields I/O-relation in frequency domain:

$$y(s) = \Big(\underbrace{C(sI_n - A)^{-1}B + D}_{=: G(s)} \Big) u(s)$$

G is the transfer function of Σ.

Summary

Approximate the dynamical system

$$\begin{aligned} \dot{x} &= Ax + Bu, \qquad A \in \mathbb{R}^{n\times n}, \quad B \in \mathbb{R}^{n\times m}, \\ y &= Cx + Du, \qquad C \in \mathbb{R}^{p\times n}, \quad D \in \mathbb{R}^{p\times m}, \end{aligned}$$

by reduced-order system

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of order $r \ll n$, such that

$$\|y - \hat{y}\| = \|Gu - \hat{G}u\| \leq \|G - \hat{G}\|\|u\| < \text{tolerance} \cdot \|u\|.$$

$\Longrightarrow$ Approximation problem: $\min_{\text{order}\,(\hat{G})\leq r} \|G - \hat{G}\|$.

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Application Areas

Feedback Control – controllers designed by LQR/LQG, H_2, H_∞ methods are LTI systems of order $\geq n$, but technological implementation needs order ~ 10.

Optimization/open-loop control – time-discretization of already large-scale systems leads to huge number of equality constraints in mathematical program.

Microelectronics – verification of VLSI/ULSI chip design requires high number of simulations for different input signals, various effects due to progressive miniaturization lead to large-scale systems of differential(-algebraic) equations (order $\sim 10^8$).

MEMS/Microsystem design – smart system integration needs compact models for efficient coupled simulation.

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Balanced Truncation

The Basic Ideas

Idea:

- A system Σ, realized by (A, B, C, D), is called balanced, if solutions P, Q of the Lyapunov equations

$$AP + PA^T + BB^T = 0, \qquad A^TQ + QA + C^TC = 0,$$

satisfy: $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

- $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- Compute balanced realization of the system via state-space transformation

$$\begin{aligned}\mathcal{T} : (A, B, C, D) &\mapsto (TAT^{-1}, TB, CT^{-1}, D) \\ &= \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix}, D \right)\end{aligned}$$

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Implementation: SR Method

1. Compute Cholesky factors of the solutions of the Lyapunov equations,
$$P = S^T S, \quad Q = R^T R.$$
2. Compute SVD
$$SR^T = [\,U_1,\; U_2\,] \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix}.$$
3. Set
$$W = R^T V_1 \Sigma_1^{-1/2}, \qquad V = S^T U_1 \Sigma_1^{-1/2}.$$
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Properties:

- Reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$.
- Adaptive choice of r via computable error bound:

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Singular Perturbation Approximation
(Balanced Residualization)

BT ROM satisfies: $\lim_{\omega\to\infty}(G(\jmath\omega) - \hat{G}(\jmath\omega)) = 0.$
Now, want zero steady-state error: $G(0) = \hat{G}(0).$

Assume system is minimal and balanced. (Can be attained using BT!)

Compute SPA reduced-order model by setting $\dot{x}_2(t) = 0$ ($x_1(t) \in \mathbb{R}^r$):

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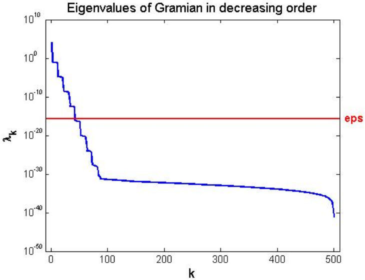
- Instead of Gramians P, Q compute $S, R \in \mathbb{R}^{n \times k}$, $k \ll n$, such that

$$P \approx SS^T, \quad Q \approx RR^T.$$

- Compute S, R with problem-specific Lyapunov solvers of "low" complexity directly.



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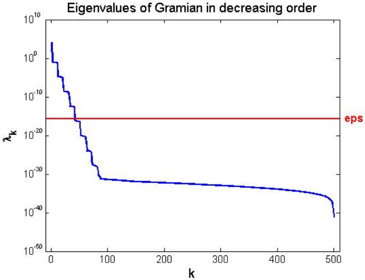

$\rightsquigarrow$ need solver for large-scale matrix equations which computes S, R directly!

Simultaneously solve

$$AP + PA^T + BB^T = 0, \qquad A^T Q + QA + C^T C = 0$$

for low-rank factors S, R of P, Q:

With $B_0 = B,\ C_0 = C,$ iterate

$$\begin{array}{lclcl} -I_n & \overset{i\rightarrow\infty}{\longleftarrow} & A_{i+1} & \leftarrow & \frac{1}{2}(A_i + A_i^{-1}), \\ \sqrt{2}S & \overset{i\rightarrow\infty}{\longleftarrow} & B_{i+1} & \leftarrow & \frac{1}{\sqrt{2}} \left[\ B_i \quad A_i^{-1} B_i\ \right], \\ \sqrt{2}R^T & \overset{i\rightarrow\infty}{\longleftarrow} & C_{i+1} & \leftarrow & \frac{1}{\sqrt{2}} \begin{bmatrix} C_i \\ C_i A_i^{-1} \end{bmatrix}, \end{array}$$

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Problem 1: Workspace doubles per iteration step.

$\Rightarrow$ apply rank-revealing QR (LQ) factorization to B_{i+1}, C_{i+1},

$\Rightarrow$ approximate low-rank factors $\tilde{S} \in \mathbb{R}^{n\times k_P}$, $\tilde{R} \in \mathbb{R}^{n\times k_Q}$.

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Problem 2:

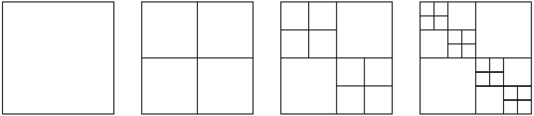
- Algorithm involves inv, add of dense matrices: $\mathcal{O}(n^3)$.
- Even if A is sparse, A^{-1} is dense $\Rightarrow$ $\mathcal{O}(n^2)$ storage.

Here: A in data-sparse $\mathcal{H}$-matrix format

$\rightsquigarrow$ use formatted arithmetic $\oplus$, $\mathrm{Inv}_{\mathcal{H}}$.

A Very Brief $\mathcal{H}$-Matrix Primer

Given index set $I = \{1, \ldots, n\}$ (e.g., numbering of FE nodes), construct block cluster tree $T_{I \times I}$:



Leaf of $T_{I \times I} \equiv$ low-rank matrix $\Rightarrow$

$\mathcal{H}$-matrix definition

$\mathcal{H}(T_{I\times I}, k) := \{M \in \mathbb{R}^{I \times I} \,|\, \mathrm{rank}\,(M|_{t \times s}) \leq k \quad \forall$ leaves $t \times s$ of $T_{I \times I}\}$.

- Storage requirements for $K \in \mathcal{H}(T_{I\times I}, k)$: $\mathcal{O}(n \log(n)\, k)$;
- arithmetic employs truncated SVD to close the set of $\mathcal{H}$-matrices;
- complexity: Kx : $\mathcal{O}(n \log(n)\, k)$
  $K \oplus M$: $\mathcal{O}(n \log(n)\, k^2)$,
  $K \odot M$, $\mathrm{Inv}_{\mathcal{H}}(K)$: $\mathcal{O}(n\, log^2(n)\, k^2)$.

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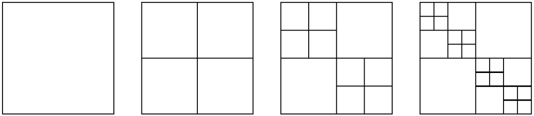


Leaf of $T_{I \times I}$ $\equiv$ low-rank matrix $\Rightarrow$

$\mathcal{H}$-matrix definition

$$\mathcal{H}(T_{I\times I}, k) := \{M \in \mathbb{R}^{I\times I} \,|\, \operatorname{rank}(M|_{t\times s}) \leq k \quad \forall \text{ leaves } t\times s \text{ of } T_{I\times I}\}.$$

- Storage requirements for $K \in \mathcal{H}(T_{I\times I}, k)$: $\mathcal{O}(n \log(n)\, k)$;
- arithmetic employs truncated SVD to close the set of $\mathcal{H}$-matrices;
- complexity: Kx : $\mathcal{O}(n \log(n)\, k)$
  $K \oplus M$: $\mathcal{O}(n \log(n)\, k^2)$,
  $K \odot M$, $\mathrm{Inv}_{\mathcal{H}}(K)$: $\mathcal{O}(n \log^2(n)\, k^2)$.

$\mathcal{H}$-Sign Function Method for Lyapunov Equations

Algorithm:

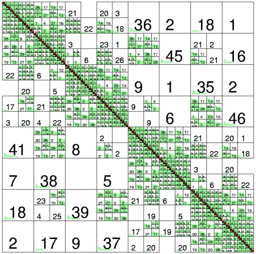
$A_0 \leftarrow (A)_{\mathcal{H}},\ B_0 \leftarrow B,\ C_0 \leftarrow C$:

WHILE $\|A_{i+1} + I_n\|_2 > \texttt{tol}$

$$A_{i+1} \leftarrow \tfrac{1}{2}(A_i \oplus \mathrm{Inv}_{\mathcal{H}}(A_i)),$$

$$B_{i+1} \leftarrow \frac{1}{\sqrt{2}}\mathrm{rrlq}\left(\left[\begin{array}{cc} B_i & \mathrm{Inv}_{\mathcal{H}}(A_i)B_i \end{array}\right]\right),$$

$$C_{i+1} \leftarrow \frac{1}{\sqrt{2}}\mathrm{rrqr}\left(\left[\begin{array}{c} C_i \\ C_i\mathrm{Inv}_{\mathcal{H}}(A_i) \end{array}\right]\right).$$



$\rightsquigarrow\ \tilde{S} \approx \frac{1}{\sqrt{2}} \lim_{i\to\infty} B_i, \quad \tilde{R} \approx \frac{1}{\sqrt{2}} \lim_{i\to\infty} C_i^T$

with linear-polylogarithmic complexity: $\mathcal{O}(n\log^2(n)k^2)$.

- Storage requirements for A: $\mathcal{O}(n\log(n)k)$.
- Adaptive rank choice k w.r.t. given $\mathcal{H}$-approximation error ϵ.

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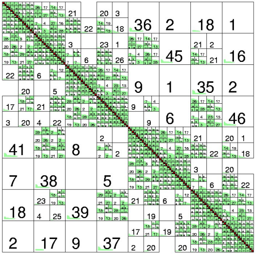

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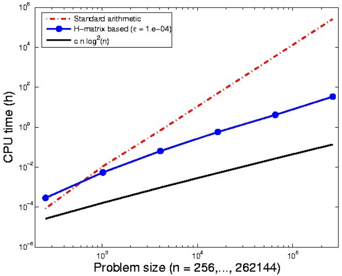
Numerical Example

Performance, accuracy of Lyapunov solver (with $\tau = \epsilon = 10^{-4}$)

- 2d heat equation, $\frac{\partial x}{\partial t} = \alpha \Delta x(t,\xi) + b(\xi)u(t),\ u(t) \in \mathbb{R}$;
- n = dim of FE space;
- use HLib 1.3 by Börm, Grasedyck, Hackbusch.

n	unknowns	k_P	$\lVert\mathcal{R}(\mathcal{P})\rVert_2$
256	32,896	11	$8.2 \cdot 10^{-8}$
1,024	524,800	13	$1.1 \cdot 10^{-6}$
4,096	8,390,656	14	$1.7 \cdot 10^{-6}$
16,384	134,225,920	15	$1.1 \cdot 10^{-6}$



$n = 262,144$: $k_P = 17 \Rightarrow$ 4.25 MB for solution instead of 64 GB!

Error Analysis for Transfer Function Approximation

For balanced truncation we have absolute error bound:

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

Worst-case error: $\|G-\hat{G}\|_\infty \le \|G-G_{\mathcal{H}}\|_\infty + \underbrace{\|G_{\mathcal{H}}-\hat{G}\|_\infty}_{\le \text{tol}}$ with

- $G(s) = C(sI_n - A)^{-1}B$: original transfer function,
- $G_{\mathcal{H}}(s) = C(sI_n - A_{\mathcal{H}})^{-1}B$: $\mathcal{H}$-approximation to $G(s)$,
- $\hat{G}(s) = \hat{C}(sI_r - \hat{A})^{-1}\hat{B}$: reduced-order system.

Theorem

For A, $A_{\mathcal{H}}$ symmetric and with $\|A-A_{\mathcal{H}}\|_2 \le c\epsilon$, we have

$$\|G-\hat{G}\|_\infty \le c\,\epsilon\,\|C\|_2\|B\|_2 \max_{\lambda\in\lambda(A)} \frac{1}{|\lambda|^2} + \underbrace{2\sum_{k=r+1}^{n}\sigma_k}_{\text{BT error}} + \mathcal{O}(\epsilon^2).$$

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Numerical Examples I

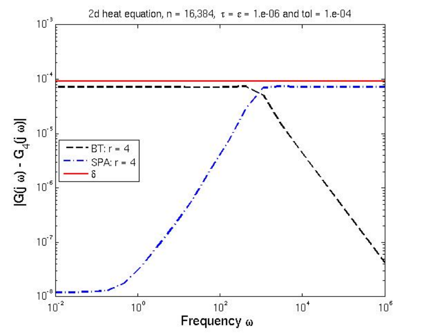
2d heat equation, FEM discretization

$$\frac{\partial x}{\partial t} = \alpha \Delta x(t,\xi) + b(\xi)u(t),$$

FEM $\rightsquigarrow$ $n = 16384$.

Lyapunov solver yields $k_P = k_Q = 16$; for given tolerance 10^{-4}, we obtain $r = 4$. The computed error bound is $9.18 \cdot 10^{-5}$.

Magnitude of absolute error



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Memory requirements

$$\begin{array}{llll} \text{for} & n & = & 16,384 \\ \text{and} & r & = & 7: \end{array} \qquad \begin{array}{lllr} \Sigma & = & (A, B, C): & 2048.2\ \text{MB}, \\ \Sigma_h & = & (A_{\mathcal{H}}, B, C): & 171.3\ \text{MB}, \\ \hat{\Sigma} & = & (\hat{A}, \hat{B}, \hat{C}): & 0.49\ \text{KB}. \end{array}$$

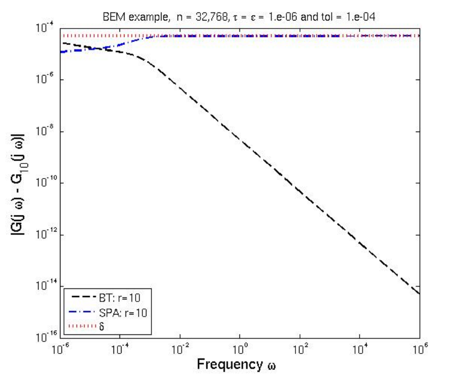
Numerical Examples II

3d heat equation, BEM discretization

$$\frac{\partial x}{\partial t} = \alpha \Delta x(t,\xi) + b(\xi)u(t),$$

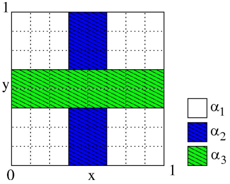
BEM $\rightsquigarrow$ $n = 8192$. Note: A is dense!

Magnitude of absolute error



Numerical Examples III, FEM discretizations

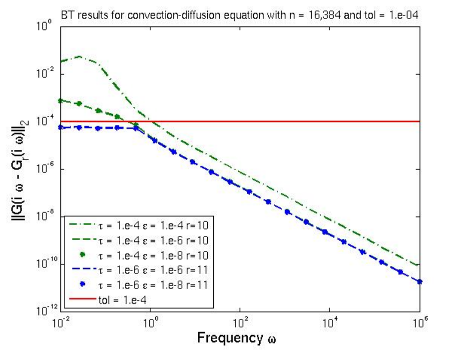
2d heat equation with jumping coefficients



$$\frac{\partial x}{\partial t} = \alpha(\xi)\Delta x(t,\xi) + b(\xi)u(t),$$

$$\alpha_1 = 1$$
$$\alpha_2 = 10^{-4}$$
$$\alpha_3 = 10$$

Magnitude of absolute error



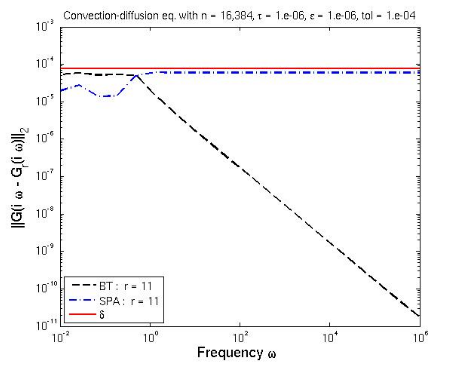
Numerical Examples IV

2d convection-diffusion equation, FEM discretization

$$\frac{\partial x}{\partial t} = \alpha \Delta x(t,\xi) + c \cdot \nabla x(t,\xi) + b(\xi)u(t),$$

with constant convection $c = (0,1)^T$ and $\alpha(\xi) \equiv 10^{-4}$.

Magnitude of absolute error



- With $\mathcal{H}$-matrix arithmetic we can solve large-scale Lyapunov, Sylvester ($\rightarrow$ next talk), and Stein equations.
- Well suited approach for solving matrix equations arising from FEM/BEM discretizations of elliptic partial differential operators (solvers for generalized Lyapunov equations, Sylvester and Stein equations also available).
- Based on Lyapunov solver we obtain efficient new implementation of model reduction method based on balanced truncation and singular perturbation approximation.
- Analogous implementation of BT and SPA for discrete-time systems available.
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References

1. A.C. Antoulas.
Lectures on the Approximation of Large-Scale Dynamical Systems.
SIAM Publications, Philadelphia, PA, 2005.

2. P. Benner, V. Mehrmann, and D. Sorensen (editors).
Dimension Reduction of Large-Scale Systems.
Lecture Notes in Computational Science and Engineering, Vol. 45,
Springer-Verlag, Berlin/Heidelberg, Germany, 2005.

3. U. Baur and P. Benner.
Factorized Solution of Lyapunov Equations Based on Hierarchical Matrix Arithmetic.
Computing, Vol. 78, No. 3, pp. 211-234, 2006.

4. U. Baur and P. Benner.
Gramian-Based Model Reduction for Data-Sparse Systems.
Chemnitz Scientific Computing Preprints 07-01, TU Chemnitz, February 2007.

5. U. Baur.
Low Rank Solution of Data-Sparse Sylvester Equations.
Numerical Linear Algebra with Applications, to appear.

6. P. Benner.
Factorized Solution of Sylvester Equations with Applications in Control.
Proc. 16th Intl. Symp. Math. Theory of Network and Systems, MTNS 2004, Leuven, Belgium, July 5-9, 2004.

7. P. Benner and E.S. Quintana-Ortí.
Solving Stable Generalized Lyapunov Equations with the Matrix Sign Function.
Numerical Algorithms, 20:75–100, 1999.