MODEL REDUCTION FOR LINEAR INVERSE PROBLEMS

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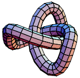


SIAM CSE 2009

Miami, March 2–6, 2009

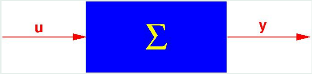
Overview

Model Reduction for Dynamical Systems

Original System

$$\Sigma : \begin{cases} E\dot{x}(t) = f(t, x(t), u(t)), \\ y(t) = g(t, x(t), u(t)). \end{cases}$$

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



Reduced-Order System

$$\widehat{\Sigma} : \begin{cases} \hat{E}\dot{\hat{x}}(t) = \widehat{f}(t, \hat{x}(t), u(t)), \\ \hat{y}(t) = \widehat{g}(t, \hat{x}(t), u(t)). \end{cases}$$

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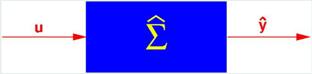

Goal:

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

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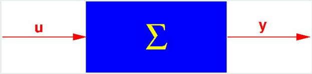

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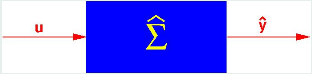

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Linear Systems

Linear, Time-Invariant (LTI) / Descriptor Systems

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

Laplace Transformation / Frequency Domain

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

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

yields I/O-relation in frequency domain:

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

G is the transfer function of Σ.

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Problem

Approximate the dynamical system

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

by reduced-order system

$$\begin{aligned} \hat{E}\dot{\hat{x}} &= \hat{A}\hat{x} + \hat{B}u, \qquad & \hat{A}, \hat{E} \in \mathbb{R}^{r\times r}, \quad & \hat{B} \in \mathbb{R}^{r\times m}, \\ \hat{y} &= \hat{C}\hat{x} + \hat{D}u, & \hat{C} \in \mathbb{R}^{p\times r}, \quad & \hat{D} \in \mathbb{R}^{p\times m}, \end{aligned}$$

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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Inverse Problems for Linear Dynamical Systems

System inversion

Assume $m = p$, $D \in \mathbb{R}^{m \times m}$ invertible (generalizations possible!), then

$$G^{-1}(s) = -D^{-1}C(sE - (A - BD^{-1}C))^{-1}BD^{-1} + D^{-1}.$$

Some applications like

- inverse-based control,
- identification of source terms,

reconstruct input function from reference trajectory/measured outputs: given $Y(s)$, the Laplace transform of $y(t)$, compute $U(s) = G^{-1}(s)Y(s)$.

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Goal: reduced-order transfer function $\hat{G}(s)$ such that

$$\hat{U}(s) = \hat{G}^{-1}(s)Y(s)$$

has small error

$$\|U - \hat{U}\| = \|G^{-1}Y - \hat{G}^{-1}Y\| \leq \|G^{-1} - \hat{G}^{-1}\|\|Y\| \leq \text{tolerance} \cdot \|Y\|.$$

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Balancing Basics
($E = I_n$ for ease of notation)

Linear, Time-Invariant (LTI) Systems

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(A, B, C, D) is a realization of Σ (nonunique).

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Model Reduction Based on Balancing

Given $P, Q \in \mathbb{R}^{n \times n}$ symmetric positive definite (spd), and a contragredient transformation $T : \mathbb{R}^n \to \mathbb{R}^n$,

$$TPT^T = T^{-T}QT^{-1} = \mathrm{diag}(\sigma_1, \ldots, \sigma_n), \quad \sigma_1 \geq \ldots \geq \sigma_n \geq 0.$$

Balancing Σ w.r.t. P, Q:

$$\Sigma \equiv (A, B, C, D) \mapsto (TAT^{-1}, TB, CT^{-1}, D) \equiv \Sigma.$$

Generalization to $P, Q \geq 0$ possible: if $\hat{n}$ is McMillan degree of Σ, then

$$T(PQ)T^{-1} = \mathrm{diag}(\sigma_1, \ldots, \sigma_{\hat{n}}, 0, \ldots, 0).$$

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Basic Model Reduction Procedure

1. Given $\Sigma \equiv (A, B, C, D)$ and balancing (w.r.t. given P, Q spd) transformation $T \in \mathbb{R}^{n\times n}$ nonsingular, compute

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

2. Truncation $\rightsquigarrow$ reduced-order model:

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Implementation: SR Method

1. Compute Cholesky (square) or full-rank (maybe rectangular, "thin") factors of P, Q

$$P = S^T S, \quad Q = R^T R.$$

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

$$W = R^T V_1 \Sigma_1^{-1/2}, \qquad V = S^T U_1 \Sigma_1^{-1/2}.$$

4. Reduced-order model is

$$(\hat{A}, \hat{B}, \hat{C}, \hat{D}) := (W^T AV, W^T B, CV, D) \quad (\equiv (A_{11}, B_1, C_1, D).)$$

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Methods

Truncate realization, balanced w.r.t. $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n) = \Sigma$, $\sigma_1 \geq \ldots \geq \sigma_r > \sigma_{r+1} \geq \ldots \sigma_n \geq 0$ at size r.

Classical Balanced Truncation (BT) — Mullis/Roberts '76, Moore '81

- P/Q = controllability/observability Gramian of $\Sigma \equiv (A, B, C, D)$.
- For asymptotically stable systems, P, Q solve dual Lyapunov equations

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

- $\{\sigma_1^{\mathrm{BT}}, \ldots, \sigma_n^{\mathrm{BT}}\}$ are the Hankel singular values (HSVs) of Σ.
- Preserves stability, extends to unstable systems w/o purely imaginary poles using frequency domain definition of the Gramians [Zhou/Salomon/Wu '99].
- Can be applied to inverse system $(A - BD^{-1}C, BD^{-1}, D^{-1}C, D^{-1})$.
- Computable error bound comes for free:

$$\|G - \hat{G}^{\mathrm{BT}}\|_{H_\infty} \leq 2 \sum_{j=r+1}^{n} \sigma_j^{\mathrm{BT}},$$

allows adaptive choice of r!

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Balanced Stochastic Truncation (BST) — Desai/Pal '84, Green '88

- $P =$ controllability Gramian of $\Sigma \equiv (A, B, C, D)$, i.e., solution of Lyapunov equation $AP + PA^T + BB^T = 0$.
- $Q =$ observability Gramian of right spectral factor of power spectrum of Σ, i.e., solution of ARE

$$A_W^T Q + QA_W + QB_W(DD^T)^{-1}B_W^T Q + C^T(DD^T)^{-1}C = 0,$$

where $A_W := A - B_W(DD^T)^{-1}C$, $B_W := BD^T + PC^T$.

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- Preserves stability; needs stability of A_W.
- Computable relative error bound [Green '88]:

$$\|\Delta^{\mathrm{BST}}\|_{H_\infty} = \|G^{-1}(G - \hat{G}^{\mathrm{BST}})\|_{H_\infty} \leq \prod_{j=r+1}^{n} \frac{1+\sigma_j^{\mathrm{BST}}}{1-\sigma_j^{\mathrm{BST}}} - 1,$$

  $\rightsquigarrow$ uniform approximation quality over full frequency range.
  Note: $|\sigma_j^{\mathrm{BST}}| \leq 1$.

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- Zeros of $G(s)$ are preserved in $\hat{G}(s) \Longrightarrow$

$G(s)$ minimum-phase $\Longrightarrow$ $\hat{G}(s)$ minimum-phase.

- Error bound for inverse system [B. '03]

If $G(s)$ is square, minimal, stable, minimum-phase, nonsingular on $\jmath\mathbb{R}$, then

$$\|G^{-1} - \hat{G}^{-1}\|_{H_\infty} \leq \left(\prod_{j=r+1}^{n} \frac{1+\sigma_j^{\mathrm{BST}}}{1-\sigma_j^{\mathrm{BST}}} - 1\right) \|\hat{G}^{-1}\|_{H_\infty}.$$

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- Error bound for inverse system [B. '03]

If $G(s)$ is square, minimal, stable, minimum-phase, nonsingular on $\jmath\mathbb{R}$, then

$$\|G^{-1} - \hat{G}^{-1}\|_{H_\infty} \leq \left(\prod_{j=r+1}^{n} \frac{1+\sigma_j^{\mathrm{BST}}}{1-\sigma_j^{\mathrm{BST}}} - 1 \right) \|\hat{G}^{-1}\|_{H_\infty}.$$

Balancing for Inverse Problems

Truncate realization, balanced w.r.t. $P = Q = \operatorname{diag}(\sigma_1, \ldots, \sigma_n) = \Sigma$, $\sigma_1 \geq \ldots \geq \sigma_r > \sigma_{r+1} \geq \ldots \sigma_n \geq 0$ at size r.

Balanced Stochastic Truncation (BST) — Desai/Pal '84, Green '88

- $P =$ controllability Gramian of $\Sigma \equiv (A, B, C, D)$, i.e., solution of Lyapunov equation $AP + PA^T + BB^T = 0$.
- $Q =$ observability Gramian of right spectral factor of power spectrum of Σ, i.e., solution of ARE

$$A_W^T Q + QA_W + QB_W(DD^T)^{-1}B_W^T Q + C^T(DD^T)^{-1}C = 0,$$

  where $A_W := A - B_W(DD^T)^{-1}C$, $B_W := BD^T + PC^T$.
- For minimum-phase systems, no ARE necessary [Obinata/Anderson '01]:
  Solving the Lyapunov equation

$$(A - BD^{-1}C)^T R + R(A - BD^{-1}C) + C^T(DD^T)^{-1}C = 0,$$

  and balancing P vs. R yields BST reduced-order model.
  Note: $\sigma_j^{\mathrm{BST}} = \alpha_j(1 + \alpha_j^2)^{-\frac{1}{2}}$,
  where the α_j's are the square roots of the eigenvalues of PR.

General form for $A, G = G^T, W = W^T \in \mathbb{R}^{n\times n}$ given and $P \in \mathbb{R}^{n\times n}$ unknown:

$$\begin{aligned} 0 &= \mathcal{L}(Q) := A^T Q + QA + W, \\ 0 &= \mathcal{R}(Q) := A^T Q + QA - QGQ + W. \end{aligned}$$

In large scale applications from semi-discretized control problems for PDEs,

- $n = 10^3 - 10^6$ ($\Longrightarrow 10^6 - 10^{12}$ unknowns!),
- A has sparse representation ($A = -M^{-1}K$ for FEM),
- G, W low-rank with $G, W \in \{BB^T, C^T C\}$, where $B \in \mathbb{R}^{n\times m}$, $m \ll n$, $C \in \mathbb{R}^{p\times n}$, $p \ll n$.
- Standard (eigenproblem-based) $\mathcal{O}(n^3)$ methods are not applicable!

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- For $A \in \mathbb{R}^{n \times n}$ stable, $B \in \mathbb{R}^{n \times m}$ $(w \ll n)$, consider Lyapunov equation
$$AX + XA^T = -BB^T.$$
- ADI Iteration: [Wachspress 1988]
$$\begin{aligned}(A + p_k I)X_{(j-1)/2} &= -BB^T - X_{k-1}(A^T - p_k I)\\ (A + \overline{p_k} I){X_k}^T &= -BB^T - X_{(j-1)/2}(A^T - \overline{p_k} I)\end{aligned}$$
with parameters $p_k \in \mathbb{C}^-$ and $p_{k+1} = \overline{p_k}$ if $p_k \notin \mathbb{R}$.
- For $X_0 = 0$ and proper choice of p_k: $\lim_{k \to \infty} X_k = X$ superlinear.
- Re-formulation using $X_k = Y_k Y_k^T$ yields iteration for Y_k...

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Factored ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$.

Setting $X_k = Y_k Y_k^T$, some algebraic manipulations $\Longrightarrow$

Algorithm [Penzl '97/'00, Li/White '99/'02, B. 04, B./Li/Penzl '99/'08]

$$V_1 \leftarrow \sqrt{-2\mathrm{Re}\,(p_1)}(A + p_1 I)^{-1}B, \qquad Y_1 \leftarrow V_1$$

FOR $j = 2, 3, \ldots$

$$V_k \leftarrow \sqrt{\frac{\mathrm{Re}\,(p_k)}{\mathrm{Re}\,(p_{k-1})}} \left(V_{k-1} - (p_k + \overline{p_{k-1}})(A + p_k I)^{-1} V_{k-1}\right)$$

$$Y_k \leftarrow \begin{bmatrix} Y_{k-1} & V_k \end{bmatrix}$$

$$Y_k \leftarrow \mathrm{rrlq}(Y_k, \tau) \qquad \text{\% column compression}$$

At convergence, $Y_{k_{\max}} Y_{k_{\max}}^T \approx X$, where

$$Y_{k_{\max}} = \begin{bmatrix} V_1 & \ldots & V_{k_{\max}} \end{bmatrix}, \qquad V_k = \Big[\,\Big] \in \mathbb{C}^{n \times m}.$$

Note: Implementation in real arithmetic possible by combining two steps.

Factored Galerkin-ADI Iteration

Lyapunov equation $0 = AX + XA^T + BB^T$

Projection-based methods for Lyapunov equations with $A + A^T < 0$:

1. Compute orthonormal basis $\mathrm{range}(Z)$, $Z \in \mathbb{R}^{n \times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, $\dim \mathcal{Z} = r$.
2. Set $\hat{A} := Z^T A Z$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
4. Use $X \approx Z\hat{X}Z^T$.

Examples:

- Krylov subspace methods, i.e., for $m = 1$:

$$\mathcal{Z} = \mathcal{K}(A, B, r) = \mathrm{span}\{B, AB, A^2B, \ldots, A^{r-1}B\}$$

  [Jaimoukha/Kasenally '94, Jbilou '02–'08].

- K-PIK [Simoncini '07],

$$\mathcal{Z} = \mathcal{K}(A, B, r) \cup \mathcal{K}(A^{-1}, B, r).$$

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Examples:

- ADI subspace [B./R.-C. Li/Truhar '08]:

$$\mathcal{Z} = \mathrm{colspan}\left[\ V_1, \quad \ldots, \quad V_r\ \right].$$

Note: ADI subspace is rational Krylov subspace [J.-R. Li/White '02].

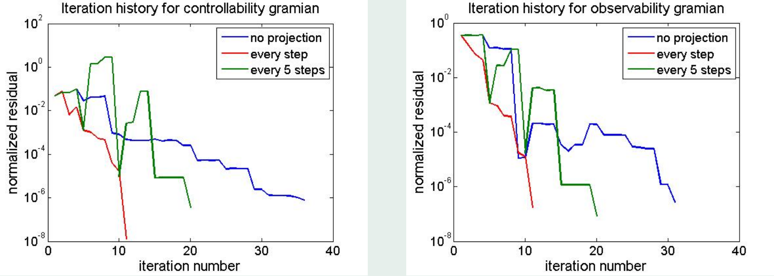
Factored Galerkin-ADI Iteration

Numerical example

FEM semi-discretized control problem for parabolic PDE:

- optimal cooling of rail profiles,
- $n = 20,209,\ m = 7,\ p = 6.$

Good ADI shifts



CPU times: 80s (projection every 5th ADI step) vs. 94s (no projection).

Computations by Jens Saak.

Factored Galerkin-ADI Iteration

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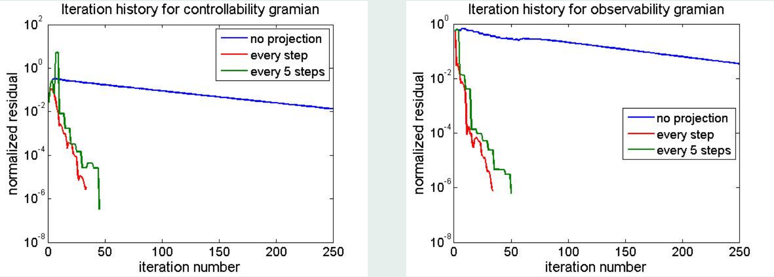

CPU times: 368s (projection every 5th ADI step) vs. 1207s (no projection).

Computations by Jens Saak.

Newton's Method for AREs
[Kleinman '68, Mehrmann '91, Lancaster/Rodman '95, B./Byers '94/'98, B. '97, Guo/Laub '99]

- Consider $0 = \mathcal{R}(Q) = C^T C + A^T Q + QA - QBB^T Q.$
- Frechét derivative of $\mathcal{R}(Q)$ at Q:

$$\mathcal{R}'_Q : Z \to (A - BB^T Q)^T Z + Z(A - BB^T Q).$$

- Newton-Kantorovich method:

$$Q_{j+1} = Q_j - \left(\mathcal{R}'_{Q_j}\right)^{-1} \mathcal{R}(Q_j), \quad j = 0, 1, 2, \ldots$$

Newton's method (with line search) for AREs

FOR $j = 0, 1, \ldots$

1. $A_j \leftarrow A - BB^T Q_j =: A - BK_j$.
2. Solve the Lyapunov equation $A_j^T N_j + N_j A_j = -\mathcal{R}(Q_j)$.
3. $Q_{j+1} \leftarrow Q_j + t_j N_j$.

END FOR j

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Low-Rank Newton-ADI for AREs

Re-write Newton's method for AREs

$$A_j^T N_j + N_j A_j = -\mathcal{R}(Q_j)$$

$$\Longleftrightarrow$$

$$A_j^T \underbrace{(Q_j + N_j)}_{=Q_{j+1}} + \underbrace{(Q_j + N_j)}_{=Q_{j+1}} A_j = \underbrace{-C^T C - Q_j B B^T Q_j}_{=:-W_j W_j^T}$$

Set $Q_j = Z_j Z_j^T$ for $\mathrm{rank}\,(Z_j) \ll n \Longrightarrow$

$$A_j^T \left(Z_{j+1} Z_{j+1}^T\right) + \left(Z_{j+1} Z_{j+1}^T\right) A_j = -W_j W_j^T$$

Factored Newton Iteration [B./Li/Penzl '99/'08]

Solve Lyapunov equations for Z_{j+1} directly by factored ADI iteration and use 'sparse + low-rank' structure of A_j.

Low-Rank Newton-ADI for AREs

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Factored Newton Iteration [B./Li/Penzl '99/'08]

Solve Lyapunov equations for Z_{j+1} directly by factored ADI iteration and use 'sparse + low-rank' structure of A_j.

- Right-hand of Lyapunov equation in jth Newton step:

$$-C^T(DD^T)^{-1}C + Q_j B(DD^T)^{-1}B^T Q_j =: -W_{j,1}W_{j,1}^T + W_{j,2}W_{j,2}^T.$$

$\rightsquigarrow$ solve two Lyapunov equations in parallel:

$$A_j^T\left(Z_{j+1,\ell}Z_{j+1,\ell}^T\right) + \left(Z_{j+1,\ell}Z_{j+1,\ell}^T\right)A_j = -W_{j,\ell}W_{j,\ell}^T, \quad \ell = 1,2.$$

- After convergence, one more Lyapunov equation to obtain final low-rank factor:

$$A^T(YY^T) + (YY^T)A + W^TW = 0,$$

where

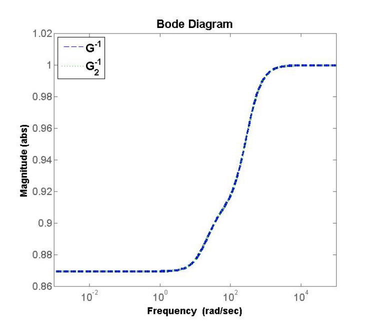
$$W = (DD^T)^{-\frac{1}{2}}C - (DD^T)^{-\frac{1}{2}}B\,[Z_{j_{\max},1},\, Z_{j_{\max},1}]\begin{bmatrix} Y_{j_{\max},2}^T \\ -Y_{j_{\max},2}^T \end{bmatrix}.$$

Numerical Examples

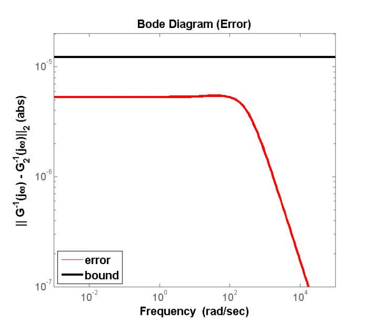
Random example

- $n = 500,\ m = 1 = p;\ D = 1.$
- Reduced order: $r = 2$; $\|G^{-1} - \hat{G}^{-1}\|_\infty \leq 6.114 \cdot 10^{-6}$.

Transfer functions

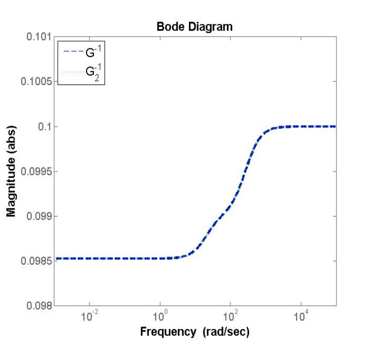


Error



- $n = 500$, $m = 1 = p$; $D = 10$.
- Reduced order: $r = 2$; $\|G^{-1} - \hat{G}^{-1}\|_\infty \leq 6.3975 \cdot 10^{-8}$.

Transfer functions



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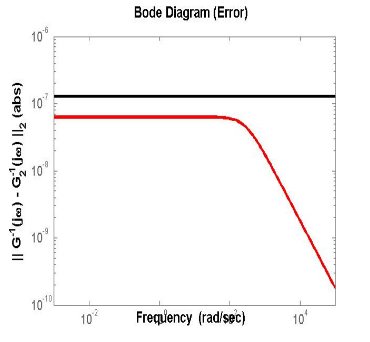
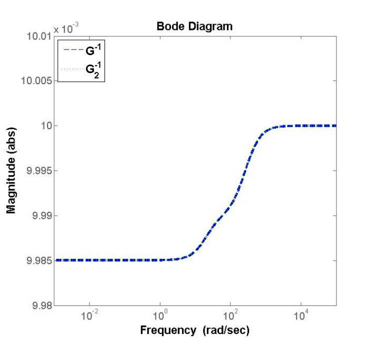


Numerical Examples

Random example

- $n = 500,\ m = 1 = p;\ D = 100.$
- Reduced order: $r = 2;\ \|G^{-1} - \hat{G}^{-1}\|_\infty \leq 6.4275 \cdot 10^{-10}.$

Transfer functions



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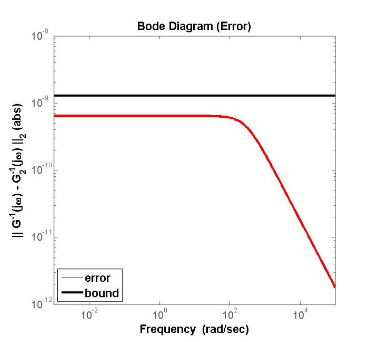
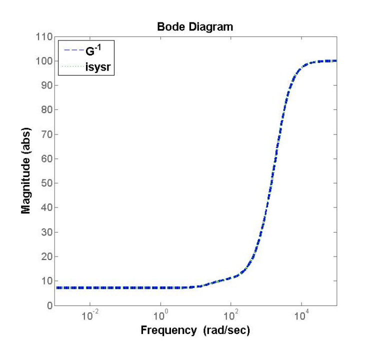


Numerical Examples

Random example

- $n = 500,\ m = 1 = p$; $D = 0.01$.
- Reduced order: $r = 2$; $\|G^{-1} - \hat{G}^{-1}\|_\infty \le 1.225 \cdot 10^{-2}$.

Transfer functions



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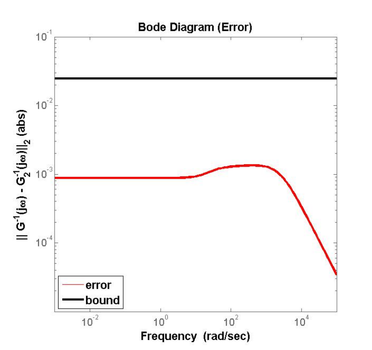

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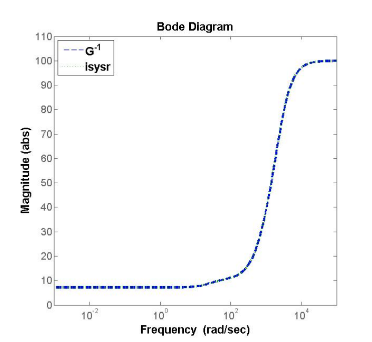
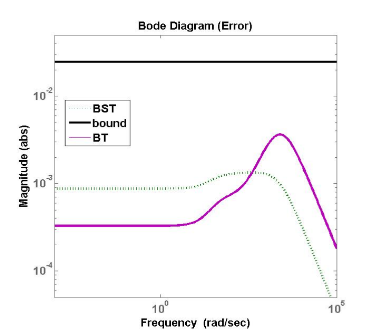


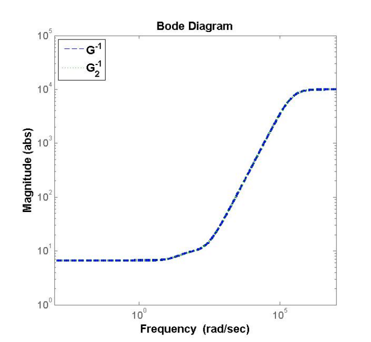
Error (including BT)



Numerical Examples
Random example

- $n = 500,\ m = 1 = p;\ D = 10^{-4}$.
- Reduced order: $r = 2$; $\|G^{-1} - \hat{G}^{-1}\|_\infty \leq 1.2392$.

Transfer functions



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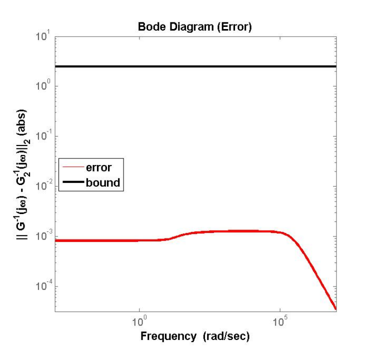

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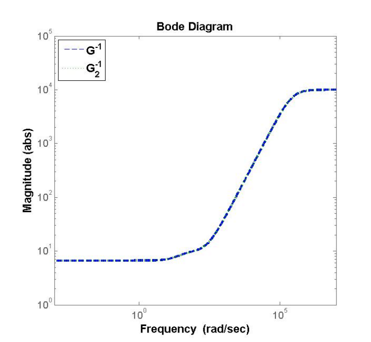

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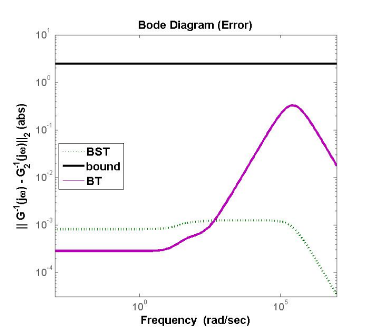
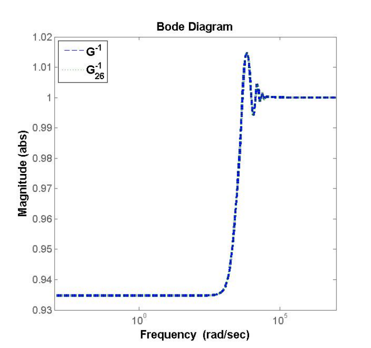


Numerical Examples

Convection-diffusion with distributed control

- $\mathbf{x}_t = \Delta \mathbf{x} - [1000,\ 0] \cdot \nabla \mathbf{x} + \mathbf{b}u.$
- 30×30 uniform grid $\rightsquigarrow$ $n = 900,\ m = 1 = p;\ D = 1.$
- Reduced order: $r = 26;\ \|G^{-1} - \hat{G}^{-1}\|_\infty \leq 3.7452 \cdot 10^{-6}.$

Transfer functions



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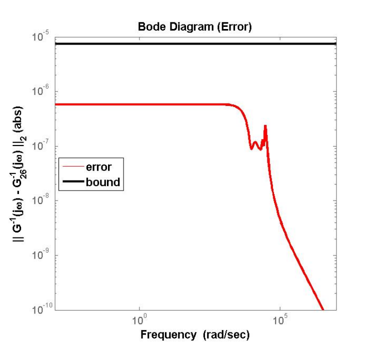

Numerical Examples

Convection-diffusion with distributed control

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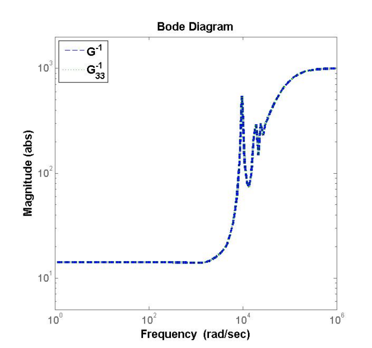
- 30×30 uniform grid $\rightsquigarrow$ $n = 900,\ m = 1 = p;\ D = 10^{-3}.$
- Reduced order: $r = 33;\ \| G^{-1} - \hat{G}^{-1} \|_\infty \leq 6.9565 \cdot 10^{-3}.$

Transfer functions



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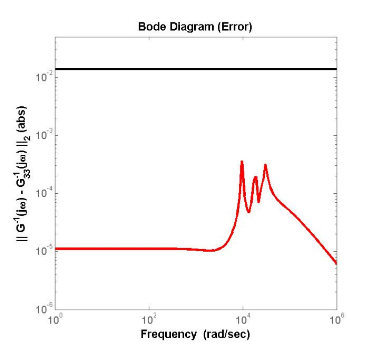

Conclusions and Outlook

- Balanced stochastic truncation yields reduced-order models that can approximate inverse systems to a prescribed tolerance.
- Main message:

  Balanced truncation and family are applicable to large-scale systems.

  (If efficient numerical algorithms are employed.)
- Efficiency of numerical algorithms can be further enhanced, several details require deeper investigation.
- Future work:
  - Better understanding of the role played by feedthrough term D: can it be used/seen as "regularization" parameter.
  - Implementation for non-square systems/approximation of left/right inverse systems.
  - Extension to descriptor systems.
  - Sharper error bound?

Announcement