SYSTEM-THEORETIC METHODS FOR MODEL REDUCTION OF LARGE-SCALE SYSTEMS: SIMULATION, CONTROL, AND INVERSE PROBLEMS

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Model Reduction for Dynamical Systems

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$\Sigma : \begin{cases} E\dot{x}(t) = f(t, x(t), u(t)), & x(t_0) = x_0, \\ y(t) = g(t, x(t), u(t)) & (b) \end{cases}$

with

- (generalized) states $x(t) \in \mathbb{R}^n$ ($E \in \mathbb{R}^{n \times n}$),
- inputs $u(t) \in \mathbb{R}^m$,

Dynamical Systems

• outputs $y(t) \in \mathbb{R}^p$, (b) is called output equation.

E singular \Rightarrow (a) is system of differential-algebraic equations (DAEs) otherwise \Rightarrow (a) is system of ordinary differential equations (ODEs)





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Original System

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

<u>u</u> <u>y</u>

Reduced-Order System

$$\widehat{\Sigma}: \left\{ egin{array}{l} \hat{E}\dot{\hat{x}}(t) = \widehat{f}(t,\hat{x}(t),oldsymbol{u}(t)), \ \hat{y}(t) = \widehat{g}(t,\hat{x}(t),oldsymbol{u}(t)). \end{array}
ight.$$

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

• inputs
$$u(t) \in \mathbb{R}^m$$
,

• outputs
$$\hat{y}(t) \in \mathbb{R}^{p}$$
.

Goal

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



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Linear Systems

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Linear, Time-Invariant (LTI) / Descriptor Systems

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

_aplace 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:

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

G is the transfer function of Σ .



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Approximate the dynamical system

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

by reduced-order system

Problem

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

of order $r \ll n$, such that

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

 \implies Approximation problem: min_{order (\hat{G}) < $r \parallel G - \hat{G} \parallel$.}



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of order $r \ll n$, such that

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

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



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Here:

■ linear systems,

- $\blacksquare n \gg m, p,$
- n so large, that A(, E) cannot be stored in main memory (RAM) as n × n array: n > 5000, say, e.g., from
 - semi-discretization of PDEs,
 - finite element modeling of MEMS,
 - VLSI design/circuit simulation, ...
- A(, E) sparse or data-sparse, i.e., A(, E) can be stored in O(n) or O(n log n) memory locations, but matrix manipulations like similarity transformations are too expensive (possible exception: permutations, sparse factorizations).



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Time-domain simulation

Evaluation of variation-of-constants formula

$$y(t) = C \exp(At) \left(x^0 + \int_0^t \exp(-A\tau) Bu(\tau) d\tau \right),$$

usually too expensive \rightsquigarrow numerical simulation, e.g., using backwards Euler

$$y_h(t_{k+1}) = C(E - h_k A)^{-1} (Ex_h(t_k) + h_k Bu(t_{k+1})) + Du(t_{k+1}),$$

Bottleneck: solution of $(E - h_k A)z = b$, computation time can be significantly reduced by using reduced-order model:

$$\hat{y}_h(t_{k+1}) = \hat{C}(\hat{E} - h_k\hat{A})^{-1} \left(\hat{E}x_h(t_k) + h_k\hat{B}u(t_{k+1})\right) + \hat{D}u(t_{k+1}).$$



Application Areas Simulation

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Frequency-domain simulation

Frequency response analysis, e.g., for Bode, Nyquist or Nichols plots, requires evaluation of transfer function

$$G(\iota\omega_k) = C(\iota\omega_k E - A)^{-1}B + D, \quad \omega_k \ge 0, \ k = 1, \dots, N_f.$$

Bottleneck: solution of $(\imath \omega_k E - A)z = b$.

Computation time can be significantly reduced by using reduced-order model:

$$\hat{G}(\imath\omega_k) = \hat{C}(\imath\omega_k\hat{E} - \hat{A})^{-1}\hat{B} + \hat{D}.$$



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But: the cost for solving the linear systems in time/frequency domain simulation may not benefit from smaller order, if efficient sparse direct solver for full-size sparse system matrices is available.



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An easy improvement

Significant reduction can be achieved by transforming (\hat{A}, \hat{E}) to Hessenberg-triangular form using QZ algorithm, i.e., compute orthogonal Q, Z such that

$$Q(\lambda \hat{E} - \hat{A})Z = \lambda \left[\swarrow \right] - \left[\swarrow \right] \equiv \left[\swarrow \right]$$

New reduced-order system: $(Q\hat{E}Z, Q\hat{A}Z, Q\hat{B}, \hat{C}Z)$, linear systems of equations

$$(\jmath\omega\hat{E}-\hat{A})x = b,$$

 $(\hat{E}-h_k\hat{A})x_{k+1} = \hat{E}x_k + \dots,$ etc

have Hessenberg form and can thus be solved using r - 1 Givens rotations only! (Needs Hessenberg solver inside simulator.)

For symmetric systems, further reduction can be achieved.



Application Areas (Optimal) Control

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Feedback Controllers

A feedback controller (dynamic compensator) is a linear system of order N, where

- input = output of plant,
- output = input of plant.

Modern (LQG- $/\mathcal{H}_2$ - $/\mathcal{H}_\infty$ -) control design: $N \ge n$.



Practical controllers require small N ($N \sim 10$, say) due to

- real-time constraints,
- increasing fragility for larger N.

 \implies reduce order of plant (*n*) and/or controller (*N*).



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Application Areas Inverse Problems

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Conclusions and Outlook 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

System inversion

- 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

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



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Automatic generation of compact models.

 Satisfy desired error tolerance for all admissible input signals, i.e., want

 $||y - \hat{y}|| < \text{tolerance} \cdot ||u|| \qquad \forall u \in L_2(\mathbb{R}, \mathbb{R}^m).$

 \implies Need computable error bound/estimate!

- Preserve physical properties:
 - stability (poles of G in \mathbb{C}^-),
 - minimum phase (zeroes of G in \mathbb{C}^-),
 - passivity ("system does not generate energy"),



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

Linear, Time-Invariant (LTI) Systems



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Model Reduction Based on Balancing

Linear, Time-Invariant (LTI) Systems

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

$$TPT^{T} = T^{-T}QT^{-1} = \operatorname{diag}(\sigma_{1}, \ldots, \sigma_{n}), \quad \sigma_{1} \geq \ldots \geq \sigma_{n} \geq 0.$$

Balancing Σ w.r.t. P, Q:

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

Generalization to $P, Q \ge 0$ possible: if \hat{n} is McMillan degree of Σ , then $T(PQ)T^{-1} = \operatorname{diag}(\sigma_1, \dots, \sigma_{\hat{n}}, 0, \dots, 0).$



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Basic Model Reduction Procedure

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Conclusions and Outlook **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

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

2 Truncation \rightsquigarrow reduced-order model:

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Implementation: SR Method

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

$$SR^{T} = \begin{bmatrix} U_1, U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^{T} \\ V_2^{T} \end{bmatrix}$$

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

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



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Balancing for Simulation, Control Truncate realization, balanced w.r.t. $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma$, $\sigma_1 \ge \dots \ge \sigma_r > \sigma_{r+1} \ge \dots = \sigma_n \ge 0$ at size r.

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Classical Balanced Truncation (BT) MULLIS/ROBERTS '76, MOORE '81

• $P/Q = \text{controllability/observability Gramian of } \Sigma \equiv (A, B, C, D).$

• For asymptotically stable systems, P, Q solve dual Lyapunov equations $AP + PA^{T} + BB^{T} = 0, \qquad A^{T}Q + QA + C^{T}C = 0.$

• $\{\sigma_1^{BT}, \ldots, \sigma_n^{BT}\}$ 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].
- Preserves passivity for certain symmetric systems.
- Computable error bound comes for free:

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

allows adaptive choice of r!



Balancing for Simulation, Control Truncate realization, balanced w.r.t. $P = Q = \text{diag}(\sigma_1, \dots, \sigma_n) = \Sigma$, $\sigma_1 \ge \dots \ge \sigma_r > \sigma_{r+1} \ge \dots = \sigma_n \ge 0$ at size r.

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Linear-Quadratic Gaussian Balanced Truncation (LQGBT) JONCKHEERE/SILVERMAN '83

■ *P*/*Q* = controllability/observability Gramian of closed-loop system based on LQG compensator.

■ *P*, *Q* solve dual algebraic Riccati equations (AREs)

$$0 = AP + PA^{T} - PC^{T}CP + B^{T}B,$$

$$0 = A^{T}Q + QA - QBB^{T}Q + C^{T}C.$$

- Applies to unstable systems! (Only stabilizability & detectability are required.)
- Computable error bound comes for free: if $G = M^{-1}N$, $\hat{G} = \hat{M}^{-1}\hat{N}$ are left coprime factorizations with stable factors, then

 $\|\begin{bmatrix} N & M \end{bmatrix} - \begin{bmatrix} \hat{N} & \hat{M} \end{bmatrix}\|_{H_{\infty}} \leq 2\sum_{j=r+1}^{n} \sigma_{j}^{\mathrm{LQG}} \left(1 + (\sigma_{j}^{\mathrm{LQG}})^{2}\right)^{\frac{1}{2}},$

allows adaptive choice of r!

■ Yields reduced-order LQR/LQG controller for free!



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Based on positive-real equations, related to positive real (Kalman-Yakubovich-Popov-Anderson) lemma.

• For m = p, P, Q solve dual AREs

Positive-Real Balanced Truncation (PRBT)

 $0 = \overline{A}P + P\overline{A}^{T} + PC^{T}\overline{R}^{-1}CP + B\overline{R}^{-1}B^{T},$ $0 = \overline{A}^{T}Q + Q\overline{A} + QB\overline{R}^{-1}B^{T}Q + C^{T}\overline{R}^{-1}C,$

where $\bar{R} = D + D^T$, $\bar{A} = A - B\bar{R}^{-1}C$.

Preserves stability, strict passivity; needs stability of \overline{A} .

Computable error bound [GUGERCIN/ANTOULAS '03,B. '05]:

 $\|G - \hat{G}^{\mathrm{PR}}\|_{H_{\infty}} \leq 2\|R\|^2 \|\hat{G}_D\|_{\infty} \|G_D\|_{\infty} \sum_{k=r+1}^n \sigma_k^{\mathrm{PR}}.$

$$(G_D(s) := G(s) + D^T, \ \hat{G}_D(s) := \hat{G}(s) + D^T.)$$

Green '88



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Balanced Stochastic Truncation (BST)

Desai/Pal '84, Green '88

- $P = \text{controllability Gramian of } \Sigma \equiv (A, B, C, D), \text{ i.e., solution of Lyapunov equation } AP + PA^T + BB^T = 0.$
- 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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where $A_W := A - B_W (DD^T)^{-1}C$, $B_W := BD^T + PC^T$.

Preserves stability; needs stability of A_W.

Balanced Stochastic Truncation (BST)

■ Computable relative error bound [GREEN '88]:

$$\|\Delta^{\mathrm{BST}}\|_{\mathcal{H}_{\infty}} = \|G^{-1}(G-\widehat{G}^{\mathrm{BST}})\|_{\mathcal{H}_{\infty}} \leq \prod_{j=r+1}^n rac{1+\sigma_j^{\mathrm{BST}}}{1-\sigma_j^{\mathrm{BST}}} - 1,$$

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



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Desai/Pal '84, Green '88

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■ Zeros of G(s) are preserved in $\hat{G}(s)$. \implies G(s) minimum-phase $\implies \hat{G}(s)$ minimum-phase.

Balanced Stochastic Truncation (BST)

 Error bound for inverse system [B. '03]
 If G(s) is square, minimal, stable, minimum-phase, nonsingular on gR then

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



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Balanced Stochastic Truncation (BST)

Error bound for inverse system [B. '03] If G(s) is square, minimal, stable, minimum-phase, nonsingular on $j\mathbb{R}$, then

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Basic Principle of Balanced Truncation

Given positive semidefinite matrices $P = S^T S$, $Q = R^T R$, compute balancing state-space transformation so that

 $P = Q = \operatorname{diag}(\sigma_1, \ldots, \sigma_n) = \Sigma, \quad \sigma_1 \ge \ldots \ge \sigma_n \ge 0,$

and truncate corresponding realization at size r with $\sigma_r > \sigma_{r+1}$.

Other Balancing-Based Methods

- Bounded-real balanced truncation (BRBT) based on bounded real lemma [OPDENACKER/JONCKHEERE '88];
- H_{∞} balanced truncation (HinfBT) closed-loop balancing based on H_{∞} compensator [MUSTAFA/GLOVER '91].

Both approaches require solution of dual AREs.

Frequency-weighted versions of the above approaches.



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All balancing-related methods have nice theoretical properties that make them appealing for applications in simulation, control, optimization, inverse problems.



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All balancing-related methods have nice theoretical properties that make them appealing for applications in simulation, control, optimization, inverse problems.

But: computationally demanding w.r.t. to memory and CPU time; need efficient solvers for linear (Lyapunov) and nonlinear (Riccati) matrix equations!



Solving Large-Scale Matrix Equations

Algebraic Lyapunov and Riccati Equations

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Conclusions and Outlook 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:

$$0 = \mathcal{L}(Q) := A^T Q + QA + W,$$

$$0 = \mathcal{R}(Q) := A^T Q + QA - QGQ + W.$$

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

- $n = 10^3 10^6 \implies 10^6 10^{12} \text{ unknowns!}$),
- A has sparse representation $(A = -M^{-1}K \text{ for FEM})$,
- 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) O(n³) methods are not applicable!



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

■
$$n = 10^3 - 10^6$$
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Low-Rank Approximation ARE $0 = A^T Q + QA - QBB^T Q + CC^T$

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Conclusions and Outlook Consider spectrum of ARE solution (analogous for Lyapunov equations).

Example:

- Linear 1D heat equation with point control,
- $\Omega = [0, 1],$
- FEM discretization using linear B-splines,

$$h = 1/100 \implies n = 101.$$

Idea: $Q = Q^T \ge 0 \implies$



$$Q = ZZ^{T} = \sum_{k=1}^{n} \lambda_{k} z_{k} z_{k}^{T} \approx Z^{(r)} (Z^{(r)})^{T} = \sum_{k=1}^{r} \lambda_{k} z_{k} z_{k}^{T}$$



Low-Rank Approximation ARE $0 = A^T Q + QA - QBB^T Q + CC^T$

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Conclusions and Outlook Consider spectrum of ARE solution (analogous for Lyapunov equations).

Example:

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Conclusions and Outlook 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]

$$(A + p_k I) \frac{X_{(j-1)/2}}{(A + \overline{p_k} I) \frac{X_k}{X_k}} = -BB^T - \frac{X_{k-1}(A^T - p_k I)}{(A + \overline{p_k} I) \frac{X_k}{X_k}}$$

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 $0 = AX + XA^{T} + BB^{T}$.

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Algorithm [PENZL '97/'00, LI/WHITE '99/'02, B. 04, B./LI/PENZL '99/'0

$$V_1 \leftarrow \sqrt{-2\operatorname{Re}(p_1)}(A + p_1I)^{-1}B, \quad Y_1 \leftarrow V_1$$

FOR $j = 2, 3, ...$
 $V_k \leftarrow \sqrt{\frac{\operatorname{Re}(p_k)}{\operatorname{Re}(p_{k-1})}} (V_{k-1} - (p_k + \overline{p_{k-1}})(A + p_kI)^{-1}V_{k-1})$
 $Y_k \leftarrow [Y_{k-1} V_k]$
 $Y_k \leftarrow \operatorname{rrlq}(Y_k, \tau)$ % column compression

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

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

$$Y_{k_{\max}} = \begin{bmatrix} V_1 & \dots & V_{k_{\max}} \end{bmatrix}, \quad V_k = \begin{bmatrix} \mathbb{C}^{n \times m} \end{bmatrix}.$$

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



Factored ADI Iteration Lyapunov equation $0 = AX + XA^{T} + BB^{T}$.

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Conclusions and Outlook $V_{1} \leftarrow \sqrt{-2\operatorname{Re}(p_{1})}(A + p_{1}I)^{-1}B, \quad Y_{1} \leftarrow V_{1}$ FOR j = 2, 3, ... $V_{k} \leftarrow \sqrt{\frac{\operatorname{Re}(p_{k})}{\operatorname{Re}(p_{k-1})}} \left(V_{k-1} - (p_{k} + \overline{p_{k-1}})(A + p_{k}I)^{-1}V_{k-1}\right)$ $Y_{k} \leftarrow \left[Y_{k-1} \quad V_{k}\right]$ $Y_{k} \leftarrow \operatorname{rrlq}(Y_{k}, \tau) \qquad \% \text{ column compression}$

Algorithm [PENZL '97/'00, LI/WHITE '99/'02, B. 04, B./LI/PENZL '99/'08]

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$$Y_{k_{\max}} = \begin{bmatrix} V_1 & \dots & V_{k_{\max}} \end{bmatrix}, \quad V_k = \begin{bmatrix} \in \mathbb{C}^{n \times m}. \end{bmatrix}$$

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Factored Galerkin-ADI Iteration Lyapunov equation $0 = AX + XA^{T} + BB^{T}$

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

1 Compute orthonormal basis range (*Z*), $Z \in \mathbb{R}^{n \times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n \dim \mathcal{Z} - r$

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:

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

[JAIMOUKHA/KASENALLY '94, JBILOU '02-'08].

■ K-PIK [Simoncini '07],

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



Factored Galerkin-ADI Iteration Lyapunov equation $0 = AX + XA^{T} + BB^{T}$

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- 2 Set $\hat{A} := Z^T A Z$, $\hat{B} := Z^T B$.
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4 Use
$$X \approx Z \hat{X} Z^T$$
.

Examples:

$$\mathcal{Z} = \operatorname{colspan} \left[\begin{array}{cc} V_1, & \dots, & V_r \end{array} \right].$$

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



Factored Galerkin-ADI Iteration

Numerical example

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FEM semi-discretized control problem for parabolic PDE:

■ optimal cooling of rail profiles (~→ later),

$$n = 20,209, m = 7, p = 6.$$

Good ADI shifts



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

Computations by Jens Saak.



Factored Galerkin-ADI Iteration

Numerical example

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Conclusions and Outlook FEM semi-discretized control problem for parabolic PDE:

■ optimal cooling of rail profiles (~→ later),

$$n = 20,209, m = 7, p = 6.$$

Bad ADI shifts



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]

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Conclusions and Outlook • 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:

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

Newton's method (with line search) for AREs

FOR j = 0, 1, ...

$$\blacksquare A_j \leftarrow A - BB^T Q_j =: A - BK_j.$$

Solve the Lyapunov equation $A_i^T N_j + N_j A_j = -\mathcal{R}(Q_j).$

END FOR j



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

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

Newton's method (with line search) for AREs

FOR j = 0, 1, ... **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



Low-Rank Newton-ADI for AREs

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

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

Set $Q_j = Z_j Z_j^T$ for rank $(Z_j) \ll n \Longrightarrow$ $A_i^T (Z_{i+1} Z_{i+1}^T) + (Z_{i+1} Z_{i+1}^T) A_j = -W_j W_j^T$

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_i .



Low-Rank Newton-ADI for AREs

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Set $Q_j = Z_j Z_j^T$ for rank $(Z_j) \ll n \Longrightarrow$

$A_{j}^{T}(Z_{j+1}Z_{j+1}^{T}) + (Z_{j+1}Z_{j+1}^{T})A_{j} = -W_{j}W_{j}^{T}$

Factored Newton Iteration [B./LI/PENZL '99/'08]

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Solving Large-Scale Matrix Equations Performance of Matrix Equation Solvers

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- Linear 2D heat equation with homogeneous Dirichlet boundary and point control/observation.
- FD discretization on uniform 150×150 grid.
- n = 22.500, m = p = 1, 10 shifts for ADI iterations.
- Convergence of large-scale matrix equation solvers:







Solving Large-Scale Matrix Equations

Performance of matrix equation solvers

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Performance of Newton's method for accuracy $\sim 1/n$

grid	unknowns	$\frac{\ \mathcal{R}(P)\ _{F}}{\ P\ _{F}}$	it. (ADI it.)	CPU (sec.)
8 × 8	2,080	4.7e-7	2 (8)	0.47
16 imes 16	32,896	1.6e-6	2 (10)	0.49
32×32	524,800	1.8e-5	2 (11)	0.91
64×64	8,390,656	1.8e-5	3 (14)	7.98
128 imes 128	134,225,920	3.7e-6	3 (19)	79.46

Here,

- Convection-diffusion equation,
- m = 1 input and p = 2 outputs,
- $P = P^T \in \mathbb{R}^{n \times n} \Rightarrow \frac{n(n+1)}{2}$ unknowns.

Confirms mesh independence principle for Newton-Kleinman [Burns/Sachs/Zietsmann 2006].


Numerical Examples: Simulation Microthruster (MEMS)

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- Co-integration of solid fuel with silicon micro-machined system.
- Goal: Ignition of solid fuel cells by electric impulse.
- Application: nano satellites.
- Thermo-dynamical model, ignition via heating an electric resistance by applying voltage source.
- Design problem: reach ignition temperature of fuel cell w/o firing neighboring cells.
- Spatial FEM discretization of thermo-dynamical model ~→ linear system, *m* = 1, *p* = 7.





Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark Courtesy of C. Rossi, LAAS-CNRS/EU project "Micropyros".

Numerical Examples: Simulation Microthruster (MEMS)

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- axial-symmetric 2D model
- FEM discretization using linear (quadratic) elements $\rightarrow n = 4,257$ (11,445) m = 1, p = 7.
- Reduced model computed using SPARED, modal truncation using ARPACK, and Z. Bai's PVL implementation.

Numerical Examples: Simulation Microthruster (MEMS)

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Relative error n = 4,257



Numerical Examples: Simulation Microthruster (MEMS)

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Numerical Examples: Simulation Microthruster (MEMS)

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Numerical Examples: Simulation Spiral Inductor (Micro Electronics)

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Conclusions and Outlook Passive device used for RF filters etc.

■
$$n = 1,434, m = 1, p = 1.$$



Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark



Numerical Examples: Simulation

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Conclusions and Outlook Passive device used for RF filters etc.

- n = 1,434, m = 1, p = 1.
- Numerical rank of Gramians is 34/41.
- r = 20 passive model computed by PRBT (MorLab).





Source: The Oberwolfach Benchmark Collection http://www.imtek.de/simulation/benchmark



Numerical Examples: Control Optimal Cooling of Steel Profiles

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Conclusions and Outlook Mathematical model: boundary control for linearized 2D heat equation.

$$c \cdot \rho \frac{\partial}{\partial t} x = \lambda \Delta x, \quad \xi \in \Omega$$

$$\lambda \frac{\partial}{\partial n} x = \kappa (u_k - x), \quad \xi \in \Gamma_k, \ 1 \le k \le 7,$$

$$\frac{\partial}{\partial n} x = 0, \qquad \xi \in \Gamma_7.$$

 $\implies m = 7, p = 6.$

■ FEM Discretization, different models for initial mesh (n = 371), 1, 2, 3, 4 steps of mesh refinement \Rightarrow n = 1357, 5177, 20209, 79841.

Source: Physical model: courtesy of Mannesmann/Demag. Math. model: TRÖLTZSCH/UNGER '99/'01, PENZL '99, SAAK '03.



Numerical Examples: Control Optimal Cooling of Steel Profiles

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- BT model computed with sign function method,
- MT w/o static condensation, same order as BT model.

n = 79841, Absolute error



- BT model computed using SpaRed,
- computation time: 8 min.

Mil

Numerical Examples: Control

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- FD discretized linear 2D heat equation with homogeneous Dirichlet boundary and point control/observation.
- n = 22.500, m = p = 1.
- Computed reduced-order model (BT): r = 6, BT error bound $\delta = 1.7 \cdot 10^{-3}$.
- Solve LQR problem: quadratic cost functional, solution is linear state feedback.

Transfer function approximation



Numerical Examples: Control

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Numerical Examples: Control BT vs. LQG BT

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- FDM \rightsquigarrow n = 4496, m = 2; 4 sensor locations $\rightsquigarrow p = 4$.
- Numerical ranks of BT Gramians are 68 and 124, respectively, for LQG BT both have rank 210.
- Computed reduced-order model: r = 10.



Hankel singular values

Source: COMPl_eib v1.1, www.compleib.de.

Numerical Examples: Control BT V5. LQG BT

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- Boundary control problem for 2D heat flow in copper on rectangular domain; control acts on two sides via Robins BC.
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Source: COMPleib v1.1, www.compleib.de.

Numerical Examples: Control BT vs. LQG BT

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Source: COMPleib v1.1, www.compleib.de.



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Balanced truncation and family are applicable to large-scale systems. (If efficient numerical algorithms are employed.)

- Applications: nanoelectronics, microsystems technology, optimal control, machine tool design, systems biology, ...
- Efficiency of numerical algorithms can be further enhanced, several details require deeper investigation.
- Algorithms for data-sparse systems using formatted arithmetic for *H*-matrices [B_{AUR}/B. '06/'08].
- Application to 2nd order systems ~→ talk of Jens Saak.
- Extension to descriptor systems possible. [Stykel since '02, B. 03/'08, Freitas/Martins/Rommes '08, Heinkenschloss/Sorensen/Sun '06/'08].
- Combination of BT with sparse grid interpolation for parametric model reduction [BAUR/B. '08/'09].



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Main message:

Balanced truncation and family are applicable to large-scale systems. (If efficient numerical algorithms are employed.)

- Applications: nanoelectronics, microsystems technology, optimal control, machine tool design, systems biology, ...
- Efficiency of numerical algorithms can be further enhanced, several details require deeper investigation.
- Extension to nonlinear systems employing Carleman bilinearization and tensor product structure of Krylov subspaces in combination with balanced truncation for bilinear systems [*B./Damm '09*] quite promising, in particular for polynomial nonlinearities as often encountered in biological systems.
- Theory and numerical algorithm for application to stochastic systems: [B./Damm '09]; need algorithmic enhancements for really large-scale problems.



Support

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BMBF research network SyreNe



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Conclusions and Outlook

O-MOORE-NICE!

Operational model order reduction for nanoscale IC electronics

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Support

Model Reduction of Large-Scale Systems

Peter Benner

Introduction

System-Theoretic Model Reduction

Numerical Examples

Conclusions and Outlook

DFG Projects

- Automatic, Parameter-Preserving Model Reduction for Applications in Microsystems Technology. Jointly with Jan Gerrit Korvink (IMTEK/U Freiburg and FRIAS).
- Integrated Simulation of the System "Machine Tool Drive System – Stock Removal Process" Using Reduced-Order Structural FE Models.

Jointly with *Michael Zäh* (iwb/TU München) and *Heike Faßbender* (ICM/TU Braunschweig).