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Numerical Solution of Linear and Nonlinear Matrix Equations Arising in Stochastic and Bilinear Control Theory

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verview



Introduction to Model Order Reduction

- Dynamical systems
- Parametric systems as bilinear systems
- Balanced truncation for linear systems
- Bilinear Lyapunov Equations
 - Bilinear systems
 - Balanced truncation for bilinear systems
 - Existence of low-rank approximations
 - Generalized alternating directions iteration (ADI)
 - Bilinear FKSM
 - Tensorized Krylov subspace methods
 - Comparison of methods
- Application to Parametric MOR
 - Fast simulation of cyclic voltammogramms
 - Anemometer design
- 4 Stochastic Systems
 - Stochastic Lyapunov and Riccati equations
 - Conclusions and Outlook





Dynamical Systems

Dynamical Systems

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

with

- (generalized) states $x(t; p) \in \mathbb{R}^n$ $(E \in \mathbb{R}^{n \times n})$,
- inputs $u(t) \in \mathbb{R}^m$,
- outputs $y(t; p) \in \mathbb{R}^q$, (b) is called output equation,
- $p \in \Omega \subset \mathbb{R}^d$ is a parameter vector, Ω is bounded.

Applications:

- Repeated simulation for varying material or geometry parameters, boundary conditions,
- control, optimization and design.

 MOR
 Bilinear Lyapunov Equations
 Application to Parametric MOR
 Stochastic Systems
 Conclusions and Outlook

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 Linear Parametric Systems
 Conclusions and Outlook
 Conclusions and Outlook

Linear, time-invariant (parametric) systems

 $\begin{array}{lll} E(p)\dot{x}(t;p) &=& A(p)x(t;p)+B(p)u(t), & A(p), E(p) \in \mathbb{R}^{n \times n}, \\ y(t;p) &=& C(p)x(t;p), & B(p) \in \mathbb{R}^{n \times m}, C(p) \in \mathbb{R}^{q \times n}. \end{array}$

Linear Parametric Systems

$E(p)\dot{x}(t;p) = A(p)x(t;p) + B(p)u(t), \quad A(p), E(p) \in \mathbb{R}^{n \times n},$ y(t;p) = C(p)x(t;p), $B(p) \in \mathbb{R}^{n \times m}, C(p) \in \mathbb{R}^{q \times n}$

Laplace Transformation / Frequency Domain

Linear, time-invariant (parametric) systems

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

$$sE(p)x(s;p) = A(p)x(s;p) + B(p)u(s), \quad y(s;p) = C(p)x(s;p),$$

yields I/O-relation in frequency domain:

$$y(s; p) = \left(\underbrace{C(p)(sE(p) - A(p))^{-1}B(p)}_{=:H(s;p)}\right)u(s).$$

H(s; p) is the parameter-dependent transfer function of $\Sigma(p)$.

Linear Parametric Systems

Linear, time-invariant (parametric) systems

$$\begin{array}{rcl} \mathsf{E}(p)\dot{x}(t;p) &=& \mathsf{A}(p)x(t;p) + \mathsf{B}(p)u(t), & \mathsf{A}(p), \mathsf{E}(p) \in \mathbb{R}^{n \times n}, \\ y(t;p) &=& \mathsf{C}(p)x(t;p), & \mathsf{B}(p) \in \mathbb{R}^{n \times m}, \mathsf{C}(p) \in \mathbb{R}^{q \times n}. \end{array}$$

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H(s; p) is the parameter-dependent transfer function of $\Sigma(p)$. **Goal:** Fast evaluation of mapping $(u, p) \rightarrow y(s; p)$.

Problem

Approximate the dynamical system

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

by reduced-order system

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

of order $r \ll n$, such that

$$\|y-\hat{y}\| = \|Hu-\hat{H}u\| \le \|H-\hat{H}\|\cdot\|u\| < ext{tolerance}\cdot\|u\| \quad orall \ p\in\Omega.$$

Intro	oduction		

Introduction Model Order Reduction (MOR) Problem

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

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Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Introduction to Model Order Reduction



Linear Parametric Systems — An Alternative Interpretation

Consider bilinear control systems:

$$\Sigma: \begin{cases} \dot{x}(t) = Ax(t) + \sum_{i=1}^{m} N_i x(t) u_i(t) + Bu(t), \\ y(t) = Cx(t), \quad x(0) = x_0, \end{cases}$$

where $A, N_i \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m}, C \in \mathbb{R}^{q \times n}$.

Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Introduction to Model Order Reduction





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where $A, N_i \in \mathbb{R}^{n \times n}, \ B \in \mathbb{R}^{n \times m}, \ C \in \mathbb{R}^{q \times n}$.

Key Observation: Regarding parameter dependencies as additional inputs, a linear parametric system

$$\dot{x}(t) = Ax(t) + \sum_{i=1}^{m_p} a_i(p)A_ix(t) + B_0u_0(t), \quad y(t) = Cx(t)$$

with $B_0 \in \mathbb{R}^{n \times m_0}$ can be interpreted as bilinear system (with $N_i \equiv A_i$): $u(t) := \begin{bmatrix} a_1(p) & \dots & a_{m_0}(p) & u_0(t) \end{bmatrix}^T$,

$$B:=\begin{bmatrix}\mathbf{0}&\ldots&\mathbf{0}&B_0\end{bmatrix}\in\mathbb{R}^{n\times m},\quad m=m_p+m_0.$$

Application to Parametric MOF

Stochastic System

Conclusions and Outlook

Balanced truncation for linear systems

Idea (for simplicity,
$$E = I_n$$
)

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$$\Sigma$$
:

$$\begin{cases}
\dot{x}(t) = Ax(t) + Bu(t), \\
y(t) = Cx(t), \\
\text{is balanced, if system Gramians, i.e., solutions } P, Q \text{ of the Lyapunov} \\
\text{equations}
\end{cases}$$

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

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



Application to Parametric MOF

Stochastic System

Conclusions and Outlook

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• $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ .



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

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



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• Truncation $\rightsquigarrow (\hat{A}, \hat{B}, \hat{C}) = (A_{11}, B_1, C_1).$



Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Balanced truncation for linear systems

Motivation:

HSV are system invariants: they are preserved under ${\cal T}$ and determine the energy transfer given by the Hankel map

$$\mathcal{H}: L_2(-\infty, 0) \mapsto L_2(0, \infty): u_- \mapsto y_+.$$

"functional analyst's point of view"

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"functional analyst's point of view"

In balanced coordinates, energy transfer from u_- to y_+ is

$$E := \sup_{\substack{u \in L_2(-\infty,0] \\ x(0) = x_0}} \frac{\int_0^\infty y(t)^T y(t) dt}{\int_{-\infty}^0 u(t)^T u(t) dt} = \frac{1}{\|x_0\|_2} \sum_{j=1}^n \sigma_j^2 x_{0,j}^2$$

"engineer's point of view"

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Stochastic System

Conclusions and Outlool

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"engineer's point of view" \implies Truncate states corresponding to "small" HSVs

 \implies analogy to best approximation via SVD, therefore balancing-related methods are sometimes called SVD methods.



Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Balanced truncation for linear systems



Implementation: SR Method

 Compute (Cholesky) factors of the solutions of the Lyapunov equations,

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

Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Balanced truncation for linear systems

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Ompute SVD

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



Balanced truncation for linear systems

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

Seduced model is $(W^T AV, W^T B, CV)$.



Stochastic System

Balanced truncation for linear systems

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Set

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

Seduced model is $(W^T AV, W^T B, CV)$.

Note: $T := \Sigma^{-\frac{1}{2}} V^T R$ yields balancing state-space transformation with $T^{-1} = S^T U \Sigma^{-\frac{1}{2}}$, so that $W^T = T(1:r,:)$ and $V = T^{-1}(:,1:r)$.

Application to Parametric MOR

Stochastic System

Conclusions and Outlool

Balanced truncation for linear systems

Properties:

• Reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$.

Balanced truncation for linear systems

Properties:

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

$$\|y-\hat{y}\|_2 \leq \left(2\sum_{k=r+1}^n \sigma_k\right) \|u\|_2.$$





LQG Balanced Truncation



Instead of system Gramians P, Q, use solutions of algebraic Riccati equations (AREs)

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

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

related to linear-quadratic Gaussian (LQG) control design. **Properties:**

- Applicable to unstable systems.
- When factorizations $P = S^T S$, $Q = R^T R$ are available, construction of reduced-order model exactly as in SR method for balanced truncation.
- Error bound: $\|H \hat{H}\|_{L_{\infty}} \leq 2 \sum_{j=r+1}^{n} \frac{\gamma_j}{\sqrt{1 + \gamma_j^2}}$, where $\{\gamma_1, \dots, \gamma_n\} = \Lambda (PQ)^{\frac{1}{2}}, \gamma_1 \geq \dots \gamma_n \geq 0.$

Summary of Introduction



Balancing-based MOR of linear systems requires the efficient numerical solution of either linear or nonlinear matrix equations: Balanced truncation: Lyapunov equations

$$0 = AP + PA^{T} + BB^{T} = \mathcal{L}(P),$$

$$0 = A^{T}Q + QA + C^{T}C = \mathcal{L}^{*}(Q).$$

LQG Balanced truncation: algebraic Riccati equations

$$0 = AP + PA^{T} - PC^{T}CP + BB^{T} = \mathcal{L}(P) - PC^{T}CP,$$

$$0 = A^{T}Q + QA - QBB^{T}Q + C^{T}C = \mathcal{L}^{*}(Q) - QBB^{T}Q.$$

Numerous mature methods exist, e.g.,

- for Lyapunov equations: (rational) Krylov subspace methods, low-rank ADI, Riemannian optimization, ...
- for AREs: (rational) Krylov subspace methods, Newton-ADI, Chandrasekhar iteration, ...

Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

Bilinear Control Systems — Theory and Background

Bilinear control systems:

$$\Sigma: \quad \begin{cases} \dot{x}(t) = Ax(t) + \sum_{i=1}^{m} N_i x(t) u_i(t) + Bu(t), \\ y(t) = Cx(t), \quad x(0) = x_0, \end{cases}$$

where $A, N_i \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times m}, C \in \mathbb{R}^{q \times n}$.

Properties:

- Approximation of (weakly) nonlinear systems by Carleman linearization yields bilinear systems.
- Appear naturally in boundary control problems, control via coefficients of PDEs, Fokker-Planck equations, ...
- Due to the close relation to linear systems, a lot of successful concepts can be extended, e.g. transfer functions, Gramians, Lyapunov equations, . . .
- Linear stochastic control systems possess an equivalent structure and can be treated alike [B./DAMM '11].



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 Bilinear Lyapunov Equations
 Application to Parametric MOR
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Bilinear Lyapunov Equations

Balanced truncation for bilinear systems



The concept of balanced truncation can be generalized to the case of bilinear systems, where we need the solutions of the generalized Lyapunov equations:

$$AP + PA^{T} + \sum_{i=1}^{m} N_{i}PA_{i}^{T} + BB^{T} = 0,$$
$$A^{T}Q + QA^{T} + \sum_{i=1}^{m} N_{i}^{T}QA_{i} + C^{T}C = 0.$$

- Due to its approximation quality, first method of choice for medium-size systems.
- These equations also appear for stochastic control systems, see [B./DAMM '11].
- For an iterative full-rank solver, see [DAMM '08].

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Application to Parametric MOR

Stochastic System

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Bilinear Lyapunov Equations

Some basic facts and assumptions

$$AX + XA^{T} + \sum_{i=1}^{m} N_{i}XN_{i}^{T} + BB^{T} = 0.$$
 (1)

• Need a positive semi-definite symmetric solution X.

Some basic facts and assumptions

$$AX + XA^{T} + \sum_{i=1}^{m} N_{i}XN_{i}^{T} + BB^{T} = 0.$$
 (1)

- Need a positive semi-definite symmetric solution X.
- In standard Lyapunov case, existence and uniqueness guaranteed if A stable (Λ(A) ⊂ C[−]); this is not sufficient here: (1) is equivalent to

$$\left(I_n \otimes A + A \otimes I_n + \sum_{i=1}^m N_i \otimes N_i\right) \operatorname{vec}(X) = -\operatorname{vec}(BB^T).$$

One sufficient condition for stable A is smallness of N_i (related to stability radius of A)

→ bounded-input bounded-output (BIBO) stability of bilinear systems. This will be assumed from here on, hence: existence and uniqueness of positive semi-definite solution $X = X^T$.

Application to Parametric MOR

Stochastic System

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• Want: solution methods for large scale problems, i.e., only matrix-matrix multiplication with *A*, *N_j*, solves with (shifted) *A* allowed!

Application to Parametric MOR



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- Want: solution methods for large scale problems, i.e., only matrix-matrix multiplication with *A*, *N_j*, solves with (shifted) *A* allowed!
- Requires to compute data-sparse approximation to generally dense X; here: X ≈ ZZ^T with Z ∈ ℝ^{n×nz}, n_Z ≪ n!



Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

Existence of low-rank approximations



Can we expect low-rank approximations $ZZ^T \approx X$ to the solution of

$$AX + XA^{T} + \sum_{j=1}^{m} N_{j}XN_{j}^{T} + BB^{T} = 0$$
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Standard Lyapunov case:

[GRASEDYCK '04]

$$AX + XA^T + BB^T = 0 \iff \underbrace{(I_n \otimes A + A \otimes I_n)}_{=:\mathcal{A}} \operatorname{vec}(X) = -\operatorname{vec}(BB^T).$$



Existence of low-rank approximations

Standard Lyapunov case:

[Grasedyck '04]

$$AX + XA^{T} + BB^{T} = 0 \iff \underbrace{(I_{n} \otimes A + A \otimes I_{n})}_{=:\mathcal{A}} \operatorname{vec}(X) = -\operatorname{vec}(BB^{T}).$$

Apply

$$M^{-1} = -\int_0^\infty \exp(tM) \mathrm{d}t$$

to ${\cal A}$ and approximate the integral via (sinc) quadrature \Rightarrow

$$\mathcal{A}^{-1} ~pprox ~- \sum_{i=-k}^k \omega_i \exp(t_k \mathcal{A}),$$

with error $\sim \exp(-\sqrt{k})$ ($\exp(-k)$ if $A = A^{T}$), then an approximate Lyapunov solution is given by

$$\operatorname{vec}(X) \approx \operatorname{vec}(X_k) = \sum_{i=-k}^{k} \omega_i \exp(t_i A) \operatorname{vec}(BB^T).$$

Existence of low-rank approximations

Standard Lyapunov case:

[GRASEDYCK '04]

$$AX + XA^{T} + BB^{T} = 0 \iff \underbrace{(I_{n} \otimes A + A \otimes I_{n})}_{=:\mathcal{A}} \operatorname{vec}(X) = -\operatorname{vec}(BB^{T}).$$
$$\operatorname{vec}(X) \approx \operatorname{vec}(X_{k}) = \sum_{i=:\mathcal{A}}^{k} \omega_{i} \exp(t_{i}\mathcal{A}) \operatorname{vec}(BB^{T}).$$

i = -k

$$\exp(t_i A) = \exp(t_i (I_n \otimes A + A \otimes I_n)) \equiv \exp(t_i A) \otimes \exp(t_i A).$$



Existence of low-rank approximations

Standard Lyapunov case:

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$$\operatorname{vec}(X) \approx \operatorname{vec}(X_k) = \sum_{i=-k} \omega_i \exp(t_i \mathcal{A}) \operatorname{vec}(BB^T).$$

Now observe that

$$\exp(t_i A) = \exp(t_i (I_n \otimes A + A \otimes I_n)) \equiv \exp(t_i A) \otimes \exp(t_i A).$$

Hence,

$$\operatorname{vec}(X_k) = \sum_{i=-k}^k \omega_i \left(\exp(t_i A) \otimes \exp(t_i A) \right) \operatorname{vec}(BB^T)$$


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Hence,

$$\operatorname{vec}(X_k) = \sum_{i=-k}^{k} \omega_i \left(\exp(t_i A) \otimes \exp(t_i A) \right) \operatorname{vec}(BB^T)$$
$$\implies X_k = \sum_{i=-k}^{k} \omega_i \exp(t_i A) BB^T \exp(t_i A^T) \equiv \sum_{i=-k}^{k} \omega_i B_i B_i^T,$$

so that $\operatorname{rank}(X_k) \leq (2k+1)m$ with

$$\|X - X_k\|_2 \lesssim \exp(-\sqrt{k})$$
 ($\exp(-k)$ for $A = A^T$)!



Application to Parametric MOR

Stochastic System

Existence of low-rank approximations

Can we expect low-rank approximations $ZZ^T \approx X$ to the solution of

$$AX + XA^{T} + \sum_{j=1}^{m} N_{j}XN_{j}^{T} + BB^{T} = 0$$
?

Problem: in general,

$$\exp\left(t_i(I\otimes A+A\otimes+\sum_{j=1}^mN_j\otimes N_j)\right)\neq (\exp(t_iA)\otimes\exp(t_iA))\exp\left(t_i(\sum_{j=1}^mN_j\otimes N_j)\right).$$

Application to Parametric MOR

Stochastic System

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Existence of low-rank approximations

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?

Assume that m = 1 and $N_1 = UV^T$ with $U, V \in \mathbb{R}^{n \times r}$ and consider

$$(\underbrace{I_n \otimes A + A \otimes I_n}_{=\mathcal{A}} + N_1 \otimes N_1) \operatorname{vec}(X) = \underbrace{-\operatorname{vec}(BB^T)}_{=:y}.$$



Application to Parametric MOR

Stochastic System

Existence of low-rank approximations

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Sherman-Morrison-Woodbury \Longrightarrow

$$(I_r \otimes I_r + (V^T \otimes V^T) \mathcal{A}^{-1} (U \otimes U)) w = (V^T \otimes V^T) \mathcal{A}^{-1} y, \mathcal{A} \operatorname{vec}(X) = y - (U \otimes U) w.$$



Lyapunov Equations

Application to Parametric MO

Stochastic Syster

Existence of low-rank approximations

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Matrix representation of r.h.s., $-BB^T - U \operatorname{vec}^{-1}(w) U^T$ has rank $\leq r+1!$ \rightsquigarrow Apply results for linear Lyapunov equations with r.h.s of rank r+1.

Application to Parametric MOR

Stochastic System

Existence of low-rank approximations

Theorem



can be approximated by X_k of rank (2k+1)(m+r), with an error satisfying

Assume existence and uniqueness assumption with stable A and

 $N_i = U_i V_i^T$, with $U_i, V_i \in \mathbb{R}^{n \times r_i}$. Set $r = \sum_{i=1}^m r_i$.

$$|X-X_k\|_2 \lesssim \exp(-\sqrt{k}).$$



[B./BREITEN 2012]

Application to Parametric MOF

Stochastic System

Conclusions and Outlook

Bilinear Lyapunov Equations

Generalized alternating directions iteration (ADI)

Let us again consider the generalized Lyapunov equation

$$AP + PA^{T} + NPN^{T} + BB^{T} = 0.$$



Application to Parametric MOF

Stochastic System

Conclusions and Outlook

Bilinear Lyapunov Equations

Generalized alternating directions iteration (ADI)

Let us again consider the generalized Lyapunov equation

$$AP + PA^{T} + NPN^{T} + BB^{T} = 0.$$

For a fixed parameter p, we can rewrite the linear Lyapunov operator as

$$AP + PA^{T} = \frac{1}{2p} \left((A + pI)P(A + pI)^{T} - (A - pI)P(A - pI)^{T} \right)$$

Application to Parametric MOR

Stochastic System

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Bilinear Lyapunov Equations

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leading to the fix point iteration

[Damm '08]

$$P_{j} = (A - pl)^{-1}(A + pl)P_{j-1}(A + pl)^{T}(A - pl)^{-T} + 2p(A - pl)^{-1}(NP_{j-1}N^{T} + BB^{T})(A - pl)^{-T}$$

Application to Parametric MOR

Stochastic System

[Damm '08]

Ø

Bilinear Lyapunov Equations

Generalized alternating directions iteration (ADI)

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leading to the fix point iteration

$$P_{j} = (A - pI)^{-1}(A + pI)P_{j-1}(A + pI)^{T}(A - pI)^{-T} + 2p(A - pI)^{-1}(NP_{j-1}N^{T} + BB^{T})(A - pI)^{-T}.$$

$$\begin{split} P_j &\approx Z_j Z_j^T \; (\operatorname{rank} \left(Z_j \right) \ll n) \; \rightsquigarrow \text{ factored iteration} \\ Z_j Z_j^T &= (A - pI)^{-1} (A + pI) Z_{j-1} Z_{j-1}^T (A + pI)^T (A - pI)^{-T} \\ &+ 2p (A - pI)^{-1} (N Z_{j-1} Z_{j-1}^T N^T + BB^T). \end{split}$$

Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

Generalized alternating directions iteration (ADI)



Hence, for a given sequence of shift parameters $\{p_1, \ldots, p_q\}$, we can extend the linear ADI iteration as follows:

$$Z_{1} = \sqrt{2p_{1}} (A - p_{1}I)^{-1} B,$$

$$Z_{j} = (A - p_{j}I)^{-1} [(A + p_{j}I) Z_{j-1} \quad \sqrt{2p_{j}}B \quad \sqrt{2p_{j}}NZ_{j-1}], \quad j \leq q.$$

Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

Generalized alternating directions iteration (ADI)



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Problems:

- A and N in general do not commute → we have to operate on full preceding subspace Z_{j-1} in each step.
- Rapid increase of rank (Z_j) → perform some kind of column compression.
- Choice of shift parameters? → No obvious generalization of minimax problem.
 Here, we will use shifts minimizing a certain *H*₂-optimization problem, see [B./BREITEN '11].

Application to Parametric MOR

Stochastic System

Conclusions and Outlook

16/27

Generalized alternating directions iteration (ADI)

Numerical Example: A Heat Transfer Model with Uncertainty

- 2-dimensional heat distribution motivated by [BENNER/SAAK '05]
- boundary control by a cooling fluid with an uncertain spraying intensity

$$\Omega = (0, 1) \times (0, 1)$$

$$x_t = \Delta x \qquad \text{in } \Omega$$

$$n \cdot \nabla x = (0.5 + d\omega_1) x \qquad \text{on } \Gamma_1$$

$$x = u \qquad \qquad \text{on } \Gamma_2$$

$$x = 0 \qquad \qquad \text{on } \Gamma_3, \Gamma_4$$

• spatial discretization $k \times k$ -grid

$$\Rightarrow dx \approx Axdt + Nxd\omega_i + Budt$$

• output: $C = \frac{1}{k^2} \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}$



Generalized alternating directions iteration (ADI)

Numerical Example: A Heat Transfer Model with Uncertainty

Conv. history for bilinear low-rank ADI method (n = 40,000)



Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Bilinear Lyapunov Equations

Generalizing the Extended Krylov Subspace Method (EKSM) [SIMONCINI '07]

Low-rank solutions of the generalized Lyapunov equation now may be obtained by projecting the original equation onto a suitable smaller subspace $\mathcal{V} = \operatorname{span}(V), \ V \in \mathbb{R}^{n \times k}$, with $V^T V = I$.

In more detail, solve

$$\left(V^{T}AV\right)\hat{X} + \hat{X}\left(V^{T}A^{T}V\right) + \left(V^{T}NV\right)\hat{X}\left(V^{T}N^{T}V\right) + \left(V^{T}B\right)\left(B^{T}V\right) = 0$$

and prolongate $X \approx V \hat{X} V^T$.



Application to Parametric MOR

Stochastic System

Conclusions and Outlook

Bilinear Lyapunov Equations

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and prolongate $X \approx V \hat{X} V^T$.

For this, one might use the extended Krylov subspace method (EKSM) algorithm in the following way:



Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

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For this, one might use the extended Krylov subspace method (EKSM) algorithm in the following way:

$$V_1 = \begin{bmatrix} B & A^{-1}B \end{bmatrix},$$

$$V_r = \begin{bmatrix} AV_{r-1} & A^{-1}V_{r-1} & NV_{r-1} \end{bmatrix}, \quad r = 2, 3, \dots$$



Application to Parametric MOR

Stochastic System

Bilinear Lyapunov Equations

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However, criteria like dissipativity of A for the linear case which ensure solvability of the projected equation have to be further investigated.



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Residua	I computation in $\mathcal{O}(k^2)$	3)	<u> </u>
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Theorem

Let $V_i \in \mathbb{R}^{n \times k_i}$ be the extendend Krylov matrix after *i* generalized EKSM steps. Denote the residual associated with the approximate solution $X_i = V_i \hat{X}_i V_i^T$ by

$$R_i := AX_i + X_i A^T + NX_i N^T + BB^T,$$

where \hat{X}_i is the solution of the reduced bilinear Lyapunov equation

$$V_i^T A V_i \hat{X}_i + \hat{X}_i V_i^T A^T V_i + V_i^T N V_i \hat{X}_i V_i^T N^T V_i + V_i^T B B^T V_i = 0.$$

Then:

- range $(R_i) \subset$ range (V_{i+1}) ,
- $||R_i|| = ||V_{i+1}^T R_i V_{i+1}||$ for the Frobenius and spectral norms.

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Then:

- range $(R_i) \subset$ range (V_{i+1}) ,
- $||R_i|| = ||V_{i+1}^T R_i V_{i+1}||$ for the Frobenius and spectral norms.

Remarks:

- Residual evaluation only requires quantities needed in *i* + 1st projection step plus O(k³_{i+1}) operations.
- No Hessenberg structure of reduced system matrix that allows to simplify residual expression as in standard Lyapunov case!

Bilinear EKSM

Numerical Example: A Heat Transfer Model with Uncertainty





Tensorized Krylov subspace methods

Another possibility is to iteratively solve the linear system

$$(I_n \otimes A + A \otimes I_n + N \otimes N) \operatorname{vec}(P) = -\operatorname{vec}(BB^T),$$

with a fixed number of ADI iteration steps used as a preconditioner ${\cal M}$

$$\mathcal{M}^{-1}(I_n \otimes A + A \otimes I_n + A_1 \otimes A_1) \operatorname{vec}(P) = -\mathcal{M}^{-1} \operatorname{vec}(BB^{\mathsf{T}}).$$

We implemented this approach for PCG and BiCGstab.

Updates like $X_{k+1} \leftarrow X_k + \omega_k P_k$ require truncation operator to preserve low-order structure.

Note, that the low-rank factorization $X \approx ZZ^T$ has to be replaced by $X \approx ZDZ^T$, *D* possibly indefinite.

Similar to more general tensorized Krylov solvers, see [Kressner/Tobler '10/'12].



Tensorized Krylov subspace methods

Vanilla implementation of tensor-PCG for bilinear matrix equations

Algorithm 1 Preconditioned CG method for $\mathcal{A}(X) - \mathcal{B}$

Input: Matrix functions $\mathcal{A}, \mathcal{M}: \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n}$, low rank factor B of right-hand side $\mathcal{B} = -BB^{T}$. Truncation operator \mathcal{T} w.r.t. relative accuracy ϵ_{rel} . **Output:** Low rank approximation $X = LDL^T$ with $||\mathcal{A}(X) - \mathcal{B}||_F < \text{tol.}$ 1: $X_0 = 0$, $R_0 = \mathcal{B}$, $Z_0 = \mathcal{M}^{-1}(R_0)$, $P_0 = Z_0$, $Q_0 = \mathcal{A}(P_0)$, $\xi_0 = \langle P_0, Q_0 \rangle$, k = 02: while $||R_k||_F > \text{tol } \mathbf{do}$ $\omega_k = \frac{\langle R_k, P_k \rangle}{\epsilon}$ 3: 4: $X_{k+1} = X_k + \omega_k P_k,$ $X_{k+1} \leftarrow \mathcal{T}(X_{k+1})$ Optionally: $R_{k+1} \leftarrow \mathcal{T}(R_{k+1})$ $R_{k+1} = \mathcal{B} - \mathcal{A}(X_{k+1}),$ 5: 6: $Z_{k+1} = \mathcal{M}^{-1}(R_{k+1})$ $\beta_k = -\frac{\langle Z_{k+1}, Q_k \rangle}{\varepsilon_k}$ 7: 8. $P_{k+1} = Z_{k+1} + \beta_k P_k.$ $P_{k+1} \leftarrow \mathcal{T}(P_{k+1})$ Optionally: $Q_{k+1} \leftarrow \mathcal{T}(Q_{k+1})$ 9: $Q_{k+1} = \mathcal{A}(P_{k+1}),$ 10. $\xi_{k+1} = \langle P_{k+1}, Q_{k+1} \rangle$ 11: k = k + 112: end while 13: $X = X_k$

Here, $\mathcal{A} : X \to AX + XA^{T} + NXN^{T}$, \mathcal{M} : ℓ steps of (bilinear) ADI, both in low-rank (" ZDZ^{T} " format).



Max Planck Institute Magdeburg





Comparison of methods

Comparison of CPU times

	Heat equation	RC circuit	Fokker-Planck
Bilin. ADI 2 \mathcal{H}_2 shifts	-	-	1.733 (1.578)
Bilin. ADI 6 \mathcal{H}_2 shifts	144,065 (2,274)	20,900 (3091)	-
Bilin. ADI 8 \mathcal{H}_2 shifts	135,711 (3,177)	-	-
Bilin. ADI 10 \mathcal{H}_2 shifts	33,051 (4,652)	-	-
Bilin. ADI 2 Wachspress shifts	-	-	6.617 (4.562)
Bilin. ADI 4 Wachspress shifts	41,883 (2,500)	18,046 (308)	-
CG (Bilin. ADI precond.)	15,640	-	-
BiCG (Bilin. ADI precond.)	-	16,131	11.581
BiCG (Linear ADI precond.)	-	12,652	9.680
EKSM	7,093	19,778	8.555

Numbers in brackets: computation of shift parameters.



Application to Parametric MOR ●○ Stochastic System

Application to Parametric MOR

Fast simulation of cyclic voltammogramms [Feng/Koziol/Rudnyi/Korvink '06]

$$\begin{aligned} E\dot{x}(t) &= (A + p_1(t)A_1 + p_2(t)A_2)x(t) + B, \\ y(t) &= Cx(t), \quad x(0) = x_0 \neq 0, \end{aligned}$$

- Rewrite as system with zero initial condition,
- FE model: n = 16,912, m = 3, q = 1,
- *p_j* ∈ [0, 10⁹] time-varying voltage functions,
- transfer function $H(i\omega, p_1, p_2)$,
- reduced system dimension r = 67,

$$\quad \underset{\substack{\omega \in \{\omega_{min}, \dots, \omega_{max}\}\\p_j \in \{p_{min}, \dots, p_{max}\}}}{\max} \frac{||H - \hat{H}||_2}{||H||_2} < 6 \cdot 10^{-4},$$

evaluation times: FOM 4.5h, ROM 38s
 → speed-up factor ≈ 426.



Application to Parametric MOF ●○ Stochastic System

Application to Parametric MOR

Fast simulation of cyclic voltammogramms [Feng/Koziol/Rudnyi/Korvink '06]





Iteration

Application to Parametric MOF ■∩ Stochastic System

Conclusions and Outlool

Application to Parametric MOR

Fast simulation of cyclic voltammogramms [Feng/Koziol/Rudnyi/Korvink '06]



 MOR
 Bilinear Lyapunov Equations
 Application to Parametric MOR
 Stochastic Systems
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Figure: [BAUR ET AL. '10]

Consider an anemometer, a flow sensing device located on a membrane used in context of minimizing heat dissipation.

$$E\dot{x}(t) = (A + pA_1)x(t) + Bu(t), \quad y(t) = Cx(t), \quad x(0) = 0,$$

- FE model: n = 29,008, m = 1, q = 3,
- $p_1 \in [0,1]$ fluid velocity,
- transfer function $H(i\omega, p_1)$, reduced system dimension r = 146,

$$\bullet \max_{\substack{\omega \in \{\omega_{min},\ldots,\omega_{max}\}\\ p_1 \in \{p_{min},\ldots,p_{max}\}}} \frac{\|H(\omega,p) - \hat{H}(\omega,p)\|_2}{\|H(\omega,p)\|_2} < 3 \cdot 10^{-5},$$

• evaluation times: FOM 51min, ROM 21s.





Iteration



 10^{-7}

 10^{-9}

0

200

400

600

800

Rank

1,200 1,400

1.000

Stochastic Systems

Itô-type linear stochastic differential equations (SDE):

$$\Sigma: \begin{cases} dx(t) = Ax(t)dt + Nx(t)d\omega(t) + Bu(t)dt, \\ y(t) = Cx(t), \quad x(0) = x_0. \end{cases}$$

Here, $A, N \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{q \times n}$ and $d\omega(t)$ are white noise processes associated with a Wiener process $\omega(t)$.

The SDE formalism is merely a notation for

$$x(t) = x(0) + \int_0^t Ax(\tau)d\tau + \int_0^t Nx(\tau)d\omega + \int_0^t Bu(\tau)d\tau,$$

with $d\omega_i$ denoting the Itô integral.

OR Bilinear Lyapunov Equations Application to Para

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Stochastic Systems

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Balanced truncation for linear SDEs requires the same steps as for deterministic systems, instead of standard Lyapunov equations need to solve again

$$AP + PA^{T} + NPN^{T} + BB^{T} = 0,$$

$$A^{T}Q + QA^{T} + N^{T}QN + C^{T}C = 0.$$
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Can show stability preservation under certain assumptions, but no error bound!

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 $AP + PA^{T} + NPN^{T} + BB^{T} = 0,$ $A^{T}Q + QA^{T} + N^{T}QN + C^{T}C = 0.$

Can show stability preservation under certain assumptions, but no error bound! **Alternative:** Applying balanced truncation using \tilde{P} and Q, where

 $\label{eq:approx_state} A\tilde{P}+\tilde{P}A^{T}+\tilde{P}N\tilde{P}^{-1}N^{T}\tilde{P}+BB^{T}=0,$

we obtain desired error bound $\|y - \hat{y}\|_{L^2_{\omega}} \leq 2\left(\sum_{j=r+1}^n \sigma_j\right) \|u\|_{L^2_{\omega}}$ [B./DAMM '12].



Itô-type linear stochastic differential equations (SDE):

$$\Sigma: \quad \begin{cases} dx(t) = Ax(t)dt + Nx(t)d\omega(t) + Bu(t)dt, \\ y(t) = Cx(t), \quad x(0) = x_0. \end{cases}$$

Balanced truncation for linear SDEs requires the same steps as for deterministic systems, instead of standard Lyapunov equations need to solve again

$$AP + PA^{T} + NPN^{T} + BB^{T} = 0,$$

$$A^{T}Q + QA^{T} + N^{T}QN + C^{T}C = 0.$$

Can show stability preservation under certain assumptions, but no error bound! **Alternative:** Applying balanced truncation using \tilde{P} and Q, where

$$A\tilde{P} + \tilde{P}A^{T} + \tilde{P}N\tilde{P}^{-1}N^{T}\tilde{P} + BB^{T} = 0,$$

we obtain desired error bound $\|y - \hat{y}\|_{L^2_{\omega}} \leq 2 \left(\sum_{j=r+1}^n \sigma_j\right) \|u\|_{L^2_{\omega}}$ [B./DAMM '12]. **Problem:** no satisfactory solution method for new nonlinear matrix equation! Note: using $\hat{P} := \tilde{P}^{-1}$, we obtain an algebraic Bernoulli equation:

$$\hat{P}A + A^T\hat{P} + N\hat{P}N^T + \hat{P}BB^T\hat{P} = 0.$$





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In analogy to LGQ BT for deterministic systems, could use solutions of stochastic LQG equations [WONHAM '68]:

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

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

- Solution for large-scale problems using Newton-ADI or Newton-EKSM [B./BREITEN ILAS 2011].
- No results regarding properties of reduced-order model.
- Might also use these equations for "LQG BT" for bilinear systems, but: these are not LQG equations from LQG design for bilinear systems; there, P, Q are state-dependent as, e.g., $B \rightarrow B + Nx!$

Bilinear Lyapunov Equations

Application to Parametric MOR

Stochastic System

Conclusions and Outlook



- Model reduction for bilinear and stochastic systems leads to the solution of generalized ("bilinear") Lyapunov equations.
- Special versions of balanced truncation for stochastic systems lead to nonlinear matrix equations.
- We have established a connection between special linear parametric and bilinear systems that automatically yields structure-preserving model reduction techniques for linear parametric systems.
- Under certain assumptions, we can expect the existence of low-rank approximations to the solution of generalized Lyapunov equations.
- Solutions strategies via extending the ADI iteration to bilinear systems and EKSM as well as using preconditioned iterative solvers like CG or BiCGstab up to dimensions n ~ 500,000 in MATLAB[®].
- Optimal choice of shift parameters for ADI is a nontrivial task.
- What about the singular value decay in case of N being full rank?

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http://www.mpi-magdeburg.mpg.de/preprints/index.php