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Solving Large-Scale Matrix Equations: Recent Progress and New Applications

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Overview

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Introduction

Linear Matrix Equations/Men with Beards

Sylvester equation

James Joseph Sylvester
(September 3, 1814 – March 15, 1897)

$$AX + XB = C.$$

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Lyapunov equation

Alexander Michailowitsch Ljapunow
(June 6, 1857 – November 3, 1918)

$$AX + XA^T = C, \quad C = C^T.$$

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Note:

- Consider only regular cases, having a unique solution!
- Solutions of symmetric cases are symmetric, $X = X^T \in \mathbb{R}^{n \times n}$; otherwise, $X \in \mathbb{R}^{n \times \ell}$ with $n \neq \ell$ in general.

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Generalizations of Sylvester ($AX + XB = C$) and Lyapunov ($AX + XA^T = C$) Equations

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$$AX + XB + \sum_{k=1}^{m} N_k X M_k = C.$$

(Generalized) discrete bilinear Lyapunov/Stein-minus-positive eq.:

$$EXE^T - AXA^T - \sum_{k=1}^{m} N_k X N_k^T = C, \quad C = C^T.$$

Note: Again consider only regular cases, symmetric equations have symmetric solutions.

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$$\underbrace{\left(D^T \otimes A + B^T \otimes E\right)}_{=:\mathcal{A}} \underbrace{\mathrm{vec}(X)}_{=:x} = \underbrace{\mathrm{vec}(C)}_{=:c} \quad \Longleftrightarrow \quad \mathcal{A}x = c.$$

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Lemma

$$\Lambda(\mathcal{A}) = \{\alpha_j + \beta_k \mid \alpha_j \in \Lambda(A, E),\ \beta_k \in \Lambda(B, D)\}.$$

Hence, (1) has unique solution $\Longrightarrow \Lambda(A, E) \cap -\Lambda(B, D) = \emptyset$.

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Example: Lyapunov equation $AX + XA^T = C$ has unique solution

$$\iff \nexists\, \mu \in \mathbb{C} : \pm\mu \in \Lambda(A).$$

Introduction

The Classical Lyapunov Theorem

Theorem (Lyapunov 1892)

Let $A \in \mathbb{R}^{n \times n}$ and consider the Lyapunov operator $\mathcal{L} : X \to AX + XA^T$. Then the following are equivalent:

(a) $\forall Y > 0$: $\exists X > 0$: $\mathcal{L}(X) = -Y$,

(b) $\exists Y > 0$: $\exists X > 0$: $\mathcal{L}(X) = -Y$,

(c) $\Lambda(A) \subset \mathbb{C}^- := \{z \in \mathbb{C} \mid \Re z < 0\}$, *i.e., A is (asymptotically) stable or Hurwitz.*

A. M. Lyapunov. *The General Problem of the Stability of Motion* (in Russian). Doctoral dissertation, Univ. Kharkov 1892. English translation: Stability of Motion, Academic Press, New-York & London, 1966.

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The proof (c) $\Rightarrow$ (a) is trivial from the necessary and sufficient condition for existence and uniqueness, apart from the positive definiteness. The latter is shown by studying $z^H Yz$ for all eigenvectors z of A.

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Important in applications: the nonnegative case:

$$\mathcal{L}(X) = AX + XA^T = -WW^T, \quad \text{where} \quad W \in \mathbb{R}^{n\times n_W}, \; n_W \ll n.$$

A Hurwitz $\Rightarrow$ $\exists$ unique solution $X = ZZ^T$ for $Z \in \mathbb{R}^{n\times n_X}$ with $1 \le n_X \le n$.

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$$\underbrace{AX + XA^T}_{=:\mathcal{L}(X)} + \underbrace{\sum_{k=1}^{m} N_k X N_k^T}_{=:\mathcal{P}(X)} = C, \quad C = C^T \leq 0.$$

Note: The operator

$$\mathcal{P}(X) \mapsto \sum_{j=1}^{m} N_k X N_k^T$$

is nonnegative in the sense that $\mathcal{P}(X) \geq 0$, whenever $X \geq 0$.

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This nonnegative Lyapunov-plus-positive equation is the one occurring in applications like model order reduction.

If A is Hurwitz and the N_k are small enough, eigenvalue perturbation theory yields existence and uniqueness of solution.
This is related to the concept of bounded-input bounded-output (BIBO) stability of dynamical systems.

Introduction

Existence of Solutions of Linear Matrix Equations II

Theorem (Schneider 1965, Damm 2004)

Let $A \in \mathbb{R}^{n\times n}$ and consider the Lyapunov operator $\mathcal{L} : X \to AX + XA^T$ and a nonnegative operator $\mathcal{P}$ (i.e., $\mathcal{P}(X) \geq 0$ if $X \geq 0$).
The following are equivalent:

(a) $\forall Y > 0$: $\exists X > 0$: $\mathcal{L}(X) + \mathcal{P}(X) = -Y$,

(b) $\exists Y > 0$: $\exists X > 0$: $\mathcal{L}(X) + \mathcal{P}(X) = -Y$,

(c) $\exists Y \geq 0$ *with* (A, Y) *controllable:* $\exists X > 0$: $\mathcal{L}(X) + \mathcal{P}(X) = -Y$,

(d) $\Lambda(\mathcal{L} + \mathcal{P}) \subset \mathbb{C}^- := \{z \in \mathbb{C} \,|\, \Re z < 0\}$,

(e) $\Lambda(\mathcal{L}) \subset \mathbb{C}^-$ *and* $\rho(\mathcal{L}^{-1}\mathcal{P}) < 1$,

where $\rho(\mathcal{T}) = \max\{|\lambda| \,\big|\, \lambda \in \Lambda(\mathcal{T})\} =$ *spectral radius of* $\mathcal{T}$.

T. Damm. *Rational Matrix Equations in Stochastic Control.* Number 297 in Lecture Notes in Control and Information Sciences. Springer-Verlag, 2004.

H. Schneider. Positive operators and an inertia theorem. Numerische Mathematik, 7:11–17, 1965.

Overview

Applications

Stability Theory I — Classical

From Lyapunov's theorem, immediately obtain characterization of asymptotic stability of linear dynamical systems

$$\dot{x}(t) = Ax(t). \qquad (2)$$

Theorem (Lyapunov)

The following are equivalent:

- *For (2), the zero state is asymptotically stable.*
- *The Lyapunov equation $AX + XA^T = Y$ has a unique solution $X = X^T > 0$ for all $Y = Y^T < 0$.*
- *A is Hurwitz.*

A. M. Lyapunov. The General Problem of the Stability of Motion (In Russian). Doctoral dissertation, Univ. Kharkov 1892. English translation: Stability of Motion, Academic Press, New-York & London, 1966.

Applications

Stability Theory II — Detecting Hopf Bifurcations

Detecting instability in large-scale dynamical systems caused by Hopf bifurcations $\rightsquigarrow$ identifying the rightmost pair of complex eigenvalues of large sparse generalized eigenvalue problems.

[Meerbergen/Spence 2010] suggest Lyapunov inverse iteration for the dynamical system with parameter $\mu \in \mathbb{R}$

$$Mx_t = f(x; \mu).$$

Task: Identify critical points (x^*, μ^*) where the steady-state solution (i.e., $x_t \equiv 0$) changes from being stable to unstable.

Their continuation algorithm involves solution of generalized Lyapunov equation

$$AX_{j+1}M^T + MX_{j+1}A^T = -F_j \equiv F(X_j),$$

where $A = D_x f(\bar{x}; \bar{\mu})$ and $(\bar{x}; \bar{\mu})$ is current estimate of critical point.

K. Meerbergen, A. Spence. Inverse iteration for purely imaginary eigenvalues with application to the detection of Hopf bifurcations in large-scale problems. SIAM Journal on Matrix Analysis and Applications, 31:1982-1999, 2010.

H.C. Elman, K. Meerbergen, A. Spence, M. Wu. Lyapunov inverse iteration for identifying Hopf bifurcations in models of incompressible flow. SIAM Journal on Scientific Computing, 34(3):A1584-A1606, 2012.

Applications

Stability Theory III — Metastable Equilibria of Stochastic Systems

Metastable states of stochastic processes

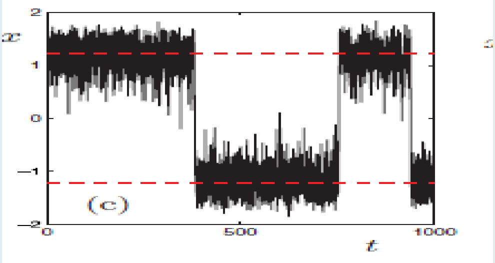

Figure: Metastable states (red dashed) and path of of a 1-dimensional stochastic ODE. This is Fig. 2.2(c) of [KUEHN 2012].

C. Kuehn. Deterministic continuation of stochastic metastable equilibria via Lyapunov equations and ellipsoids. SIAM Journal on Scientific Computing, 34(3):A1635-A1658, 2012.

Applications

Stability Theory III — Metastable Equilibria of Stochastic Systems

Tracking (w.r.t. a parameter $\mu \in \mathbb{R}$) metastable equilibrium points of stochastic differential equations (SDEs) via continuation methods:

Let $x \in \mathbb{R}^n$ and consider the SDE

$$dx_t = f(x_t;\mu)dt + \sigma F(x_t;\mu)dW_t,$$

where W_t = k-dimensional Brownian motion, $\sigma > 0$ controls the noise level and f, F sufficiently smooth.

For metastable equilibrium points $x^* := x^*(\mu)$, stochastic paths with high probability stay in regions characterized by covariance matrix C of x_t, linearized at x^*, defined by Lyapunov equation

$$A(x^*;\mu)C + CA(x^*;\mu)^T + \sigma^2 F(x^*;\mu)F(x^*;\mu)^T = 0.$$

where $A(x;\mu) := (D_x f)(x;\mu)$.

C. Kuehn. Deterministic continuation of stochastic metastable equilibria via Lyapunov equations and ellipsoids. SIAM Journal on Scientific Computing, 34(3):A1635-A1658, 2012.

Applications

Biochemical Engineering

Biochemical reaction networks under certain assumptions can be described by

$$\dot{c}(t) = Sv(c(t), q), \qquad (2)$$

where $S \in \mathbb{R}^{n\times m}$ is the stoichiometric matrix, $c(t) \in \mathbb{R}^n$ denotes the species concentrations, $v(t) \in \mathbb{R}^m$ the reaction rates, and q the rate constants.

In order to take molecular fluctuations (or intrinsic noise) due the stochasticity of the biochemical reactions into account, need the covariance matrix $C \in \mathbb{R}^{n\times n}$ of the concentrations. With

- the diffusion matrix $D \in \mathbb{R}^{n\times n}$ reflecting the randomness of the reaction events, and
- the drift matrix $A = \frac{\partial v}{\partial c}(c^0) \in \mathbb{R}^{n\times n}$ denoting the Jacobian of (2) along the macroscopic state trajectory at the equilibrium state c^0,

C is determined by the Lyapunov equation

$$AC + CA^T + D = 0.$$

P. Kügler, W. Yang. Identification of alterations in the Jacobian of biochemical reaction networks from steady state covariance data at two conditions. Journal of Mathematical Biology, 68:1757-1783, 2013.

Applications

Fractional Differential Equations

Fractional partial differential equations have received recent interest in various fields, e.g.,

- viscoelasticity (e.g., Kelvin-Voigt fractional derivative model),
- image processing,
- electro-analytical chemistry,
- biomedical engineering.

T. Breiten, V. Simoncini, M. Stoll. Fast iterative solvers for fractional differential equations. Max Planck Institute Magdeburg Preprints MPIMD/14-02, January 2014.

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Definition (Caputo derivative)

Given $f \in C^n(a,b)$, $\alpha \in [n-1, n)$, Caputo derivative of real order α is defined by:

$$ {}_a^C D_t^\alpha f(t) := \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{f^{(n)}(s)}{(t-s)^{\alpha-n+1}} ds. $$

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Definition (Riemann-Liouville derivative)

Given integrable $f(t)$ with $t \in [a, b]$, $\beta \in [n-1, n)$, left sided Riemann-Liouville derivative of real order β is defined by:

$$ {}_{a}^{RL}D_t^{\beta} f(t) := \frac{1}{\Gamma(n-\beta)} \left(\frac{d}{dt}\right)^n \int_a^t \frac{f(s)}{(t-s)^{\beta-n+1}} ds. $$

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Applications

Fractional Differential Equations

Consider fractional "heat equation"

$$ {}_{0}^{C}D_t^{\alpha} u(x,t) - {}_{a}^{RL}D_x^{\beta} u(x,t) = f(x,t). $$

For discretization use Grünwald-Letnikov formula ($\beta \in (1,2)$)

$$ {}_{a}^{RL}D_x^{\beta} u(x,t) = \lim_{M\to\infty} \frac{1}{h^{\alpha}} \sum_{k=0}^{M} g_{\beta,k}\, u(x-(k-1)h, t) $$

and as an approximation get

$$ {}_{a}^{RL}D_x^{\beta} u_i^{n+1} \approx \frac{1}{h_x^{\beta}} \sum_{k=0}^{i+1} g_{\beta,k}\, u_{i-k+1}^{n+1}. $$

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and as an approximation get in (Toeplitz) matrix form

$$ \underbrace{h_x^{-\beta} \begin{bmatrix} g_{\beta,1} & g_{\beta,0} & & & & & 0 \\ g_{\beta,2} & g_{\beta,1} & g_{\beta,0} & & & & \\ g_{\beta,3} & g_{\beta,2} & g_{\beta,1} & g_{\beta,0} & & & \\ \vdots & \ddots & g_{\beta,2} & g_{\beta,1} & \ddots & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & g_{\beta,0} & 0 \\ \vdots & \ddots & \ddots & \ddots & g_{\beta,2} & g_{\beta,1} & g_{\beta,0} \\ g_{\beta,n_x} & g_{\beta,n_x-1} & \cdots & \cdots & & g_{\beta,2} & g_{\beta,1} \end{bmatrix}}_{\mathbf{T}_{\beta}^{n_x}} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ u_{n_x-1}^{n+1} \\ u_{n_x}^{n+1} \end{bmatrix}. $$

Applications

Fractional Differential Equations

For fractional heat equation equation

$$ {}_{0}^{C}D_t^{\alpha} u(x,t) - {}_{a}^{RL}D_x^{\beta} u(x,t) = f(x,t) $$

get

$$ \left((\mathbf{T}_{\alpha}^{n_t} \otimes \mathbf{I}^{n_x}) - (\mathbf{I}^{n_t} \otimes \mathbf{L}_{\beta}^{n_x}) \right) \mathbf{u} = \mathbf{f} $$

where $\mathbf{T}_{\alpha}^{n_t}$ and $\mathbf{L}_{\beta}^{n_x}$ are Toeplitz matrices. With $\mathbf{u} = \mathrm{vec}(\mathbf{U})$ and dropping all superscripts this corresponds to the Sylvester equation

$$ \mathbf{U}\mathbf{T}_{\alpha}^{T} - \mathbf{L}_{\beta}\mathbf{U} = \mathbf{F}. $$

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Some Classical Applications

Algebraic Riccati Equations (ARE)

Solving AREs by Newtons's Method

Feedback control design often involves solution of

$$A^T X + XA - XGX + H = 0, \quad G = G^T, H = H^T.$$

$\rightsquigarrow$ In each Newton step, solve Lyapunov equation

$$(A - GX_j)^T X_{j+1} + X_{j+1}(A - GX_j) = -X_j G X_j - H.$$

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⇝ In each Newton step, solve Lyapunov equation

$$(A - GX_j)^T X_{j+1} + X_{j+1}(A - GX_j) = -X_j GX_j - H.$$

Decoupling of dynamical systems, e.g., in slow/fast modes, requires solution of nonsymmetric ARE

$$AX + XF - XGX + H = 0.$$

⇝ In each Newton step, solve Sylvester equation

$$(A - X_j G)X_{j+1} + X_{j+1}(F - GX_j) = -X_j GX_j - H.$$

Some Classical Applications

Model Reduction

Model Reduction via Balanced Truncation

For linear dynamical system

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx_r(t), \qquad x(t) \in \mathbb{R}^n$$

find reduced-order system

$$\dot{x}_r(t) = A_r x_r(t) + B_r u(t), \quad y_r(t) = C_r x_r(t), \qquad x(t) \in \mathbb{R}^r, \quad r \ll n$$

such that $\|y(t) - y_r(t)\| < \delta$.

The popular method balanced truncation requires the solution of the dual Lyapunov equations

$$AX + XA^T + BB^T = 0, \qquad A^T Y + YA + C^T C = 0.$$

Overview

This part: joint work with Patrick Kürschner and Jens Saak (MPI Magdeburg)

Solving Large-Scale Sylvester and Lyapunov Equations

The Low-Rank Structure

Sylvester Equations

Find $X \in \mathbb{R}^{n\times m}$ solving

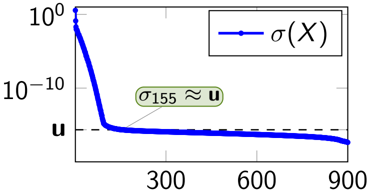
$$AX - XB = FG^T,$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{m\times m}$, $F \in \mathbb{R}^{n\times r}$, $G \in \mathbb{R}^{m\times r}$.

If n, m large, but $r \ll n, m$
$\rightsquigarrow$ X has a small numerical rank.
[Penzl 1999, Grasedyck 2004, Antoulas/Sorensen/Zhou 2002]

$$\operatorname{rank}(X, \tau) = f \ll \min(n, m)$$

singular values of 1600 × 900 example



$\rightsquigarrow$ Compute low-rank solution factors $Z \in \mathbb{R}^{n\times f}$, $Y \in \mathbb{R}^{m\times f}$, $D \in \mathbb{R}^{f\times f}$, such that $X \approx ZDY^T$ with $f \ll \min(n, m)$.

Solving Large-Scale Sylvester and Lyapunov Equations

The Low-Rank Structure

Lyapunov Equations

Find $X \in \mathbb{R}^{n\times n}$ solving

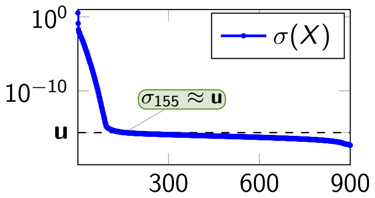
$$AX + XA^T = -FF^T,$$

where $A \in \mathbb{R}^{n\times n}$, $F \in \mathbb{R}^{n\times r}$.

If n large, but $r \ll n$
$\rightsquigarrow$ X has a small numerical rank.
[Penzl 1999, Grasedyck 2004, Antoulas/Sorensen/Zhou 2002]

$$\operatorname{rank}(X,\tau) = f \ll n$$

singular values of 1600×900 example



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Solving Large-Scale Sylvester and Lyapunov Equations

Some Basics

Sylvester equation $AX - XB = FG^T$ is equivalent to linear system of equations

$$\left(I_m \otimes A - B^T \otimes I_n\right) \mathrm{vec}(x) = \mathrm{vec}(FG^T).$$

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- in Lyapunov case, symmetry and possible definiteness are not respected.

Possible solvers:

- Standard Krylov subspace solvers in operator from [Hochbruck, Starke, Reichel, Bao, ...].
- Block-Tensor-Krylov subspace methods with truncation [Kressner/Tobler, Bollhöfer/Eppler, B./Breiten, ...].
- Galerkin-type methods based on (extended, rational) Krylov subspace methods [Jaimoukha, Kasenally, Jbilou, Simoncini, Druskin, Knizhermann,...]
- Doubling-type methods [Smith, Chu et al., B./Sadkane/El Khoury, ...].
- ADI methods [Wachspress, Reichel et al., Li, Penzl, B., Saak, Kürschner, ...].

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

Sylvester and Stein equations

Let $\alpha \neq \beta$ with $\alpha \notin \Lambda(B)$, $\beta \notin \Lambda(A)$, then

$$\underbrace{AX - XB = FG^T}_{\text{Sylvester equation}} \quad \Leftrightarrow \quad \underbrace{X = \mathcal{A} X \mathcal{B} + (\beta - \alpha) \mathcal{F} \mathcal{G}^H}_{\text{Stein equation}}$$

with the Cayley like transformations

$$\mathcal{A} := (A - \beta I_n)^{-1}(A - \alpha I_n), \qquad \mathcal{B} := (B - \alpha I_m)^{-1}(B - \beta I_m),$$
$$\mathcal{F} := (A - \beta I_n)^{-1} F, \qquad \mathcal{G} := (B - \alpha I_m)^{-H} G.$$

$\leadsto$ fix point iteration

$$X_k = \mathcal{A} X_{k-1} \mathcal{B} + (\beta - \alpha) \mathcal{F} \mathcal{G}^H$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$.

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

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Let $\alpha_{\mathbf{k}} \neq \beta_{\mathbf{k}}$ with $\alpha_{\mathbf{k}} \notin \Lambda(B)$, $\beta_{\mathbf{k}} \notin \Lambda(A)$, then

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$$\mathcal{A} := (A - \beta_{\mathbf{k}} I_n)^{-1}(A - \alpha_{\mathbf{k}} I_n), \qquad \mathcal{B} := (B - \alpha_{\mathbf{k}} I_m)^{-1}(B - \beta_{\mathbf{k}} I_m),$$
$$\mathcal{F} := (A - \beta_{\mathbf{k}} I_n)^{-1} F, \qquad \mathcal{G} := (B - \alpha_{\mathbf{k}} I_m)^{-H} G.$$

$\rightsquigarrow$ **alternating directions implicit (ADI)** iteration

$$X_k = \mathcal{A}_{\mathbf{k}} X_{k-1} \mathcal{B}_{\mathbf{k}} + (\beta_{\mathbf{k}} - \alpha_{\mathbf{k}}) \mathcal{F}_{\mathbf{k}} \mathcal{G}^H{}_{\mathbf{k}}$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$. [Wachspress 1988]

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H,$$
$$\mathcal{A}_k := (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m),$$
$$\mathcal{F}_k := (A - \beta_k I_n)^{-1} F \in \mathbb{R}^{n \times r}, \quad \mathcal{G}_k := (B - \alpha_k I_m)^{-H} G \in \mathbb{C}^{m \times r}.$$

Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = \mathcal{A}_1 X_0 \mathcal{B}_1 + (\beta_1 - \alpha_1)\mathcal{F}_1 \mathcal{G}_1^H$$

,

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H,$$

$$\mathcal{A}_k := (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m),$$

$$\mathcal{F}_k := (A - \beta_k I_n)^{-1} F \in \mathbb{R}^{n \times r}, \quad \mathcal{G}_k := (B - \alpha_k I_m)^{-H} G \in \mathbb{C}^{m \times r}.$$

Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = (\beta_1 - \alpha_1)(A - \beta_1 I_n)^{-1} F G^T (B - \alpha_1 I_m)^{-1}$$

$$\Rightarrow V_1 := Z_1 = (A - \beta_1 I_n)^{-1} F \in \mathbb{R}^{n \times r},$$

$$D_1 = (\beta_1 - \alpha_1) I_r \in \mathbb{R}^{r \times r},$$

$$W_1 := Y_1 = (B - \alpha_1 I_m)^{-H} G \in \mathbb{C}^{m \times r}.$$

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

Sylvester ADI iteration [Wachspress 1988]

$$
\begin{aligned}
X_k &= \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H, \\
\mathcal{A}_k &:= (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m), \\
\mathcal{F}_k &:= (A - \beta_k I_n)^{-1} F \in \mathbb{R}^{n \times r}, \quad \mathcal{G}_k := (B - \alpha_k I_m)^{-H} G \in \mathbb{C}^{m \times r}.
\end{aligned}
$$

Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$
\begin{aligned}
X_2 &= \mathcal{A}_2 X_1 \mathcal{B}_2 + (\beta_2 - \alpha_2)\mathcal{F}_2 \mathcal{G}_2^H = \ldots = \\
V_2 &= V_1 + (\beta_2 - \alpha_1)(A + \beta_2 I)^{-1} V_1 \in \mathbb{R}^{n \times r}, \\
W_2 &= W_1 + \overline{(\alpha_2 - \beta_1)}(B + \alpha_2 I)^{-H} W_1 \in \mathbb{R}^{m \times r}, \\
Z_2 &= [Z_1, \;\; V_2], \\
D_2 &= \operatorname{diag}(D_1, (\beta_2 - \alpha_2) I_r), \\
Y_2 &= [Y_1, \;\; W_2].
\end{aligned}
$$

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Algorithm

[B. 2005, Li/Truhar 2008, B./Li/Truhar 2009]

Algorithm 1: Low-rank Sylvester ADI / factored ADI (fADI)

Input : Matrices defining $AX - XB = FG^T$ and shift parameters $\{\alpha_1, \ldots, \alpha_{k_{\max}}\}$, $\{\beta_1, \ldots, \beta_{k_{\max}}\}$.

Output: Z, D, Y such that $ZDY^H \approx X$.

$Z_1 = V_1 = (A - \beta_1 I_n)^{-1} F$,

$Y_1 = W_1 = (B - \alpha_1 I_m)^{-H} G$.

$D_1 = (\beta_1 - \alpha_1) I_r$

for $k = 2, \ldots, k_{\max}$ **do**

$V_k = V_{k-1} + (\beta_k - \alpha_{k-1})(A - \beta_k I_n)^{-1} V_{k-1}$.

$W_k = W_{k-1} + \overline{(\alpha_k - \beta_{k-1})}(B - \alpha_k I_n)^{-H} W_{k-1}$.

Update solution factors

$$Z_k = [Z_{k-1}, V_k], \quad Y_k = [Y_{k-1}, W_k], \quad D_k = \operatorname{diag}(D_{k-1}, (\beta_k - \alpha_k) I_r).$$

Solving Large-Scale Sylvester and Lyapunov Equations

ADI Shifts

Optimal Shifts

Solution of rational optimization problem

$$\min_{\substack{\alpha_j \in \mathbb{C} \\ \beta_j \in \mathbb{C}}} \max_{\substack{\lambda \in \Lambda(A) \\ \mu \in \Lambda(B)}} \prod_{j=1}^{k} \left| \frac{(\lambda - \alpha_j)(\mu - \beta_j)}{(\lambda - \beta_j)(\mu - \alpha_j)} \right|,$$

for which no analytic solution is known in general.

Some shift generation approaches:

- generalized Bagby points, [Levenberg/Reichel 1993]
- adaption of Penzl's cheap heuristic approach available [Penzl 1999, Li/Truhar 2008]
  $\rightsquigarrow$ approximate $\Lambda(A)$, $\Lambda(B)$ by small number of Ritz values w.r.t. A, A^{-1}, B, B^{-1} via Arnoldi,
- just taking these Ritz values alone also works well quite often.

Solving Large-Scale Sylvester and Lyapunov Equations

LR-ADI Derivation

Disadvantages of Low-Rank ADI as of 2012:

1. No efficient stopping criteria:
   - Difference in iterates $\rightsquigarrow$ norm of added columns/step: not reliable, stops often too late.
   - Residual is a full dense matrix, can not be calculated as such.
2. Requires complex arithmetic for real coefficients when complex shifts are used.
3. Expensive (only semi-automatic) set-up phase to precompute ADI shifts.

Solving Large-Scale Sylvester and Lyapunov Equations

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Will show: none of these disadvantages exists as of today
$\Longrightarrow$ speed-ups old vs. new LR-ADI can be up to 20!

Solving Large-Scale Sylvester and Lyapunov Equations

Low-Rank Structure of the Residual

Low-rank Structure of $\mathcal{S}_k$ in LR-ADI [B./Kürschner 2013]

$$\mathcal{S}_k := \underbrace{A\left(Z_k D_k Y_k^H\right) - \left(Z_k D_k Y_k^H\right) B - FG^T}_{\text{large, dense } n \times m \text{ matrix}} = -Q_k U_k^H \in \mathbb{C}^{n\times m},$$

$$Q_k = Q_{k-1} + (\beta_k - \alpha_k) V_k \in \mathbb{C}^{n\times r},$$

$$U_k = U_{k-1} - \overline{(\beta_k - \alpha_k)} W_k \in \mathbb{C}^{m\times r}.$$

$\Rightarrow \quad \operatorname{rank}(\mathcal{S}_k) \leq r.$

Moreover, with $Q_0 = F$, $U_0 = G$ it holds for the LR-ADI iterations

$$V_k = (A - \alpha_k I_n)^{-1} Q_{k-1},$$

$$W_k = (B - \beta_k I_m)^{-H} U_{k-1}, \quad \forall k \geq 1.$$

$\rightsquigarrow$ Holds also similarly in LR-ADI for Lyapunov equations.

[B./Kürschner/Saak 2013]

Solving Large-Scale Sylvester and Lyapunov Equations

⇝ Low-rank Sylvester ADI reloaded

[B./Kürschner 2013]

Algorithm 2: Reformulated Factored ADI iteration (fADI 2.0)

Input : Matrices defining $AX - XB = FG^T$ and shift parameters $\{\alpha_1, \ldots, \alpha_{k_{\max}}\}$, $\{\beta_1, \ldots, \beta_{k_{\max}}\}$, tolerance τ.

Output: Z, Y, D such that $ZDY^H \approx X$.

$Q_0 = F$, $U_0 = G$, $k = 1$.

while $\|Q_{k-1}U_{k-1}^H\| \geq \tau \|FG^T\|$ **do**

  $\gamma_k = \beta_k - \alpha_k$.

  $V_k = (A - \beta_k I_n)^{-1} Q_{k-1}$, $\quad W_k = (B - \alpha_k I_m)^{-H} U_{k-1}$,

  $Q_k = Q_{k-1} + \gamma_k V_k$, $\quad U_k = U_{k-1} - \overline{\gamma_k} W_k$.

  Update solution factors

$$Z_k = [Z_{k-1}, V_k],\ \ Y_k = [Y_{k-1}, W_k],\ \ D_k = \operatorname{diag}(D_{k-1}, \gamma_k I_r).$$

  $k++$

Solving Large-Scale Sylvester and Lyapunov Equations

Computing the Residual Norm

Low-rank factors $Q_k,\ U_k$ of the residual $\mathcal{S}_k$ now integral part of the iteration.
Allows a cheap computation of $\|\mathcal{S}_k\|_2$ via, e.g.,

$$\|\mathcal{S}_k\|_2 = \|Q_k U_k^H\|_2 = \|U_k R_k^H\|_2,\ Q_k = H_k R_k,\ H_k^H H_k = I_r$$

$\rightsquigarrow$ requires thin QR factorization of an $n \times r$ matrix and $\|\cdot\|_2$ computation of an $r \times r$ matrix.

Much cheaper than the traditional approach: apply Lanczos to $\mathcal{S}_k^H \mathcal{S}_k$ to get $\|\mathcal{S}_k\|_2 = \sqrt{\lambda_{\max}(\mathcal{S}_k^H \mathcal{S}_k)}$
$\rightsquigarrow$ requires several matrix vector products with $A,\ B$ (and $A^T,\ B^T$) and additional scalar products.

Note: In Lyapunov case, residual evaluation is almost "free" as no QR factorization is required.

Solving Large-Scale Sylvester and Lyapunov Equations

Low-Rank Structure of the Residual

Example I: 5-point discretizations of the operator ∼[Jbilou 2006]

$$L(x) := \Delta x - v.\nabla x - f(\xi_1, \xi_2)x$$

on $\Omega = (0,1)^2$ for $x = x(\xi_1,\ \xi_2)$, homogeneous Dirichlet BC.

A: 150 grid points, $v = [e^{\xi_1+\xi_2},\ 1000\xi_2]$, $f(\xi_1, \xi_2) = \xi_1$,

B: 120 grid points, $v = [\sin(\xi_1 + 2\xi_2),\ 20e^{\xi_1+\xi_2}]$, $f(\xi_1, \xi_2) = \xi_1\xi_2$.

$\Rightarrow n = 22500,\ m = 14400$, F, G random with $r = 4$ columns.

Shifts: 10 Ritz values w.r.t. A, A^{-1}, B, B^{-1} yield
20 α- shifts, 20 β- shifts

Solving Large-Scale Sylvester and Lyapunov Equations

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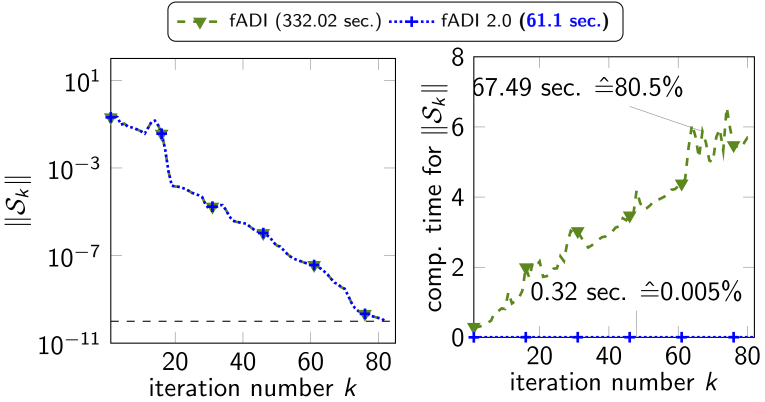


Solving Large-Scale Sylvester and Lyapunov Equations

Realification of LR-ADI

We have real matrices $A,\ B,\ F,\ G$ defining the Sylvester equation.
If $\Lambda(A),\ \Lambda(B) \subset \mathbb{C} \rightsquigarrow$ some $\alpha_k,\ \beta_k$ might be complex
$\rightsquigarrow$ complex operations in LR-ADI $\rightsquigarrow$ $Z,\ D,\ Y$ complex.

To generate real solution factors we need that $\{\alpha_k\},\ \{\beta_k\}$ form

Proper and suitably ordered sets of shifts

- If $\alpha_k \in \mathbb{C}$ then $\alpha_{k+1} = \overline{\alpha_k}$ and either $\beta_k, \beta_{k+1} = \overline{\beta_k} \in \mathbb{C}$ or $\beta_k, \beta_{k+1} \in \mathbb{R}$.
- If $\beta_k \in \mathbb{C}$ then $\beta_{k+1} = \overline{\beta_k}$ and either $\alpha_k, \alpha_{k+1} = \overline{\alpha_k} \in \mathbb{C}$ or $\alpha_k, \alpha_{k+1} \in \mathbb{R}$.

No restriction, since ADI is independent of the order of shifts.
Can be achieved by simple permutation of the sets of shifts.

Solving Large-Scale Sylvester and Lyapunov Equations

Realification of LR-ADI

Relation of Iterates [B./Kürschner 2013]

If $\alpha_k, \alpha_{k+1} = \overline{\alpha_k} \in \mathbb{C}$ and $\beta_k, \beta_{k+1} = \overline{\beta_k} \in \mathbb{C}$ then

$$V_{k+1} = \overline{V_k} + \frac{\beta_k - \gamma_k}{\operatorname{Im}(\beta_k)} \operatorname{Im}(V_k), \quad W_{k+1} = \overline{W_k} + \frac{\overline{\beta_k - \gamma_k}}{\operatorname{Im}(\alpha_k)} \operatorname{Im}(W_k).$$

- Linear systems with $A - \overline{\alpha_k} I_n$, $B - \overline{\beta_k} I_m$ not required,
- low-rank factors always augmented by real data:

$$\begin{aligned} Z_{k+1} &= \left[Z_{k-1}, [\operatorname{Re}(V_k), \operatorname{Im}(V_k)] \in \mathbb{R}^{n \times \mathbf{2r}} \right], \\ Y_{k+1} &= \left[Y_{k-1}, [\operatorname{Re}(W_k), \operatorname{Im}(W_k)] \in \mathbb{R}^{m \times \mathbf{2r}} \right], \\ D_{k+1} &= \operatorname{diag}\left(D_{k-1}, \left[\begin{smallmatrix} * & * \\ * & * \end{smallmatrix}\right] \in \mathbb{R}^{\mathbf{2r} \times \mathbf{2r}} \right), \end{aligned}$$

- similar relations for residual factors $Q_{k+1} \in \mathbb{R}^{n \times r}$, $U_{k+1} \in \mathbb{R}^{m \times r}$ and for the other shift sequences.

(Generalization of Lyapunov case as in [B./Kürschner/Saak 2012/13].)

Solving Large-Scale Sylvester and Lyapunov Equations

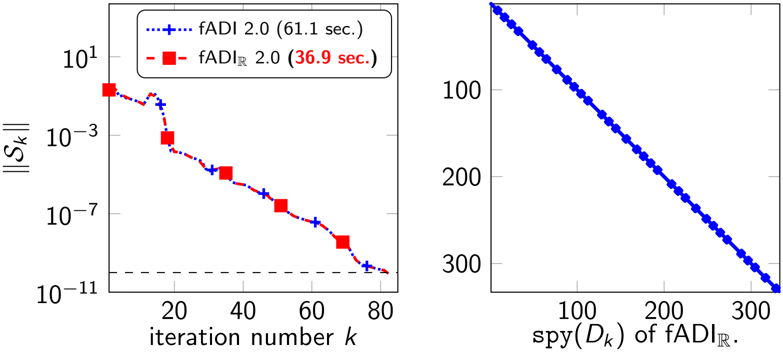
Realification of LR-ADI

Example I, cont.:

Shifts: 10 Ritz values w.r.t. A, A^{-1}, B, B^{-1} yield

20 α- shifts (4 real, 8 complex),

20 β- shifts (12 real, 4 complex).



Solving Large-Scale Sylvester and Lyapunov Equations

Self-generating Shifts

Problems with heuristic shifts:

- low-rank structure of solution not embraced,
- **no known rules for the numbers**
  - $\mathbf{k}_{\text{max}}$ of $\boldsymbol{\alpha}$ / $\boldsymbol{\beta}$ shifts,
  - Ritz values (i.e., Arnoldi steps)

$$\mathbf{k}_+^A,\ \mathbf{k}_-^A,\ \mathbf{k}_+^B,\ \mathbf{k}_-^B \quad \text{w.r.t.} \quad A,\ A^{-1},\ B,\ B^{-1},$$

- Arnoldi process brings additional costs.

Solving Large-Scale Sylvester and Lyapunov Equations

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- Arnoldi process brings additional costs.

Observation:

Even small changes in these numbers can lead to significantly different convergence results.

Solving Large-Scale Sylvester and Lyapunov Equations

Self-generating Shifts

A cheap but powerful way out [Hund 2012, B./Kürschner/Saak 2013]

1. Choose initial shifts, e.g,

$$\tilde{Q} = \texttt{orth}(F), \quad \tilde{U} = \texttt{orth}(G),$$
$$\{\alpha\} = \Lambda(\tilde{Q}^T A \tilde{Q}), \quad \{\beta\} = \Lambda(\tilde{U}^T B \tilde{U}).$$

2. If these are depleted during ADI compute new shifts via

$$\{\alpha_{\text{new}}\} = \Lambda(\tilde{Q}^T A \tilde{Q}), \quad \{\beta_{\text{new}}\} = \Lambda(\tilde{U}^T B \tilde{U}),$$

where

Variant 1: $\tilde{Q} = \texttt{orth}(\operatorname{Re}(V), \operatorname{Im}(V))$,
$\tilde{U} = \texttt{orth}(\operatorname{Re}(W), \operatorname{Im}(W))$ (iterates),

Variant 2: $\tilde{Q} = \texttt{orth}(Q)$, $\tilde{U} = \texttt{orth}(U)$ (residual factors).

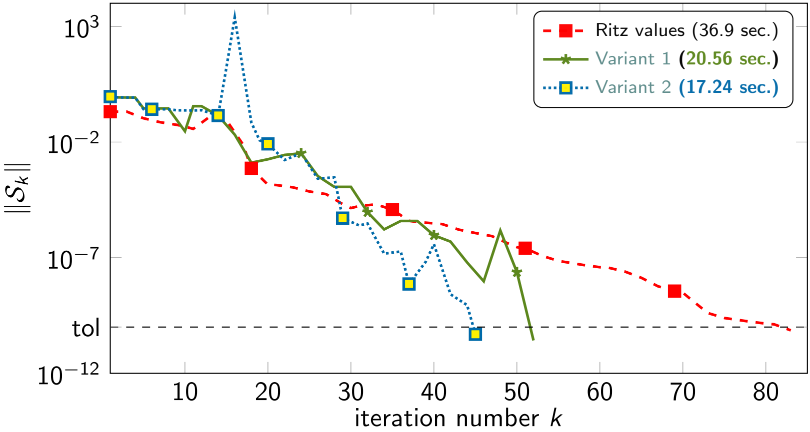
⇝ Works surprisingly well although **no setup parameters** are needed.

⇝ Theoretical foundation is current research.

Solving Large-Scale Sylvester and Lyapunov Equations

Self-generating Shifts

Example I, cont.:



Projection-Based Lyapunov Solvers. . .

. . . for 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 $\hat{A} := Z^T AZ$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
4. Use $X \approx Z\hat{X}Z^T$.

Projection-Based Lyapunov Solvers...

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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 $\hat{A} := Z^T AZ$, $\hat{B} := Z^T B$.
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 $m = 1$:

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

[Saad 1990, Jaimoukha/Kasenally 1994, Jbilou 2002–2008].

- Extended Krylov subspace method (EKSM) [Simoncini 2007],

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

- Rational Krylov subspace methods (RKSM) [Druskin/Simoncini 2011].

Solving Large-Scale Sylvester and Lyapunov Equations

The New LR-ADI Applied to Lyapunov Equations

Comparison of the new LR-ADI and EKSM

- Both methods require a system solve and several matvecs per iteration.

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- EKSM requires dissipativity of A, i.e., $A + A^T < 0$, to guarantee convergence, ADI only needs $\Lambda(A) \subset \mathbb{C}^-$.
- If it converges, EKSM is usually faster for SISO systems with $A = A^T < 0$.

The New LR-ADI Applied to Lyapunov Equations

Example II: an ocean circulation problem [Van Gijzen et al. 1998]

- FEM discretization of a simple 3D ocean circulation model (barotropic, constant depth) $\rightsquigarrow$ stiffness matrix $-A$ with $n = 42,249$, choose artificial constant term $B =$ `rand(n,5)`.

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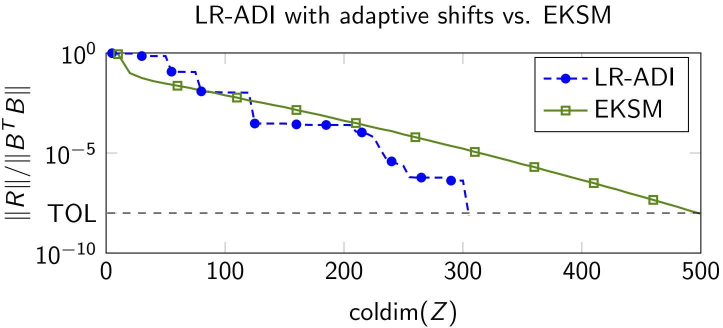
- **Convergence history:**



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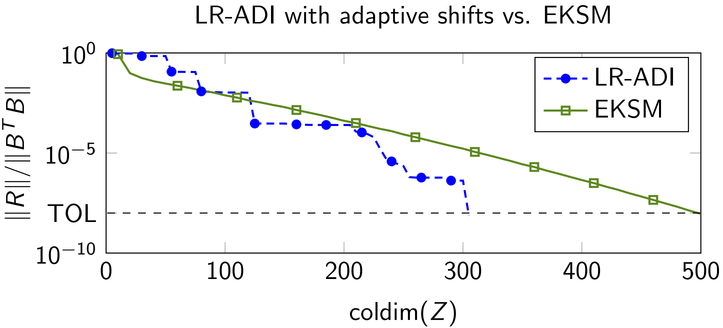
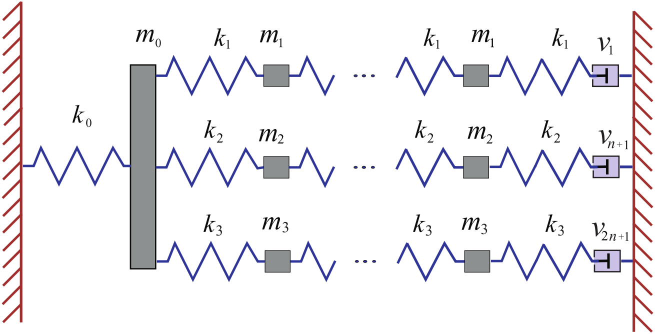


- CPU times: LR-ADI $\approx$ 110 sec, EKSM $\approx$ 135 sec.

The New LR-ADI Applied to Lyapunov Equations

Example III: the triple-chain-ocillator [Truhar/Veselic 2009]

- Standard vibrational system



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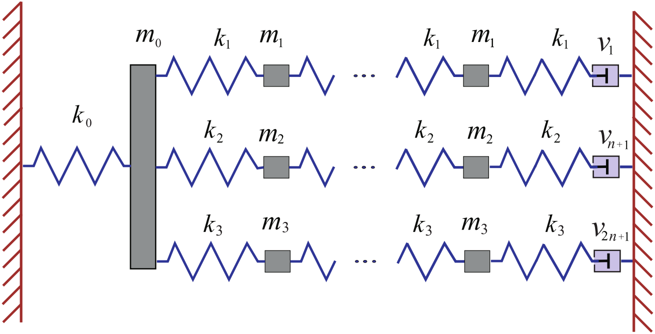

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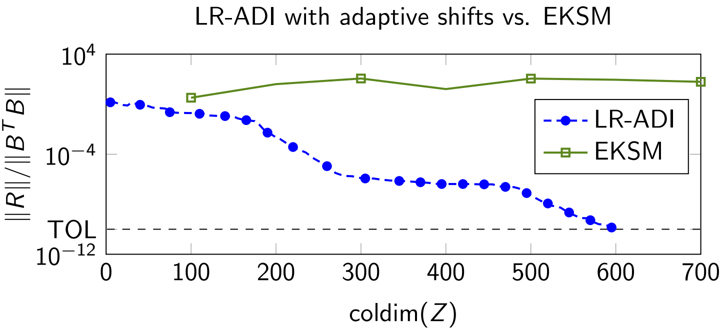

Solving Large-Scale Sylvester and Lyapunov Equations

Summary & Outlook

- Numerical enhancements of low-rank ADI for large Sylvester/Lyapunov equations:
  1. low-rank residuals, reformulated implementation,
  2. compute real low-rank factors in the presence of complex shifts,
  3. self-generating shift strategies (quantification in progress).

Recall the example:
332.02 sec. down to **17.24 sec.** $\rightsquigarrow$ acceleration by factor almost **20**.

- Generalized version enables derivation of low-rank solvers for various generalized Sylvester equations.
- Ongoing work:
  - Apply LR-ADI in Newton methods for algebraic Riccati equations

$$\mathcal{N}(X) = AX + XB + FG^T - XST^TX = 0,$$

$$\mathcal{D}(X) = AXA^T - EXE^T + SS^T + A^TXF(I_r + F^TXF)^{-1}F^TXA = 0.$$

Overview

This part: joint work with Tobias Breiten (KFU Graz, Austria)

Solving Large-Scale Lyapunov-plus-Positive Equations

Application: Balanced Truncation for Bilinear Systems

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].

Solving Large-Scale Lyapunov-plus-Positive Equations

Application: 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 Lyapunov-plus-positive equations:

$$AP + PA^T + \sum_{i=1}^{m} N_i P A_i^T + BB^T = 0,$$

$$A^T Q + QA^T + \sum_{i=1}^{m} N_i^T Q A_i + C^T C = 0.$$

- Due to its approximation quality, balanced truncation is method of choice for model reduction of medium-size biliner systems.
- For stationary iterative solvers, see [Damm 2008], extended to low-rank solutions recently by [Szyld/Shank/Simoncini 2014].

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Further applications:

- Analysis and model reduction for linear stochastic control systems driven by Wiener noise [B./Damm 2011], Lévy processes [B./Redmann 2011].
- Model reduction of linear parameter-varying (LPV) systems using bilinearization approach [B./Breiten 2011].
- Model reduction for Fokker-Planck equations [Hartmann et al. 2013].

Solving Large-Scale Lyapunov-plus-Positive Equations

Some basic facts and assumptions

$$AX + XA^T + \sum_{i=1}^{m} N_i X N_i^T + BB^T = 0. \tag{3}$$

- Need a positive semi-definite symmetric solution X.

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- As discussed before, solution theory for Lyapuonv-plus-positive equation is more involved then in standard Lyapuonv case. Here, existence and uniqueness of positive semi-definite solution $X = X^T$ is assumed.

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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: $X \approx ZZ^T$ with $Z \in \mathbb{R}^{n \times n_Z}$, $n_Z \ll n$!

Solving Large-Scale Lyapunov-plus-Positive Equations

Existence of Low-Rank Approximations

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

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Standard Lyapunov case: [Grasedyck '04]

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

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Apply

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

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

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

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

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

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Now observe that

$$\exp(t_i \mathcal{A}) = \exp\left(t_i(I_n \otimes A + A \otimes I_n)\right) \equiv \exp(t_i A) \otimes \exp(t_i A).$$

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$$\begin{aligned} \operatorname{vec}(X_k) &= \sum_{i=-k}^{k} \omega_i \left(\exp(t_i A) \otimes \exp(t_i A)\right) \operatorname{vec}(BB^T) \\ \Longrightarrow\ X_k &= \sum_{i=-k}^{k} \omega_i \exp(t_i A) B B^T \exp(t_i A^T) \equiv \sum_{i=-k}^{k} \omega_i B_i B_i^T, \end{aligned}$$

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

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

Solving Large-Scale Lyapunov-plus-Positive Equations

Existence of Low-Rank Approximations

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

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

Problem: in general,

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

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

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

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Sherman-Morrison-Woodbury $\Longrightarrow$

$$\begin{aligned}\left(I_r \otimes I_r + (V^T \otimes V^T)\mathcal{A}^{-1}(U \otimes U)\right) w &= (V^T \otimes V^T)\mathcal{A}^{-1} y,\\ \mathcal{A}\,\mathrm{vec}(X) &= y - (U \otimes U) w.\end{aligned}$$

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Rank of matrix representation of r.h.s. $-BB^T - U\,\mathrm{vec}^{-1}(w)\,U^T$ is $\leq\ r+1$!

$\rightsquigarrow$ Apply results for linear Lyapunov equations with r.h.s of rank $r+1$.

Solving Large-Scale Lyapunov-plus-Positive Equations

Existence of Low-Rank Approximations

Theorem [B./Breiten 2012]

Assume existence and uniqueness assumption with stable A and $N_j = U_j V_j^T$, with $U_j, V_j \in \mathbb{R}^{n \times r_j}$. Set $r = \sum_{j=1}^{m} r_j$.
Then the solution X of

$$AX + XA^T + \sum_{j=1}^{m} N_j X N_j^T + BB^T = 0$$

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

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

Solving Large-Scale Lyapunov-plus-Positive Equations

Generalized ADI Iteration

Let us again consider the Lyapunov-plus-positive equation

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

Solving Large-Scale Lyapunov-plus-Positive Equations

Generalized ADI Iteration

Let us again consider the Lyapunov-plus-positive equation

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

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

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

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leading to the fix point iteration [Damm 2008]

$$\begin{aligned} P_j = {} & (A - pI)^{-1}(A + pI)P_{j-1}(A + pI)^T(A - pI)^{-T} \\ & + 2p(A - pI)^{-1}(NP_{j-1}N^T + BB^T)(A - pI)^{-T}. \end{aligned}$$

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$P_j \approx Z_j Z_j^T$ $(\mathrm{rank}\,(Z_j) \ll n)$ $\rightsquigarrow$ factored iteration

$$\begin{aligned} Z_j Z_j^T = {} & (A-pI)^{-1}(A+pI)Z_{j-1}Z_{j-1}^T(A+pI)^T(A-pI)^{-T} \\ & + 2p(A-pI)^{-1}(NZ_{j-1}Z_{j-1}^T N^T + BB^T)(A-pI)^{-T}. \end{aligned}$$

Solving Large-Scale Lyapunov-plus-Positive Equations

Generalized ADI Iteration

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

$$Z_1 = \sqrt{2p_1}\,(A - p_1 I)^{-1}\,B,$$

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

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Z_j &= (A - p_j I)^{-1}\left[(A + p_j I)\, Z_{j-1} \quad \sqrt{2p_j} B \quad \sqrt{2p_j} N Z_{j-1}\right], \quad j \le q.
\end{aligned}
$$

Problems:

- A and N in general do not commute $\rightsquigarrow$ we have to operate on full preceding subspace Z_{j-1} in each step.
- Rapid increase of $\mathrm{rank}\,(Z_j)$ $\rightsquigarrow$ perform some kind of column compression.
- Choice of shift parameters? $\rightsquigarrow$ No obvious generalization of minimax problem.
  Here, we will use shifts minimizing a certain $\mathcal{H}_2$-optimization problem, see [B./Breiten 2011/14].

Generalized ADI Iteration

Numerical Example: A Heat Transfer Model with Uncertainty

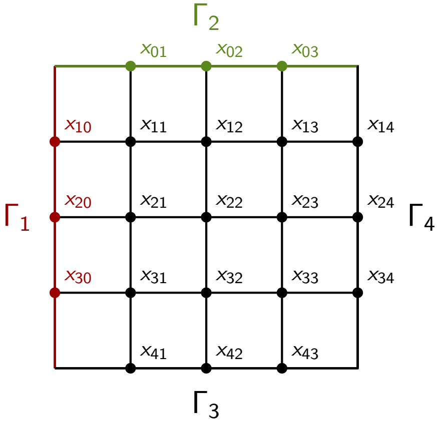
- 2-dimensional heat distribution motivated by [Benner/Saak '05]
- boundary control by a cooling fluid with an uncertain spraying intensity

$$\begin{aligned} \Omega &= (0,1) \times (0,1) & \\ x_t &= \Delta x & \text{in } \Omega \\ n \cdot \nabla x &= (0.5 + d\omega_1)x & \text{on } \Gamma_1 \\ x &= u & \text{on } \Gamma_2 \\ x &= 0 & \text{on } \Gamma_3, \Gamma_4 \end{aligned}$$

- spatial discretization $k \times k$-grid

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

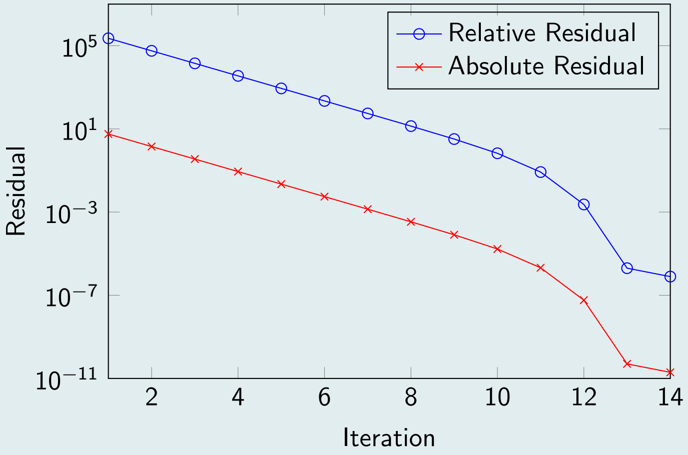
- output: $C = \frac{1}{k^2} \begin{bmatrix} 1 & \dots & 1 \end{bmatrix}$



Generalized ADI Iteration

Numerical Example: A Heat Transfer Model with Uncertainty

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



Solving Large-Scale Lyapunov-plus-Positive Equations

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

Low-rank solutions of the Lyapunov-plus-positive equation 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

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

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

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

$$V_1 = \begin{bmatrix} B & A^{-1}B \end{bmatrix},$$
$$V_r = \begin{bmatrix} AV_{r-1} & A^{-1}V_{r-1} & NV_{r-1} \end{bmatrix}, \quad r = 2, 3, \ldots$$

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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.

Bilinear EKSM

Residual Computation in $\mathcal{O}(k^3)$

Theorem (B./Breiten 2012)

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 Lyapunov-plus-positive equation

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

Then:

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

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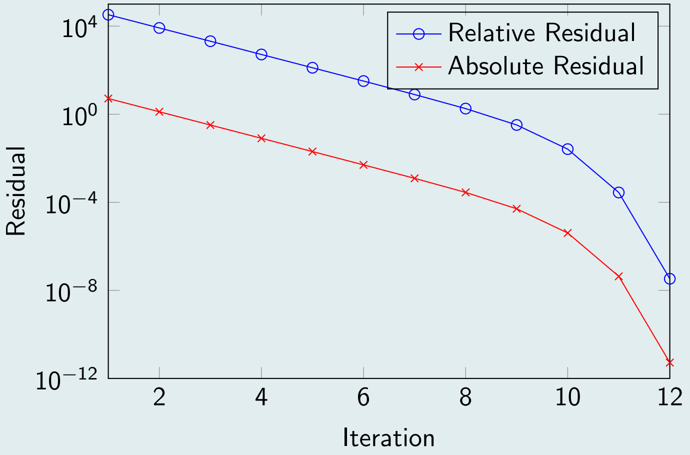
Remarks:

- Residual evaluation only requires quantities needed in $i+1$st projection step plus $\mathcal{O}(k_{i+1}^3)$ 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

Convergence history for bilinear EKSM variant ($n = 6,400$)



Solving Large-Scale Lyapunov-plus-Positive Equations

Tensorized Krylov Subspace Methods

Another possibility is to iteratively solve the linear system

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

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

$$\mathcal{M}^{-1}(I_n \otimes A + A \otimes I_n + N \otimes N)\,\mathrm{vec}(X) = -\mathcal{M}^{-1}\,\mathrm{vec}(BB^T).$$

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 2010/12].

Tensorized Krylov Subspace Methods

Vanilla Implementation of Tensor-PCG for Matrix Equations

Algorithm 3: 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 $||\mathcal{A}(X) - \mathcal{B}||_F \leq$ tol.

$X_0 = 0,\ R_0 = \mathcal{B},\ Z_0 = \mathcal{M}^{-1}(R_0),\ P_0 = Z_0,\ Q_0 = \mathcal{A}(P_0),\ \xi_0 = \langle P_0, Q_0\rangle, k = 0$

while $||R_k||_F > tol$ **do**

- $\omega_k = \frac{\langle R_k, P_k\rangle}{\xi_k}$
- $X_{k+1} = X_k + \omega_k P_k, \quad X_{k+1} \leftarrow \mathcal{T}(X_{k+1})$
- $R_{k+1} = \mathcal{B} - \mathcal{A}(X_{k+1}),$ *Optionally:* $R_{k+1} \leftarrow \mathcal{T}(R_{k+1})$
- $Z_{k+1} = \mathcal{M}^{-1}(R_{k+1})$
- $\beta_k = -\frac{\langle Z_{k+1}, Q_k\rangle}{\xi_k}$
- $P_{k+1} = Z_{k+1} + \beta_k P_k, \quad P_{k+1} \leftarrow \mathcal{T}(P_{k+1})$
- $Q_{k+1} = \mathcal{A}(P_{k+1}),$ *Optionally:* $Q_{k+1} \leftarrow \mathcal{T}(Q_{k+1})$
- $\xi_{k+1} = \langle P_{k+1}, Q_{k+1}\rangle$
- $k = k + 1$

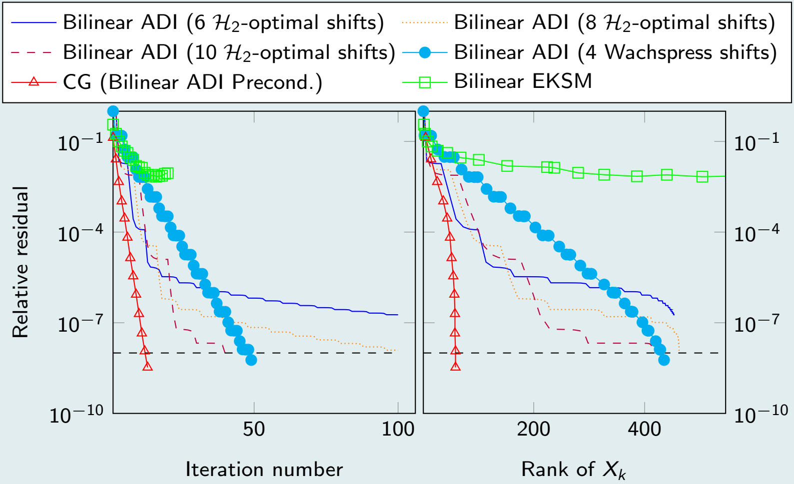
$X = X_k$

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

Comparison of Methods

Heat Equation with Boundary Control

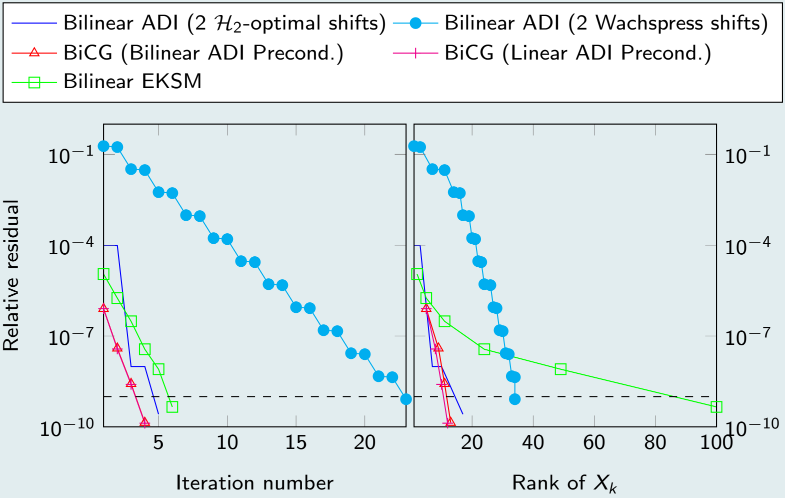
Comparison of low rank solution methods for $n = 562,500$.



Comparison of Methods

Fokker-Planck Equation

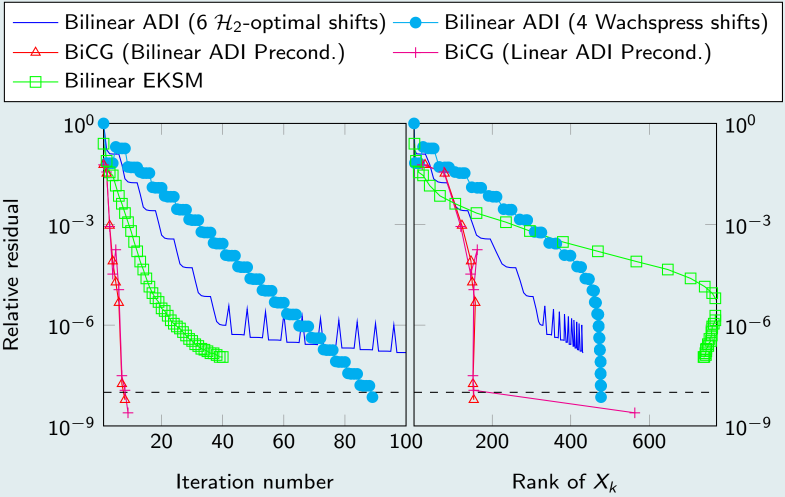
Comparison of low rank solution methods for $n = 10,000$.



Comparison of Methods

RC Circuit Simulation

Comparison of low rank solution methods for $n = 250,000$.



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.

Solving Large-Scale Lyapunov-plus-Positive Equations

Summary & Outlook

- Under certain assumptions, we can expect the existence of low-rank approximations to the solution of Lyapunov-plus-positive 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 $n \sim 500,000$ in MATLAB®.
- Optimal choice of shift parameters for ADI is a nontrivial task.
- Other "tricks" (realification, low-rank residuals) not adapted from standard case so far.
- What about the singular value decay in case of N being full rank?
- Need efficient implementation!

Further Reading

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(Upcoming) preprints available at

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