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Krylov Subspace Methods for Matrix Equations Which Include Matrix Functions

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Introduction

1. Problem - Matrix Equations

Large-scale Lyapunov equations

$$AX + XA^T = -R$$

Assumptions:

- $A \in \mathbb{R}^{n \times n}$ Hurwitz ($\Lambda(A) \subset \mathbb{C}_-$), large, sparse
  - We can efficiently compute matrix-vector products,
  - solve linear systems $Au = v$ (e.g., with Krylov methods),
  - but **cannot** compute Schur-, eigen-, singular value decompositions ($\mathcal{O}(n^3)$ complexity).
- right hand side $R = R^T \in \mathbb{R}^{n \times n}$,
- $X = X^T \in \mathbb{R}^{n \times n}$ is the sought solution
  - which we **cannot** store ($\mathcal{O}(n^2)$ storage) explicitly.

Introduction

Low-rank Phenomena

Large-scale Lyapunov equations, low-rank right hand side

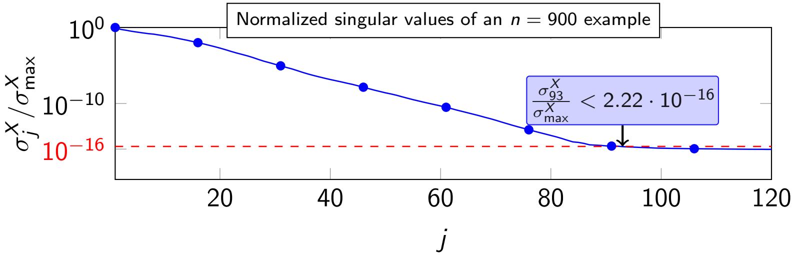
$$AX + XA^T = -BB^T, \quad B \in \mathbb{R}^{n\times r}, \quad r \ll n$$

Observation in practice, theoretical investigations

[Penzl '99, Antoulas/Sorenson/Zhou '02, Grasedyck '04]

$\rightsquigarrow$ X has small numerical rank:

$$\operatorname{rank}(X,\epsilon) := \operatorname*{argmin}_{j=1,\dots,n}\left(\frac{\sigma_j^X}{\sigma_{\max}^X} > \epsilon\right) \ll n, \quad \epsilon \ll 1$$



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$$\operatorname{rank}(X, \epsilon) := \operatorname*{argmin}_{j=1,\ldots,n} \left(\frac{\sigma_j^X}{\sigma_{\max}^X} > \epsilon \right) \ll n, \quad \epsilon \ll 1$$

Hence, we can approximate P by a low-rank factorization:

$$X \approx X_\ell = ZDZ^T, \quad Z \in \mathbb{R}^{n\times \ell}, \ D = D^T \in \mathbb{R}^{\ell\times\ell} \quad \text{with} \quad \ell \ll n.$$

Z, D are called **low-rank solution factors**.

Krylov Subspace Methods for Lyapunov Equations

Low-rank Solvers

Algorithms for computing low-rank solutions

- Low-rank (alternating directions implicit) ADI iteration (LR-ADI)

  [Penzl '99, Li/White '02, Benner/K./Saak '14]

Krylov Subspace Methods for Lyapunov Equations

Low-rank Solvers

Algorithms for computing low-rank solutions

- Low-rank (alternating directions implicit) ADI iteration (LR-ADI)
  [Penzl '99, Li/White '02, Benner/K./Saak '14]
- Projection methods: let $\mathcal{V} = \operatorname{span}\{V\} \subset \mathbb{R}^n$, $\dim(\mathcal{V}) = h \ll n$.
  Perform Galerkin projection to $AX + XA^T = -BB^T$ and solve small Lyapunov equation

$$(V^T AV)\tilde{X} + \tilde{X}(V^T A^T V) = -(V^T B)(B^T V)$$

by standard, dense methods for $\tilde{X}$. Then $V\tilde{X}V^T := X_k \approx X$.

Popular choices for $\mathcal{V}$:

- ordinary (block) Krylov subspaces $\mathcal{K}_k(A, B)$
  [Jaimoukha/Kasenally '94, ...]
- rational Krylov subspaces [Druskin/Knizherman/Simoncini '07/'11]

$$\mathcal{RK}_k(A, B, \xi) = d_{k-1}(A)^{-1}\mathcal{K}_k(A, B), \quad d_{k-1}(z) = \prod_{j=1}^{k-1}(1 - \tfrac{z}{\xi_j})$$

Krylov Methods for Matrix Functions

2. Problem - Matrix Function Times Vectors

Problem Statement

Given: $B \in \mathbb{R}^{n \times r}$, (smooth), nonlinear function f
Sought: Approximation to $B_f = f(A)B$.

Direct computation of $f(A)$ uses Schur-, eigen decomposition of A

$\rightsquigarrow$ not possible!

Again, a projection approach saves the day!
Let $B \in \mathcal{V} = \operatorname{span}\{V\} \subset \mathbb{C}^n$, $\dim(\mathcal{V}) = h \ll n$, $V^H V = I$.
Approximation: $B_f \approx VV^H B_f = V\hat{B}_f \in \mathcal{V}$, $\hat{B}_f := V^H B_f$.
Impose Ritz-Galerkin condition:

$$V\hat{B}_f - f(A)VV^H B \quad \perp \quad \mathcal{V} \quad \Longrightarrow \quad B_f \approx Vf(V^H AV)V^H B$$

$V^H AV \in \mathbb{C}^{h \times h} \Rightarrow f(V^H AV)$ can be computed.

Krylov Methods for Matrix Functions

2. Problem - Matrix Function Times Vectors

Popular choices for $\mathcal{V}$:

- Block Krylov subspace $\mathcal{V} = \mathcal{K}_k(A,\ B) \quad \Rightarrow f \approx p_{k-1} \in \mathcal{P}_{r(k-1)}$.
  Slow convergence for general functions f!
- Rational Krylov subspace $\mathcal{RK}_k(A, B, \xi) = d_{k-1}(A)^{-1}\mathcal{K}_k(A, B)$
  [Druskin/Knizherman '98, Beckermann/Reichel '09, Güttel '10]
  $\Rightarrow\ f \approx r_k = p_{k-1}/d_{k-1} \rightsquigarrow$ much better convergence for most f!

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- The shifts ξ_i (roots of d_{k-1}, poles of r_k) heavily influence the convergence speed.
- E.g., adaptive computation via [Druskin/Simoncini '11]

  $$\xi_{k+1} = \underset{s \in \mathcal{D}}{\operatorname{argmax}} |r_k(s)|^{-1},$$

  where $\mathcal{D}$ contains discrete points from boundary of the convex hull of $\Lambda(-V^H AV)$. $\rightsquigarrow$ RKSM$_{\mathcal{D}}$
- Choosing $\xi_{2k} = \infty$ and $\xi_{2k-1} = 0$ yields extended Krylov subspace
  $\mathcal{EK}_k(A, B) := \mathcal{K}_k(A,\ B) \cup \mathcal{K}_k(A^{-1},\ A^{-1}B)$ $\rightsquigarrow$ EKSM

Krylov Methods for Matrix Functions

Consider the Lyapunov equation

$$AX_f + X_f A^T = -f(A)BB^T - BB^T f(A).$$

Application: [Gawronski/Juang '90, Petterson '13]

Frequency-limited balanced truncation model order reduction of

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t).$$

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Frequency-limited balanced truncation model order reduction of

$$\dot{x}(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t).$$

There, $$f(A) = \frac{1}{2\pi}\int_{\Omega}(\mathrm{i}\omega I - A)^{-1}\mathrm{d}\omega = \frac{1}{\pi}\mathrm{Re}\left(\int_{\omega_1}^{\omega_2}(\mathrm{i}\omega I - A)^{-1}\mathrm{d}\omega\right)$$
$$= \mathrm{Re}\left(\frac{\mathrm{i}}{\pi}\log\left((A+\mathrm{i}\omega_1 I)^{-1}(A+\mathrm{i}\omega_2 I)\right)\right)$$

with frequency region $\Omega = -[\omega_1,\ \omega_2] \cup [\omega_1,\ \omega_2]$, $0 \leq \omega_1 < \omega_2 < \infty$.

Here, $\log M$ is the principal branch of the complex, matrix-valued, natural logarithm for $M \in \mathbb{C}^{n\times n}$ with $\Lambda(M) \in \mathbb{C}\backslash\mathbb{R}_-$.

Matrix Equations with Matrix Functions

Consider the Lyapunov equation

$$AX_f + X_f A^T = -f(A)BB^T - BB^T f(A).$$

Before we can compute a low-rank solution $Z_f D_f Z_f^T \approx X_f$ we have to approximate $f(A)B =: B_f$!

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Procedure part 1. [Benner/K./Saak '14/'15]

Employ rational (block) Krylov subspace method (RKSM) to get

- $\tilde{B}_f \approx B_f$ and orthonormal basis matrix V $(\mathrm{span}\,\{V\} = \mathcal{RK}_k(A, B, \xi))$.
- Recall $f(A) = \frac{1}{\pi}\,\mathrm{Re}\left(\int_{\omega_1}^{\omega_2} (\mathrm{i}\omega I - A)^{-1}\mathrm{d}\omega\right) = \mathrm{Re}\,\left(\frac{\mathrm{i}}{\pi}\log\ldots\right)$
- $\rightsquigarrow$ better adaptive shifts

$$\xi_{k+1} = \underset{s\in\mathrm{i}\hat{\Omega}}{\mathrm{argmax}}\,|r_k(s)|^{-1},$$

where $\hat{\Omega}$ contains discrete points from $[\omega_1,\ \omega_2]$ $\rightsquigarrow$ RKSM$_\Omega$

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Procedure part 2.

- Reuse V to solve Lyap.eqn. via Galerkin, i.e., solve

$$(V^T AV)\tilde{X}_f + \tilde{X}_f(V^T A^T V) = -(V^T \tilde{B}_f)(B^T V) - (V^T B)(\tilde{B}_f^T V)$$

  for $\tilde{X}_f$ and obtain $X_f \approx X_{f,k} := V\tilde{X}_f V^T$.
- If required (often not), continue RKSM until $\|AX_{f,k} + X_{f,k}A^T + \tilde{B}_f B^T + B\tilde{B}_f^T\| < \mathrm{tol}$

Numerical Examples

$AX_f \quad + \quad X_f A^T = -B_f B^T - BB_f^T, \quad f(z) = \mathrm{Re}\left(\frac{\mathrm{i}}{\pi}\log\frac{z+\mathrm{i}\omega_2}{z+\mathrm{i}\omega_1}\right)$

Example `fdm_2d`: $A \hat{=}$ FDM Discretization of

$$L(x) := \Delta x - 100\xi_1 \frac{\partial x}{\partial \xi_1} - 1000\xi_2 \frac{\partial x}{\partial \xi_2} \quad \text{on} \quad (0,1)^2$$

for $x = x(\xi_1,\ \xi_2)$, homogeneous Dirichlet BC.
350 grid points $\Rightarrow n = 122\ 500$, $B =$ `rand(n,5)`,
frequency interval limits $\omega_1 = 10$, $\omega_2 = 10^3$.

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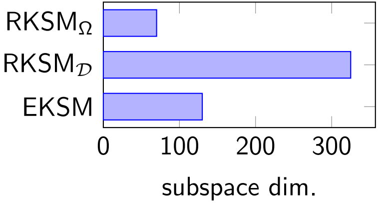
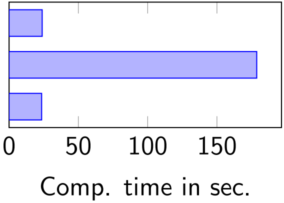
We apply EKSM, RKSM$_\mathcal{D}$, RKSM$_\Omega$ to compute low-rank solutions of X_f





Ranks of low-rank solutions: $\mathrm{rank}(Z_f D_f Z_f^T) = 38$.

Numerical Examples

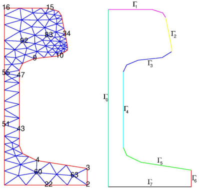
$AX_fE + EX_fA^T = -B_fB^T - BB_f^T, \quad f(z) = \mathrm{Re}\left(\frac{\mathrm{i}}{\pi}\log\frac{z+\mathrm{i}\omega_2}{z+\mathrm{i}\omega_1}\right)$

Example `rail`: Cooling of steel profiles,

A, E from FEM discretization of heat equation

[Benner/Saak '04]

$\Rightarrow n = 79\,841$, $B \in \mathbb{R}^{n\times 7}$,
frequency interval limits $\omega_1 = 10^{-2}$, $\omega_2 = 10$.



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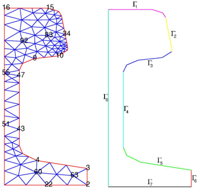

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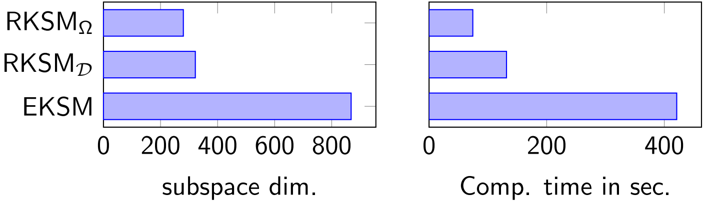

Ranks of low-rank solutions: $\mathrm{rank}(Z_fD_fZ_f^T) = 170, \ldots, 190$.

Summary / Outlook

Conclusion:

- Large-scale Lyapunov equations, where $f(A)$ appears in the right hand side, can be solved efficiently for low-rank solutions.
- Approximation of $f(A)B$ by, e.g., rational Krylov subspace methods $\rightsquigarrow$ recycling data to approximate X_f leads to very efficient *all-at-once* algorithms.
- Intelligent choice of (adaptive) shifts mandatory for fast convergence.

Further topics:

- Theoretical results w.r.t. influence of $f(A)$ to $\sigma_j(X_f)$. ✓
- Other similar applications lead to
  - $f(A) = \exp(A)$,
  - $f(A) = A^m$, $m \in \mathbb{N}$, (✓)
  - $f(A) = \frac{1}{2\pi}\,\mathrm{Re}\,(\omega_1 I - 2\mathrm{i}\log(I - A\exp(-\mathrm{i}\omega_1)))$

  or products of thereof.
- Todo: Usage of tangential rational Krylov subspaces.