On convergence of Krylov subspace approximations of time-invariant dynamical systems

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Outline, I

$$Au + u_t = b\delta(t), \quad u_{t\le 0} = 0,$$

$$u, b \in \mathbf{R}^N, \;\; 0 \prec A = A^* \in \mathbf{R}^{N\times N}.$$

Semi-discretization of parabolic equations (large N),

e.g., diffusion equation: $A \approx -\Delta.$

Our objective is the 3D diffusion Maxwell's equation (Zaslavsky's talk)

- **Rational Krylov subspace (RKS) reduction for the 1st order Hermitian problem**
  - **Rational approximation+subspace reduction=RKS reduction**
  - **Error bound via rational approximation (with prescribed poles) on the spectrum of the operator**
  - **A well known simplest case: (conventional) Krylov subspace, spectral Lanczos decomposition, quadratic convergence**
  - **Pole optimization, the third Zolotarev problem on complex plane**

Outline, II

$$\sum_{i=1}^{m} A_i \frac{d^i}{dt^i} u = b, \qquad u\,|_{t\le 0} = 0,$$

$$A_i = A_i^* \in \mathbf{R}^{\mathbf{N}\times\mathbf{N}},\ \ b(t), u(t) \in \mathbf{R}^{\mathbf{N}},\ \ b\,|_{t\le 0} = 0.$$

Semidiscretization of time-dependend PDEs, exponential integrators.

$m = 2:$ wave propagation in lossy media,

e.g., $A_0 \approx -\Delta,\ A_1$ and A_2 are the dumping and mass matrices resp.

$m = \infty:$ Maxwell's eqs. in dispersive media (Zaslavsky talk); viscoelasticity equations;

fractional diffusion, e.g., $-\Delta u + g * u = b,$

$g\, *$ is the time-convolution operator (variable in space).

- **Extension to stable high order dynamic systems**
  - **Parameter-dependent Krylov subspace (PDKS) reduction**
  - **Spectral estimate (resonance domain)**
  - **A priori error bound via for instant pulse and arbitrary time-dependent r.h.s. via rational approximation of the exponential on the resonance domain.**

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I. 1st order problem with Hermitian matrix

$$Au + u_t = b\delta(t), \quad u_{t\le 0} = 0,$$

$$u, b \in \mathbf{R}^N, \; 0 \prec A = A^* \in \mathbf{R}^{N\times N}.$$

$$\Downarrow$$

$$u(t) = e^{-tA}b = \sum_{i=0}^{\infty} \frac{(-1)^i A^i}{i!} b$$

Rational approximation of matrix functions

- **Matrix exponential is a particular case of matrix functions**

$$f(A)b$$

- **Generally, matrix function can be computed via rational approximants [Varga et al, 60s; Tal-Ezer et al, 1989; Trefethen et al, 00s; etc.]**

$$f(z) \approx p_n(z)/q_m(z)$$

Spectral estimate

$$f(A)b = \sum_{i=1}^{N} f(\lambda_i) y_i y_i^{*} b,$$

$$Ay_i - \lambda_i y_i = 0, \|y\| = 1.$$

$$\Downarrow$$

$$\left\| f(A)b - \frac{p}{q}(A)b \right\| \leq \max_{z \in [\lambda_1, \lambda_N]} \left| f(z) - \frac{p(z)}{q(z)} \right| \| b \|$$

- **Approximation (not necessary rational) of matrix function==approximation on the spectrum**

Subspace reduction

$$\text{Let } \mathbf{U}_n \subset \mathbf{R}^N,\ n \ll N,$$

$$G_n \in \mathbf{R}^{N\times n} \text{ be an orthonormal basis on } \mathbf{U}_n.$$

$$f(\overset{N\times N}{A})\overset{N}{b} \approx \overset{N\times n}{G_n}\, f(\overset{n\times n}{V_n})\overset{n}{b_n},$$

where

$$\mathrm{V}_n = G_n^{\,*} A G_n \in \mathbf{R}^{n\times n},\ \ b_n = G_n^{\,*} b \in \mathbf{R}^n.$$

- **Need a good subspace!**

Rational Krylov Subspace (RKS)

The subdiagonal rational Krylov subspace:

$$\mathbf{U}_n = \mathrm{span}\{\varphi, A\varphi, \ldots, A^{n-1}\varphi\}, \quad \varphi = q_n(A)b,$$

$$q_n(z) = \prod_{i=1}^{n} (z + z_i)^{-1}$$

z_i are real or come in complex conjugate pairs.

Krylov and Rational Krylov, history

- **Krylov subspaces were originally introduced for the solution of eigenproblem and linear systems by Lanczos, Hestenes , Stiefel and Arnoldi (for nonsymmetric *A*) in 1950s. Application to more general matrix functions In 1980s (Moro&Freed, Nour-Amid, van der Vorst etc)**
- **RKS (includes the Kryllov subspace as a particular case for *q=1*) was introduced by Ruhe in 1994 for eigenproblems.**
- **The RKS reduction == the reduction on the rational Krylov subspaces, or equivalently the Galerkin method on such subspaces. Model reduction: Bai, Freund, Grimme, Sorensen, Van Dooren, etc (90s). Matrix functions: Dr.&Kn,98; Moret&Novatti, 03;van Eshof&Hochbruck, 06; BÄorner, Ernst, Spitzer, 08; Beckerman&Reichel, 2008**

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Error bound for the RKS reduction main result

$$\| f(A)b - G_n(V_n)b_n \| \leq 2 \min_{p\ ,\deg p\ \leq n-1} \max_{[\lambda_1,\lambda_N]} \left| f(z) - \frac{p\ (z)}{q_n(z)} \right| \| b \|$$

- **Dr&Kn&Z., Submitted to SISC, 2008; Beckermann&Reichel, Submitted to SINUM, 2008 (also for nonsymmetric *A* the field of values instead of the spectral interval)**

The simplest case: Krylov subspace, SLDM

$q_n = 1, \quad \mathbf{K}_m = \mathrm{span}\{b, Ab, \ldots, A^{n-1}b\},$

three-term Gram-Schmidt (Lanczos algorithm),

tri-diagonal V_n, $b_n = e_1$.

$\exp(-tA)b$: strictly monotonic convergence, Dr., LAA,08;

$$\| \exp(-tA)b - G_n \exp(-tV_n) b_n \|$$

$$< 2 \min_{p, \deg p \le n} \max_{[\lambda_1, \lambda_N]} | \exp(-tz) - p(z) | \, \| b \|$$

$$< \| b \| \frac{c}{s} e^{-s^2}, \quad s = \frac{n}{\sqrt{t\|A\|}}, \qquad n \le 0.5t \| A \| .$$

Dr&Kn., Sov.J.Comp.Math.&Math.Phys., 89.

Cost per step is similar to the explicit time-stepping but better convergence! Still strong dependence on $\|A\|$

RKS reduction: pole optimization

- **RKS reduction== rational approximation with prescribed poles. The poles can be taking from the optimal rational approximants for corresponding problems. The cost per step is similar to the implicit time stepping.**
- **For the solution of multiscale inverse problems in geophysical oil exploration we need the time domain solutions on very large (practically infinite) time intervals, i.e., equivalently we need to solve the frequency domain problem for all harmonic frequencies.**

Pole optimization, Zolotarev problem

$$\min_{z_1,\cdots,z_n} \max_{z\in i\mathbf{R}} \| b-(A+zI)G_n(V_n+zI)^{-1}b \| <$$

$$2 \min_{\lambda_1,\cdots,\lambda_n,\, z_1,\cdots,z_n} \frac{\max\limits_{[\lambda_1,\lambda_N]} |r(\lambda)\|}{\inf\limits_{i\mathbf{R}} |r(z)|} \|b\| < 4\rho^n \|b\|,$$

$$\rho \approx e^{-\frac{\pi^2}{2\ln(\lambda_N/\lambda_1)}}, \quad r(z) = \frac{\prod_{i=1}^{n} z-\lambda_i}{\prod_{i=1}^{n} z+z_i}.$$

- **Closed form asymptotically optimal solution with real poles; Zolotarev, 1893; Le Bailly&Thiran, SINUM, 2000; Ingerman, Dr&Kn, CPAM, 2000; Kn., Dr.,&Z, SINUM 2008.**

2. Hermitian high order dynamic systems

$$\sum_{i=1}^{m} A_i \left(\frac{d}{dt} + sI \right)^i u = b,$$

$$u\,|_{t\le 0} = 0,$$

$$A_i = A_i^* \in \mathbf{R}^{\mathrm{N}\times\mathrm{N}},\ b(t), u(t) \in \mathbf{R}^{\mathrm{N}},\ b\,|_{t\le 0} = 0,$$

$$m \le \infty$$

- **Stability is assumed**

Standard approach i: the *m-*th order dynamical problem can be transformed to the 1st order (nonHermitian) system at expense of *m-*fold increase of the dimensionality. Approaches to Krylov subspace model reduction for the 1st formulation are developed in 90s: Freund, Grimme, Sorensen, Van Dooren, etc. How about the infinite *m* ?!

LET US MAKE IT EVEN MORE COMPLICATED

Time-dependent force term, two cases

- **Conventional formulation: pulse (instant) source**

$$b(t) = b_0 \delta(t), \quad b_0 \in \mathbf{R}^{\mathbf{N}}.$$

- **Arbitrary Laplace-transformable *b(t)*, not assuming that its evolution to be described by a low-dimensional subspace as in the conventional approaches (Gu&Simoncini, 05; etc.).**

Can we extend the rational Krylov subspace approach for this?

YES, WE CAN!!!

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Frequency domain formulation

Let $\tilde{b}(z)$, $\tilde{u}(z)$ and $\tilde{A}(z)$, are the Laplace transforms of resp.

$b(t)$, $u(t)$ and $\sum_{i=1}^{m} A_i \left(\dfrac{d}{dt} + sI \right)^i$ assuming

$\tilde{A}(z) = \sum_{i=0}^{m} A_i (z+s)^i$ or its analytic cont.

Then

$$\tilde{A}\tilde{u} = \tilde{b},$$

$$u(t) = \frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} e^{zt} \tilde{u}(z)\, dz.$$

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Well-posedness assumption

There exist positive constant $c_1,\ c_2$, such that

$$\sqrt{\alpha(z)^2+\beta(z)^2} > c_1 + c_2 z$$

on $\mathbf{C}_+$, where $\alpha(z)$ and $\beta(z)$ are the distances from the origin to the spectral intervals of $\mathrm{Re}\ \tilde{A}$ and $\mathrm{Im}\ \tilde{A}$ respectively.

- **Stability of the time domain problem and existence of the inverse Fourier transform**

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Parameter-dependent Krylov subspace

The parameter-dependent Krylov subspace (PDKS):

$\mathbf{U_n} = \mathrm{span}\{\tilde{u}(z_1), \ldots, \tilde{u}(z_n)\},$

z_i do not coinside, are outside of the nonlinear spectrum and real or come in the conjugate pairs.

- **For the instant pulse==nonlinear Krylov subspace, Voss , 04; for *m=2* and the infinite shifts == second order Krylov subspace, Bai 02.**

PDKS reduction

$$\overset{N\times N}{\tilde{A}}(z)^{-1}\overset{N}{\tilde{b}}(z) \approx \overset{N\times n}{G_n}\overset{n\times n}{V_n}(z)^{-1}\overset{n}{\tilde{b}_n}(z),$$

$$G_n \in \mathbf{R}^{N\times n},\ G_n G_n^{\,*} = \mathbf{I},\ \text{colspan}(G_n) = \mathbf{U}_n,$$

$$V(z) = G_n^{\,*}\tilde{A}(z)G_n \in \mathbf{R}^{n\times n},\ \tilde{b}_n(z) = G_n^{\,*}\tilde{b}(z) \in \mathbf{R}^{n}.$$

$$\text{T-domain}: u(t) \approx u_n(t) = \frac{1}{2i\pi} G_n \int_{-i\infty}^{+i\infty} e^{zt}\, V_n(z)^{-1}\tilde{b}_n(z)\, dz$$

- **Cost does not depend on *m*!**

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Why do we need new analysis

- **A straightforward approach would be to transform a high order problem to the first order form and apply the estimates via the approximation of the exponential on the field of values (Lothar's talk). Not good even for the stable second order Hermitian problems, because their field of values includes the origin.**
- **We obtain bounds for the PDKSR reduction via the approximation on an easily computable domain in the left complex half-plane. Apparently it gives the sharp estimate of the nonlinear spectrum from given spectral intervals of** $\operatorname{Re}\tilde{A}$ and $\operatorname{Im}\tilde{A}$.

The bounds on the pseudospectrum

$$\| \tilde{A}(z)^{-1} \| \leq \frac{1}{\sqrt{\alpha(\mathrm{z})^2 + \beta(\mathrm{z})^2}},$$

$$\| V(z)^{-1} \| \leq \frac{1}{\sqrt{\alpha(\mathrm{z})^2 + \beta(\mathrm{z})^2}}.$$

Nonlinear spectra of $\tilde{A}(z)$ and $V(z)$ are in

the resonance domain S, that is the set of solutions of

$\alpha(\mathrm{z})^2 + \beta(\mathrm{z})^2 = 0$. From the assumption on $\tilde{A}(z)$

we obtain $S \subset \mathbf{C}_-$ $\Rightarrow$ stability of the reduced problem.

- **Functions** $\alpha(\mathrm{z})$ and $\beta(\mathrm{z})$ **can be easily computed from the estimates of the spectral intervals of resp.** $\mathrm{Re}\,\tilde{A}$ and $\mathrm{Im}\,\tilde{A}$

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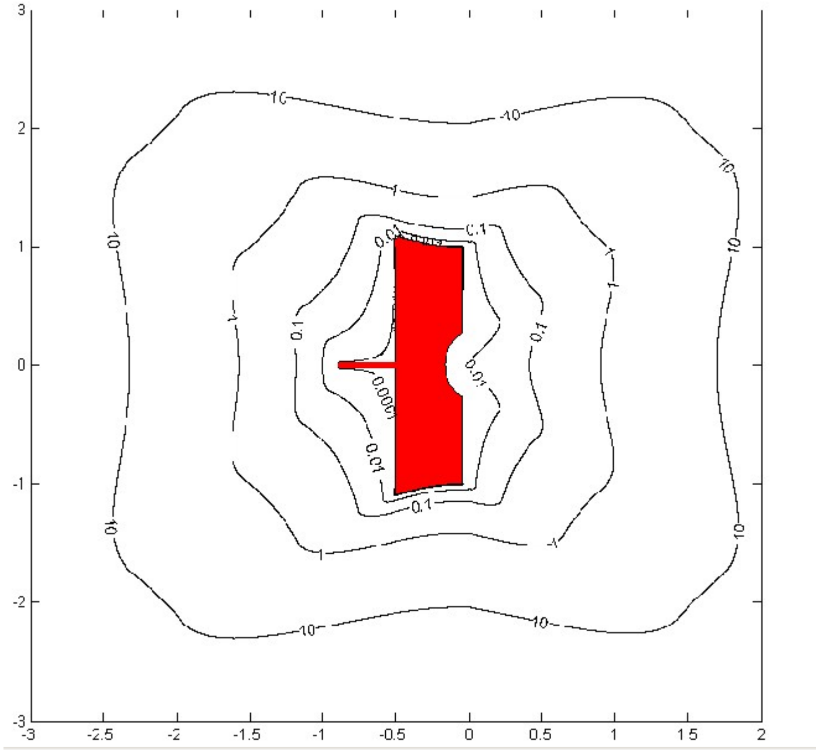
Example: the 2nd order problem



$\tilde{A}(z) = A_0 + A_1 z + A_2 z^2,$

$A_i \succ 0.$

For given spectral intervals of the pencils (A_0, A_2) and $(A_1, A_2),$ the resonance domain S gives sharp estimate of nonlinear spectrum of $\tilde{A}(z)$.

$$\sqrt{\alpha(z)^2 + \beta(z)^2}$$

the spectral intervals of the both pencils are equal to $[0.1, 1]$

Error bound for the pulse

Denote isoline $\Gamma_\varepsilon = \left\{ z : \sqrt{\alpha(z)^2 + \beta(z)^2} = \varepsilon > 0 \right\}$. By construction $\lim_{\varepsilon \to 0} \Gamma_\varepsilon = \partial S.$

Theorem 1.

If $b(t) = b_0 \delta(t)$ and $q = \prod_{i=1}^{n} (z + z_i),$

then

$$\|u(t) - u_n(t)\| \le \frac{|\Gamma_\varepsilon|}{\pi\varepsilon} \min_{p\ ,\deg p\ \le n-1} \max_{\Gamma_\varepsilon} \left| e^{zt} - \frac{p_n(z)}{q_n(z)} \right| \| b_0 \|.$$

Theorem 1 the estimates the PDKS reduction error for the the pulse via the (absolute) error of the rational approximation with prescribed poles on the boundary of the resonance domain *S*. For the first order symmetric problem it coincides with the spectral interval.

Error bound for the general r.h.s. the solution at one time

Theorem 2

If $b(t) = 0$ for $t > t_0 > 0$ (causality restriction) and $q = \prod_{i=1}^{n} (z + z_i)$,

then

$$\left\| u(t_0) - u_n(t_0) \right\| \le \int_0^{t_0} \left\| b(t) \right\| dt \, \frac{|\Gamma_\varepsilon|}{\pi\varepsilon} \min_{p\ ,\deg p\ \le n-1} \ \max_{\Gamma_\varepsilon} \left| 1 - \frac{p_n(z)}{q_n(z)} \exp\left(-z t_0\right) \right|.$$

- **The causality restriction does not affect the solution at t_0, i.e., it's effective for the solution for a single time point, e.g., for exponential integrators.**
- **The estimate is reduced to the relative rational approximation of the exponential**

Single input/output reduced order modeling

Single input/out z-domain model reduction $b_0^{\,*}\tilde{A}(z)^{-1}b_0 \approx b_n^{\,*}V_n(z)^{-1}b_n$.

For $z_1 = \cdots = z_n$ the reduced model matches the same $2n$ moments as the SPRIM model reduction (Freund, 2008) and it is stable as well.

Corollary (of Theorem 1)

If $b(t) = b_0\delta(t)$ and $q = \prod_{i=1}^{n}(z+z_i)$,

then

$$\left\| b_0\left[u(t)-u_n(t)\right]\right\| \le \frac{|\Gamma_\varepsilon|}{\pi\varepsilon} \min_{p,\ \deg p\ \le 2n-1} \ \max_{\Gamma_\varepsilon} \left| e^{zt} - \frac{p(z)}{q_n(z)^2} \right| \| b_0 \|.$$

- **The degree of the rational approximant is doubled for the reduced order model**

Conclusions I

- **The error of the Rational Krylov subspace reduction of the solution of the 1st order Hermitian problem (with instant pulse r.h.s.) can be estimated via the error of the rational approximation (with prescribed denominator) of the exponential function on the spectral interval.**
  - **the pole optimization can be obtained using methods of rational approximation . In the case of the infinite time interval the optimization is reduced to the third Zolotarev problem on complex plane, that can be solved in closed form**

Conclusion II.

- **The parameter-dependent Krylov subspace reduction allows to extend the above results to the high order stable dynamic systems with Hermitian coefficients.**
  - **The algorithm works for both pulse and arbitrary r.h.s. satisfying a natuarl causality principles.**
  - **It preserves stability of the original problem.**
  - **The error can be estimated via the error of the rational approximation (with prescribed poles) of exponential function on an easily computable estimate (resonance domain) of the nonlinear spectrum that always belongs to the complex right half plain.**

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Conclusions, Conclusion

- **Applications and future research.**
  - **Obtained results are applied to the 1st order diffusion and fractional order Maxwell systems for dispersive media arising in geophysical oil exploration, very good agreement with the theory (Mike Zaslavsky talk)**
  - **Obvious potential applications are wave equation n lossy media, model reduction for circuit simulation, fractional diffusion, exponential integrations etc.**
  - **Connection with structure-preserving model reduction Krylov methods SPRIM should be further investigated. Our approach may provide time domain error bounds for the latter.**
  - **Pole optimization when the resonance domain has significant imaginary part,**

Error bound for the RKS reduction, two lemmas

- **Minmax property (true for all Ritz approximations of Hermitian matrices)**

$$[\lambda_1, \lambda_N] \supset [\theta_1, \theta_n],$$

$$[\theta_1, \theta_n] \text{ is the spectral interval of } V_n.$$

- **Interpolation property**

$$\text{For } \forall \;\; p_{n-1} \;\; \text{of degree} \;\; \leq n\text{-}1$$

$$G_n p_{n-1}(V_n) q_n(V_n)^{-1} b_n = p_{n-1}(A) q_n(A)^{-1} b$$