Variable accuracy of matrix-vector products in eigencomputation

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The problem

Approximation of some of the eigenpairs of

$$Ax = \lambda x \qquad n \times n \qquad n \gg 1000$$

using Krylov subspace type methods

$$K_m(A, v_1) = \mathrm{span}\{v_1, Av_1, \ldots, A^{m-1}v_1\} \qquad \|v_1\| = 1$$

when A is either:

- Not known exactly
- Computationally expensive to deal with (e.g. shift-and-invert, Generalized eigenproblem)

Exact vs. Inexact

At each iteration,

$$\underbrace{y = Av}_{\text{exact}} \quad \Rightarrow \quad \underbrace{y = Av + f}_{\text{inexact}} \qquad \|f\| =?$$

$\Rightarrow$ Still get Ritz pairs $(\theta, \tilde{x})$

Questions:

- Do $(\theta, \tilde{x})$ still approximate eigenpairs of A?
- Can we act on $\|f\|$ to make computation cheaper ?
  (Bouras & Frayssé, 2000)

The exact approach

Assume A can be applied exactly.

Key relation in Krylov subspace methods:

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^* \qquad v_1 = V_m e_1$$

$(\lambda, x) \approx (\theta, V_m u)$ where $H_m u = \theta u$ Ritz pairs

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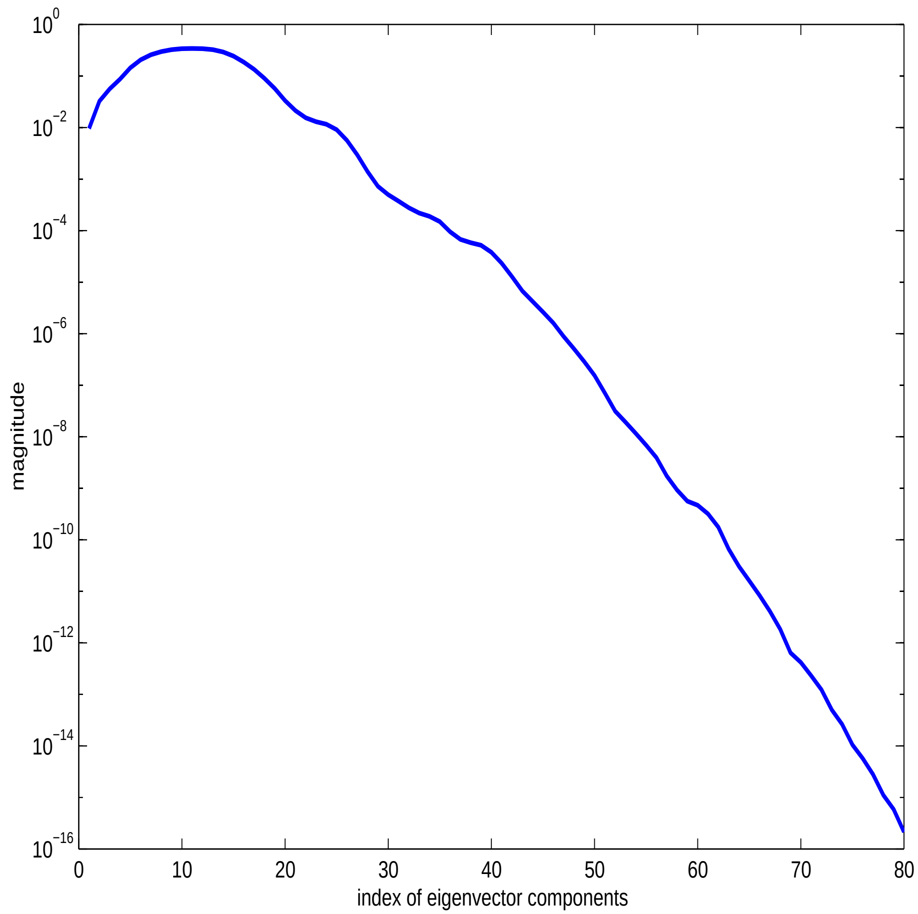
For $r_m = AV_m u - \theta V_m u$:

$$r_m = v_{m+1} h_{m+1,m} e_m^* u$$

A : $L\varphi = -\Delta\varphi + 100((x+y)\varphi)_x + 100((x+y)\varphi)_y \quad n = 900$



Components of an eigenvector of H_m: $H_m u = \lambda u \qquad m = 80$

The key relation in the inexact case

$$AV_m + \underbrace{F_m}_{[f_1,\ldots,f_m]} = V_m H_m + h_{m+1,m} v_{m+1} e_m^* \qquad V_m^T V_m = I$$

How large can F_m be allowed to be?

$$\begin{aligned} AV_m u - \theta V_m u &= V_m H_m u - \theta V_m u + h_{m+1,m} v_{m+1} e_m^* u + F_m u \\ &= \underbrace{h_{m+1,m} v_{m+1} e_m^* u}_{r_m} + F_m u \end{aligned}$$

$$\|(AV_m u - \theta V_m u) - r_m\| = \|F_m u\|$$

$(AV_m u - \theta V_m u)$: true residual | r_m : computed residual

The true residual and the residual gap

$$\|(AV_m u - \theta V_m u) - r_m\| \quad = \quad \|F_m u\|$$

$$\|AV_m u - \theta V_m u\| \quad \leq \quad \|(AV_m u - \theta V_m u) - r_m\| + \|r_m\|$$

The right question is: How large is $F_m u$ allowed to be ?

$$\begin{aligned} \|(AV_m u - \theta V_m u) - r_m\| &= \|F_m u\| = \|[f_1, \ldots, f_m]u\| \\ &\le \sum_{k=1}^{m} \|f_k\| \, |e_k^* u| \end{aligned}$$

Note: After m iterations,

u is given (eig. of H_m) whereas $\|f_k\|, k = 1, \ldots, m$ is controllable

Dynamic accuracy

$$AV_m u - V_m H_m u = h_{m+1,m} v_{m+1} e_m^* u + F_m u$$

In the error *vector*

$$F_m u = [f_1, f_2, \ldots, f_m] u = \sum_{k=1}^{m} f_k u_k$$

◇ The terms $f_k u_k$ need to be small:

If $\quad \|f_k u_k\| < \frac{1}{m}\varepsilon \quad \forall k \quad \Rightarrow \quad \|F_m u\| \leq \sum_{k=1}^{m} \|f_k u_k\| < \varepsilon$

◇ If u_k small $\quad \Rightarrow \quad f_k$ is allowed to be large

The components of the eigenvector u

Under certain conditions,

$$|e_{k+1}^* u| \leq 2 \frac{\|r_k\|}{\delta_{m,k}}$$

where

$\|r_k\|$ residual of certain eigenpair of H_k (kth iteration)

$\delta_{m,k}$ measure of eigen-sensitivity (close to "reduced" resolvent)

We next provide more precise statements

The components of the eigenvector u (cont'd)

$\star$ $H_k u^{(k)} = \theta^{(k)} u^{(k)}$, $k < m$ and $\left[\begin{pmatrix} u^{(k)} \\ \underline{0} \end{pmatrix}, Y\right] \in \mathbb{C}^{m\times m}$ unitary

$\star$ $\delta_{m,k} = \sigma_{\min}(Y^* H_m Y - \theta^{(k)} I) > 0$

$\star$ $r_k = v_{k+1} h_{k+1,k} e_k^* u^{(k)}$ computed residual kth it. s_m left residual

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If $\|r_k\| \leq \frac{\delta_{m,k}^2}{4\|s_m\|}$, there exists $u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$, $u_1 \in \mathbb{C}^k$, eigvec of H_m s.t.

$$\|u_2\| \leq \frac{\tau}{\sqrt{1+\tau^2}} \qquad \text{with} \quad 0 \leq \tau < 2\frac{\|r_k\|}{\delta_{m,k}}$$

$\Rightarrow$ $\begin{bmatrix} u^{(k)} \\ \underline{0} \end{bmatrix}$ perturbation of u Stewart & Sun (1990)

The components of the eigenvector u (cont'd)

There exists $u = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$, $u_1 \in \mathbb{C}^k$, eigvec of H_m s.t.

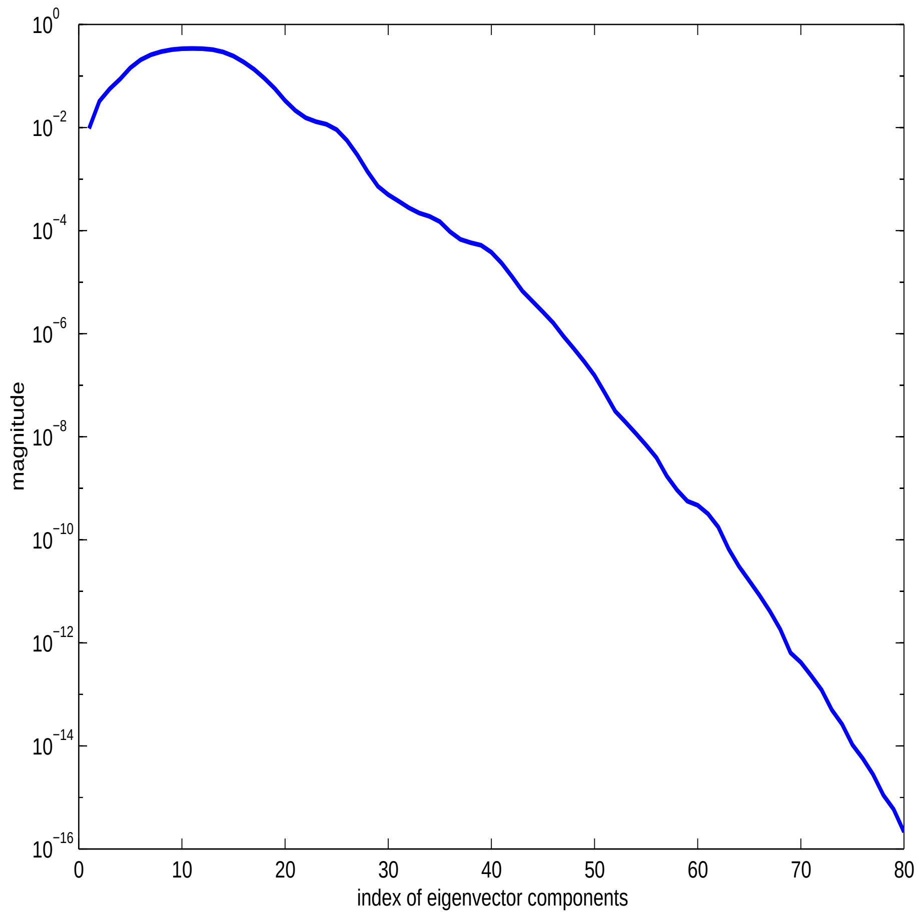
$$\|u_2\| \leq \frac{\tau}{\sqrt{1+\tau^2}} \qquad \text{with} \quad 0 \leq \tau < 2\frac{\|r_k\|}{\delta_{m,k}}$$

From which

$$|e_j^* u| \leq \frac{\tau}{\sqrt{1+\tau^2}} \leq \tau \leq 2\frac{\|r_k\|}{\delta_{m,k}}, \qquad j = k+1, \ldots, m$$

$\Rightarrow$ Of special interest: $j = k+1$

$A\ :\qquad L\varphi = -\Delta\varphi + 100((x+y)\varphi)_x + 100((x+y)\varphi)_y$



Components of eigenvector of H_m: $\qquad H_m u = \lambda u \qquad m = 80$

Flexible Accuracy of A

At each iteration $k = 1, \ldots, m$, $\qquad \widehat{v} = Av_k + f_k$

Variable accuracy result (simplified version):

Let (θ, u) be an eigenpair of H_m and $\varepsilon \in \mathbb{R}$, $\varepsilon > 0$

If, for any $k = 1, \ldots, m$, $\quad \|r_{k-1}\| \leq \dfrac{\delta_{m,k-1}^2}{4\|s_m\|} \quad$ and

$$\|f_k\| \leq \frac{\delta_{m,k-1}}{2m\|r_{k-1}\|}\varepsilon$$

then

$$\|(AV_m u - \theta V_m u) - r_m\| \leq \varepsilon$$

Empirically (Bouras e Frayssé, 2000):

$$\|f_k\| \leq \frac{10^{-\alpha}}{\|r_{k-1}\|}\varepsilon, \qquad \alpha = 0, 1, 2$$

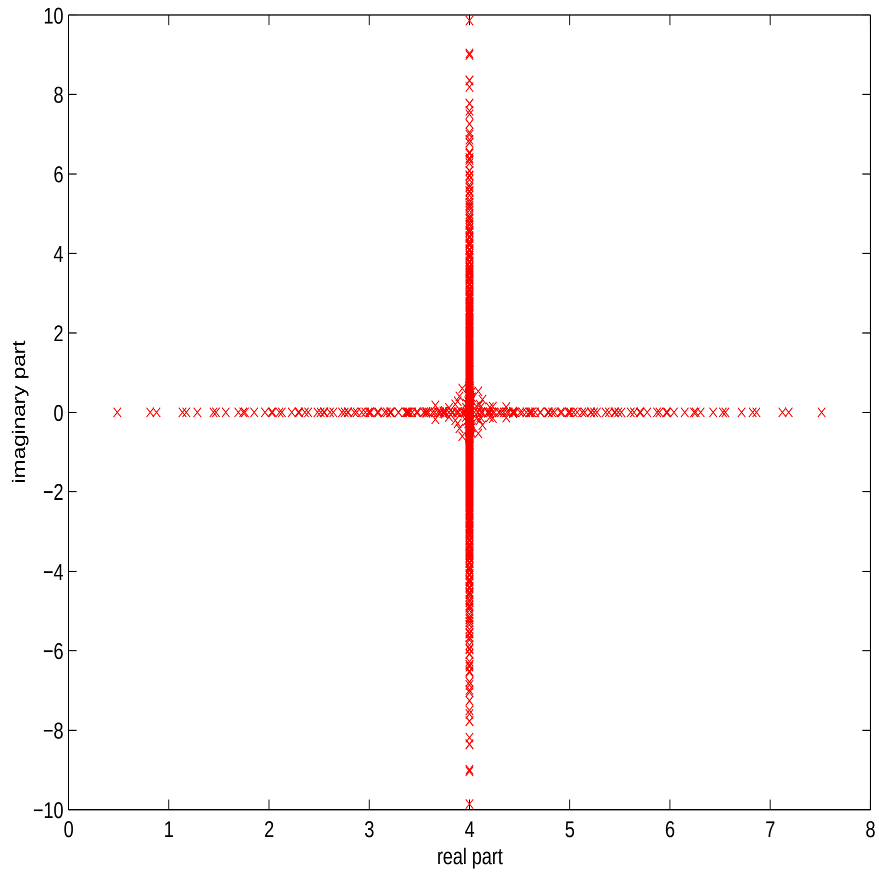
New computable bound:

$$\|f_k\| \leq \frac{\min\{1, \delta^{(k-1)}\}}{2m\|r_{k-1}\|}\varepsilon$$

where

$$\delta^{(k-1)} := \min_{\theta_j \in \Lambda(H_{k-1}) \setminus \{\theta^{(k-1)}\}} |\theta^{(k-1)} - \theta_j|$$

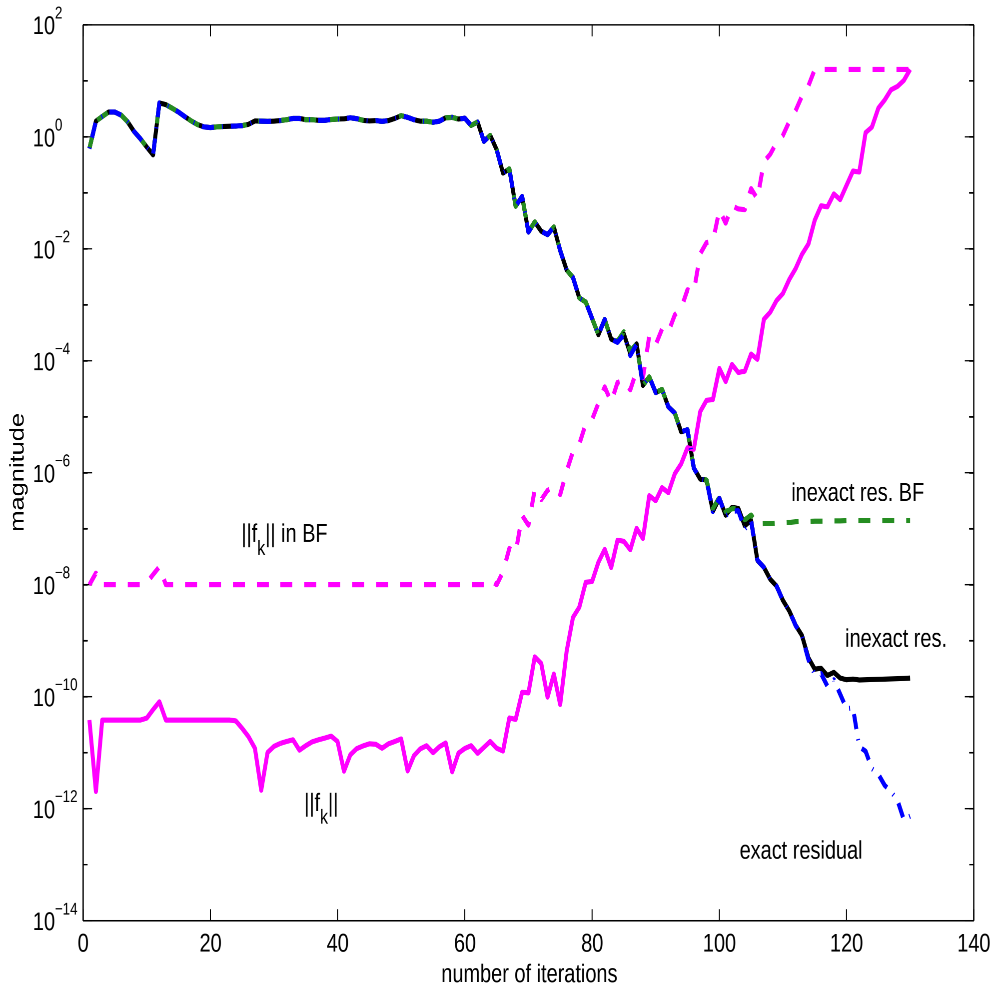
Example 1



$L\varphi = -\Delta\varphi + 100((x+y)\varphi)_x + 100((x+y)\varphi)_y$ Approx. $\Re(\lambda_{\max})$

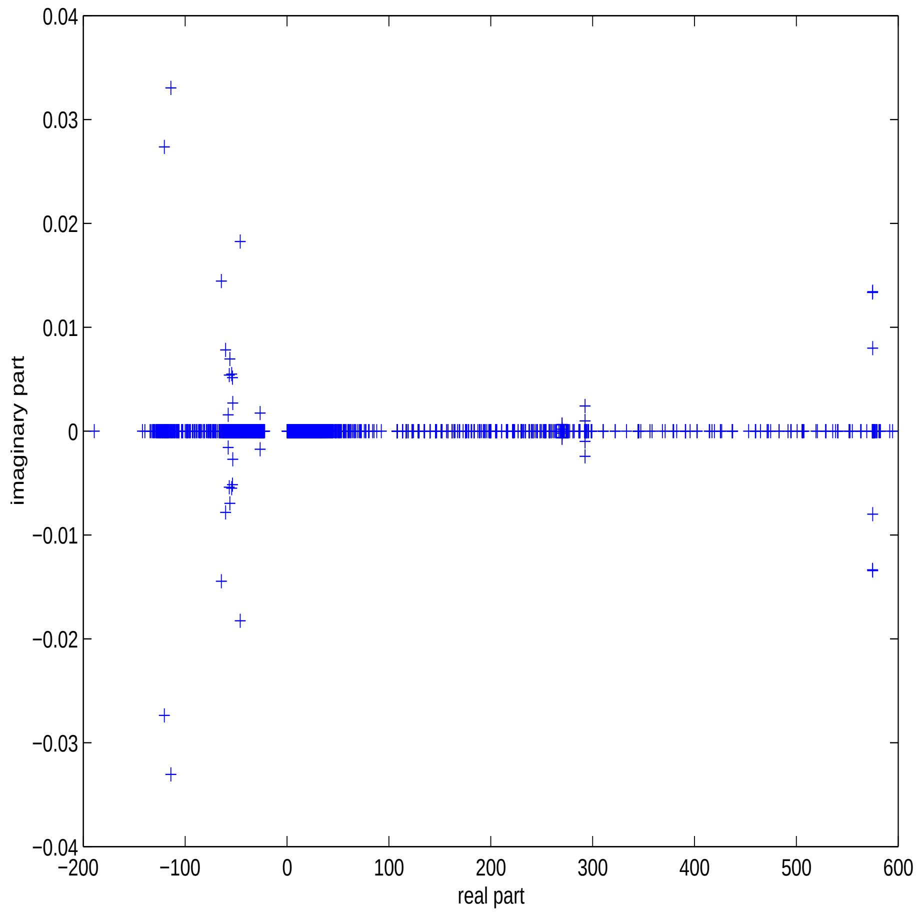
inexact residual: $\|AV_k u^{(k)} - \theta V_k u^{(k)}\|$

Example 1



$$L\varphi = -\Delta\varphi + 100((x+y)\varphi)_x + 100((x+y)\varphi)_y \qquad \text{Approx. } \Re(\lambda_{\max})$$

Example 2



SHERMAN5 MatrixMarket. Approx. $\min|\lambda|$ with "inverted" Arnoldi

Inverted Arnoldi

At each iteration:

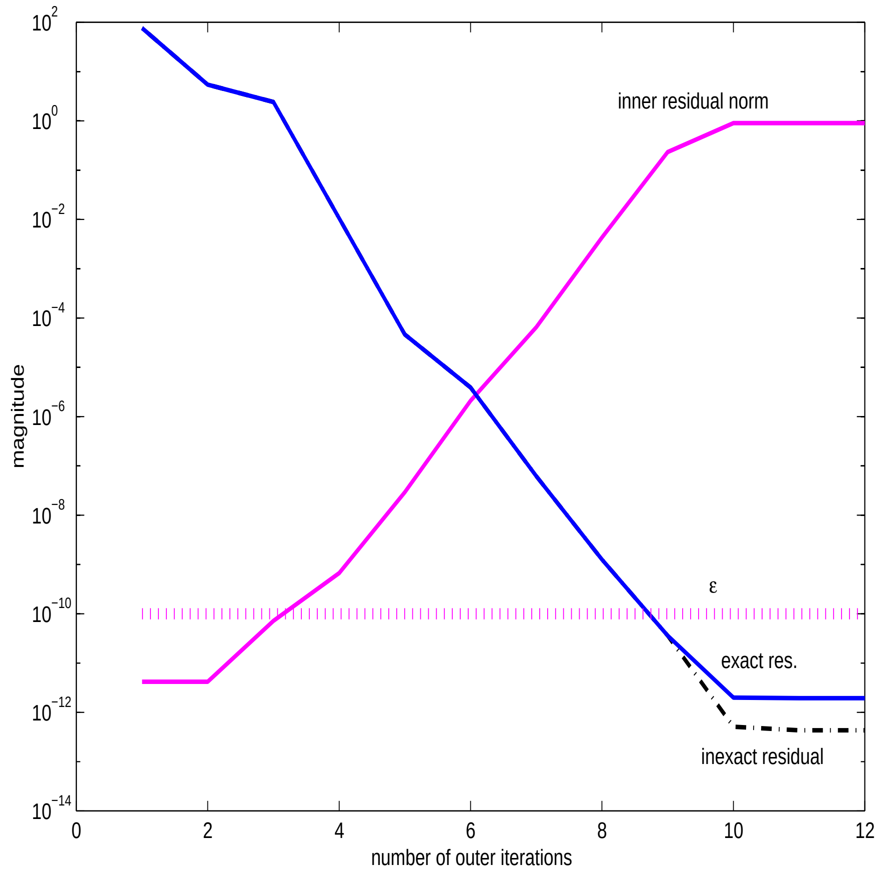
$$y \leftarrow S^{-1} v$$

Iterative solution with $S \Rightarrow$ Inner-Outer procedure

Inner stopping criterion:

$$\|v - S y_i\| \leq \frac{\min\{1, \delta^{(k-1)}\}}{2m\|r_{k-1}\|/|\theta^{(k-1)}|}\varepsilon, \qquad \varepsilon = 10^{-10}$$

Example 2



SHERMAN5 MatrixMarket. Approx. $\min|\lambda|$ with "inverted" Arnoldi

The inexact Arnoldi relation

$$(A + \mathcal{E}_m)V_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^*, \qquad \mathcal{E}_m = \sum_{k=1}^{m} f_k v_k^*$$

$\mathcal{E}_m$ perturbs the problem in a special manner!

In particular:

inexact Ritz value to target eigenvalue is close to exact Ritz value

but other Ritz values change!

Example 1

$m = 100$

eigenvalues of A	Arnoldi Ritz values	Flexible accuracy $\|\|f_{100}\|\| = 9.38\,10^{-5}$
6.528963528	6.5012 + 0.7235i	6.5010 + 0.7208i
6.553808631	6.5012 – 0.7235i	6.5010 – 0.7208i
6.714551208	6.6933 + 0.3818i	6.6949 + 0.3793i
6.825884813	6.6933 – 0.3818i	6.6949 – 0.3793i
6.863220504	6.8832 + 0.1068i	6.8846 + 0.1070i
7.122198478	6.8832 – 0.1068i	6.8846 – 0.1070i
7.185702959	7.123532521	7.123544655
7.512696262	7.512695900	7.512695904

Generalizations

- Invariant subspaces
- Harmonic Ritz values
- Inexact Non-Hermitian Lanczos method
- A comment on A Hermitian

Open problems

- More accurate estimate for $\delta_{m,k-1}$
- (Implicitly) restarted methods ?
- Convergence behavior in the inexact case

Bibliography

1. A. Bouras and V. Frayssé, A relaxation strategy for the Arnoldi method in eigenproblems, Tech. Rep. 16, CERFACS, Toulouse, France, 2000.

2. V. Simoncini. Variable accuracy of matrix-vector products in inexact eigencomputation. March 2004. http://www.imati.cnr.it/~val/list.html