



Recent advances in approximation using Krylov subspaces

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The framework

It is given an operator $v \rightarrow \mathcal{A}_\epsilon(v)$.

Efficiently solve the given problem in the approximation space

$$\mathcal{K}_m = \text{span}\{v, \mathcal{A}_{\epsilon_1}(v), \mathcal{A}_{\epsilon_2}(\mathcal{A}_{\epsilon_1}(v)), \dots\}, \quad v \in \mathbb{C}^n$$

with $\dim(\mathcal{K}_m) = m$, where $\mathcal{A}_\epsilon \rightarrow \mathcal{A}$ for $\epsilon \rightarrow 0$ (ϵ may be tuned)

★ for $\mathcal{A} = A$, $\epsilon = 0 \Rightarrow \mathcal{K}_m = \text{span}\{v, Av, A^2v, \dots, A^{m-1}v\}$

Examples of \mathcal{A} :

- Solution of (preconditioned) large linear systems,

$$Ax = b \quad n \times n \quad \mathcal{A} = A$$

- Shift-and invert eigensolvers

$$Ax = \lambda Mx, \quad \|x\| = 1, \quad \mathcal{A} = (\sigma M - A)^{-1}$$

- Preconditioned exponential approximation

$$x = \exp(A)v, \quad \mathcal{A} = (\gamma I - A)^{-1}$$

- ...

Goal: Achieve approximation x_m to x within a fixed tolerance, by using \mathcal{A}_ϵ (and *not* \mathcal{A}), with variable ϵ

Many applications in Scientific Computing

$\mathcal{A}(v)$ function (linear in v):

- Shift-and-Invert procedures for interior eigenvalues
- Schur complement: $A = B^T S^{-1} B$ S expensive to invert
- Preconditioned system: $AP^{-1}x = b$, where

$$P^{-1}v_i \approx P_i^{-1}v_i$$

- etc.

The exact approach

To focus our attention: $\mathcal{A} = A$.

\mathcal{K}_m Krylov subspace V_m orthogonal basis

Key relation in Krylov subspace methods:

$$AV_m = V_{m+1}\underline{H}_m \quad v = V_{m+1}e_1\beta \quad \underline{H}_m = \begin{bmatrix} H_m \\ h_{m+1,m}e_m^T \end{bmatrix}$$

System: $x_m \in \mathcal{K}_m \Rightarrow x_m = V_m y_m \quad (x_0 = 0)$

Eigenpb: (θ, y) eigenpair of $H_m \Rightarrow (\theta, V_m y)$ Ritz pair for (λ, x)

The inexact key relation

$$A = A \quad \rightarrow \quad A_\epsilon \approx A$$

$$AV_m = V_{m+1}\underline{H}_m + \underbrace{F_m}_{[f_1, f_2, \dots, f_m]} \quad F_m \text{ error matrix, } \|f_j\| = O(\epsilon_j)$$

How large is F_m allowed to be?

system:

$$\begin{aligned} r_m &= b - AV_m y_m = b - V_{m+1}\underline{H}_m y_m - F_m y_m \\ &= \underbrace{V_{m+1}(e_1 \beta - \underline{H}_m y_m)}_{\text{computed residual } =: \tilde{r}_m} - F_m y_m \end{aligned}$$

eigenproblem: $(\theta, V_m y)$

$$r_m = \theta V_m y - AV_m y = v_{m+1} h_{m+1,m} e_m^T y - F_m y$$

A dynamic setting

$$F_m y = [f_1, f_2, \dots, f_m] \begin{bmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_m \end{bmatrix} = \sum_{i=1}^m f_i \eta_i$$

◇ The terms $f_i \eta_i$ need to be small:

$$\|f_i \eta_i\| < \frac{1}{m} \epsilon \quad \forall i \quad \Rightarrow \quad \|F_m y\| < \epsilon$$

◇ If η_i small $\Rightarrow f_i$ is allowed to be large

Linear systems: The solution pattern

$y_m = [\eta_1; \eta_2; \dots; \eta_m]$ depends on the chosen method, e.g.

- Petrov-Galerkin (e.g. GMRES): $y_m = \operatorname{argmin}_y \|e_1 \beta - \underline{H}_m y\|,$

$$|\eta_i| \leq \frac{1}{\sigma_{\min}(\underline{H}_m)} \|\tilde{r}_{i-1}\|$$

\tilde{r}_{i-1} : GMRES computed residual at iteration $i - 1$.

Simoncini & Szyld, SISC 2003 (see also Sleijpen & van den Eshof, SIMAX 2004)

Analogous result for Galerkin methods (e.g. FOM)

Eigenproblem: The structure of the Ritz pair

Ritz approximation:

(θ, y) eigenpair of H_m

$$y = [\eta_1; \eta_2; \dots; \eta_m],$$

$$|\eta_i| \leq \frac{2}{\delta_{m,i}} \|\tilde{r}_{i-1}\|$$

$\delta_{m,i}$ quantity related to the spectral gap of θ with H_m

\tilde{r}_{i-1} : Computed eigenresidual at iteration $i - 1$

Analogous results for Harmonic Ritz values and Lanczos approx.

Simoncini, SINUM To appear

Relaxing the inexactness in A

$$A \cdot v_i \text{ not performed exactly} \quad \Rightarrow \quad (A + E_i) \cdot v_i$$

True (unobservable) vs. computed residuals:

$$r_m = b - AV_m y_m = V_{m+1}(e_1 \beta - \underline{H}_m y_m) - F_m y_m$$

GMRES: If

(Similar result for FOM)

$$\|E_i\| \leq \frac{\sigma_{\min}(\underline{H}_m)}{m} \frac{1}{\|\tilde{r}_{i-1}\|} \varepsilon \quad i = 1, \dots, m$$

$$\text{then } \|F_m y_m\| \leq \varepsilon \quad \Rightarrow \quad \|r_m - V_{m+1}(e_1 \beta - \underline{H}_m y_m)\| \leq \varepsilon$$

\tilde{r}_{i-1} : GMRES computed residual at iteration $i - 1$

An example: Schur complement

$$\underbrace{B^T S^{-1} B}_A x = b$$

$$y_i \leftarrow B^T S^{-1} B v_i$$

Inexact matrix-vector product:

$$\left\{ \begin{array}{l} \text{Solve } Sw_i = Bv_i \\ \text{Compute } y_i = B^T w_i \end{array} \right. \xrightarrow{\text{Inexact}} \left\{ \begin{array}{l} \text{Approx solve } Sw_i = Bv_i \Rightarrow \hat{w}_i \\ \text{Compute } \hat{y}_i = B^T \hat{w}_i \end{array} \right.$$

$w_i = \hat{w}_i + \epsilon_i$ ϵ_i error in inner solution so that

$$Av_i \quad \rightarrow \quad B^T \hat{w}_i = \underbrace{B^T w_i}_{Av_i} - \underbrace{B^T \epsilon_i}_{-E_i v_i} = (A + E_i)v_i$$

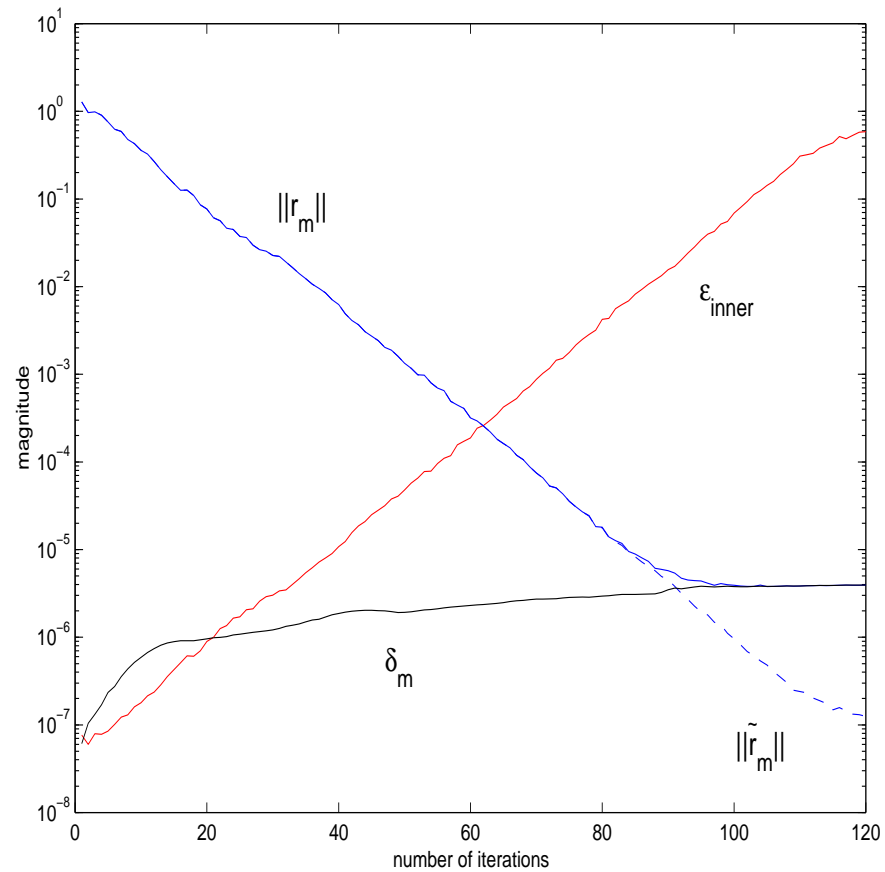
Numerical experiment

$$\underbrace{B^T S^{-1} B}_A x = b$$

at each it. i solve $Sw_i = Bv_i$

Inexact FOM

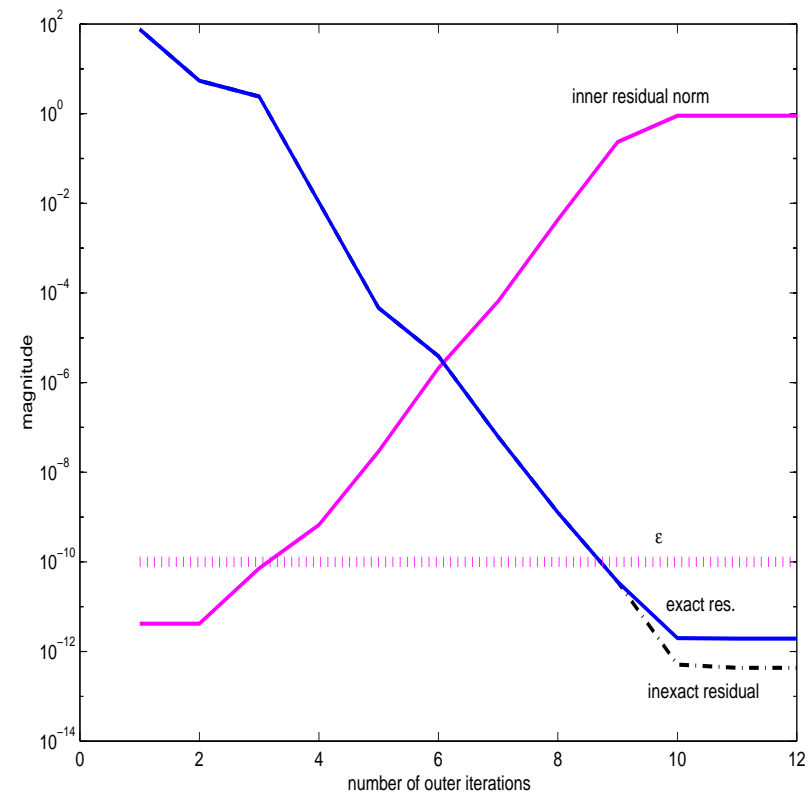
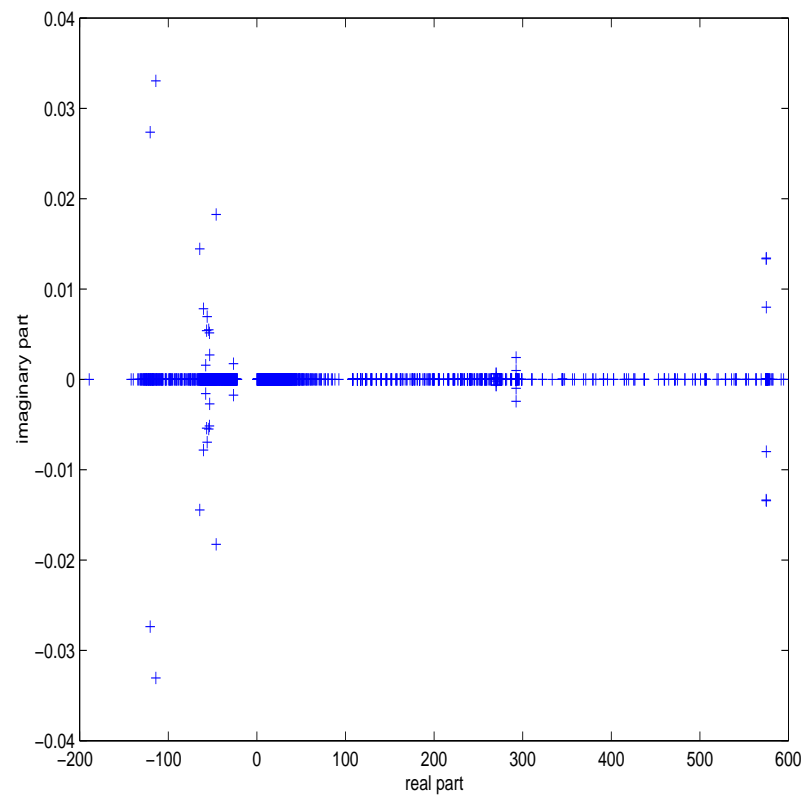
$$\delta_m = \|r_m - (b - V_{m+1} \underline{H}_m y_m)\|$$



Eigenproblem

Inverted Arnoldi: $Ax = \lambda x$ Find $\min |\lambda|$ $y \leftarrow \mathcal{A}(v) = A^{-1}v$

Matrix SHERMAN5



Problems to be faced

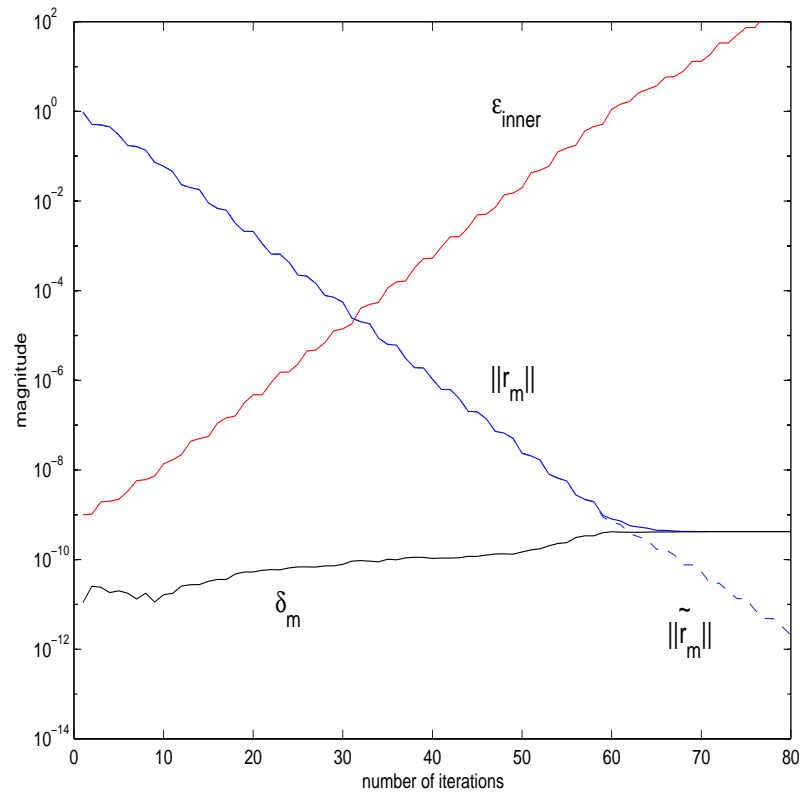
- Make the inexactness criterion practical

$$\|E_i\| \leq \frac{\sigma_{\min}(H_{m_*})}{m_*} \frac{1}{\|\tilde{r}_{i-1}\|} \varepsilon \quad \Rightarrow \quad \|E_i\| \leq \ell_{m_*} \frac{1}{\|\tilde{r}_{i-1}\|} \varepsilon$$

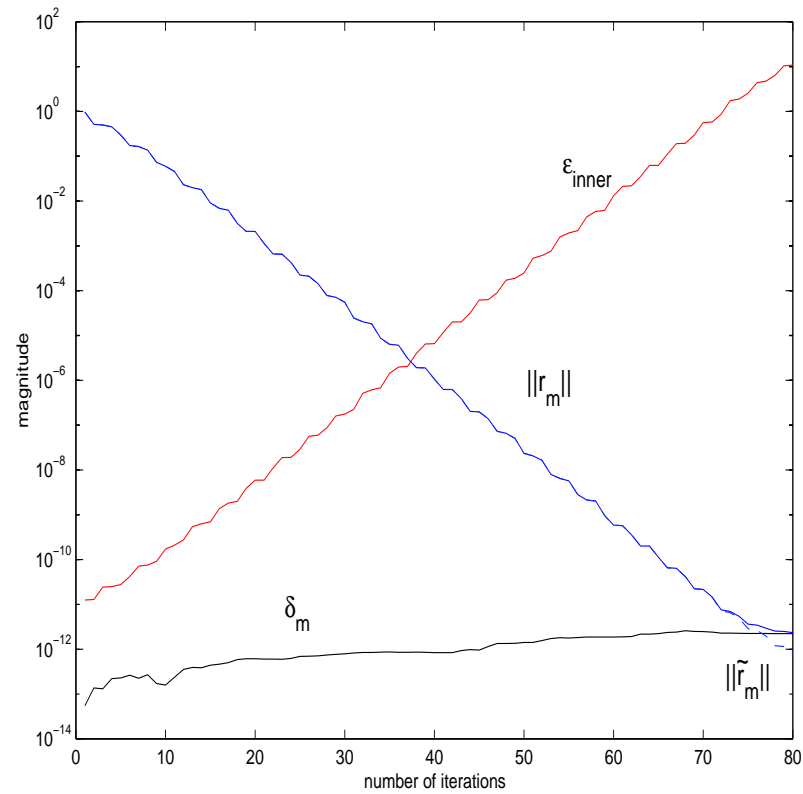
(CERFACS tr's of Bouras, Frayssè, Giraud, 2000, Bouras, Frayssè SIMAX05)

- What is the convergence behavior?
- What if original \mathcal{A} was symmetric?

Selecting ℓ_{m_*} : system $AP^{-1}x = b$



Left: $\ell_{m_*} = 1$



Right: estimated ℓ_{m_*}

Convergence behavior

Does the **inexact** procedure behave as if $\|E_i\| = 0$?

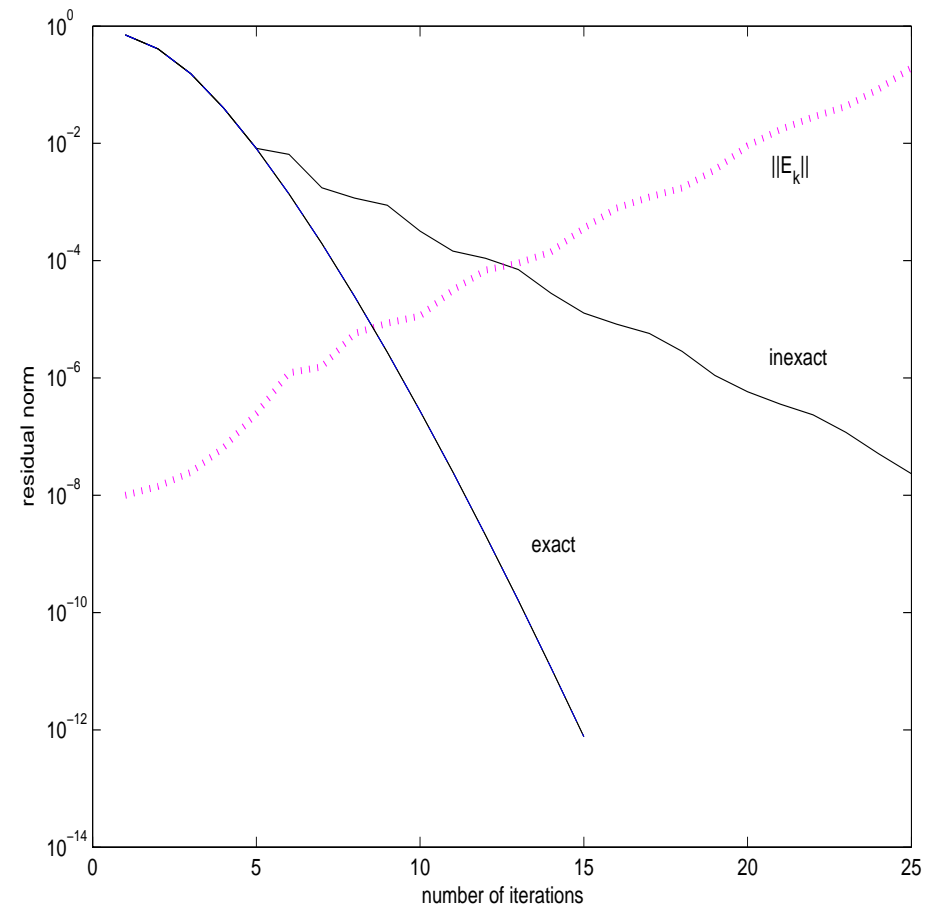
The Sleijpen & van den Eshof's example:

Exact vs. Inexact GMRES

$$b = e_1$$

E_i random entries

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 2 & 0 & \cdots & 0 \\ 0 & 1 & 3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 100 \end{bmatrix}$$



Inexactness and convergence

$$Av_i \quad \rightarrow \quad (A + E_i)v_i$$

For general A and b convergence is the same as exact A

Problems for:

- Sensitive A (highly nonnormal)
 - Special starting vector / right-hand side
- ★ Superlinear convergence as for A (Simoncini & Szyld, SIREV 2005)

Flexible preconditioning

$$AP^{-1}\hat{x} = b \quad x = P^{-1}\hat{x}$$

Flexible:

$$P^{-1}v_i \rightarrow P_i^{-1}v_i, \quad \hat{x}_m \in \text{span}\{v_1, AP_1^{-1}v_1, AP_2^{-1}v_2, \dots, AP_{m-1}^{-1}v_{m-1}\}$$

Directly recover x_m (Saad, 1993):

$$[P_1^{-1}v_1, P_2^{-1}v_2, \dots, P_m^{-1}v_m] = Z_m \quad \Rightarrow \quad x_m = Z_m y_m$$

\Rightarrow Inexact framework but exact residual

A practical example

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix} \quad \mathcal{P} = \begin{bmatrix} I & 0 \\ 0 & B^T B \end{bmatrix}$$

Application of \mathcal{P}^{-1} corresponds to solves with $B^T B$

⇓

$\tilde{\mathcal{P}}$ ⇒ Use CG to solve systems with $B^T B$

Variable inner tolerance: At each outer iteration m ,

$$\|r_k^{inner}\| \leq \frac{\ell_{m_*}}{\|r_{m-1}^{outer}\|} \varepsilon$$

Electromagnetic 2D problem

Outer tolerance: 10^{-8}

$$\|r_k^{inner}\| \leq \frac{\ell_{m_*}}{\|r_{m-1}^{outer}\|} \varepsilon_0 \equiv \varepsilon$$

Elapsed Time

Pb. Size	Fixed Inner Tol $\varepsilon = 10^{-10}$	Var. Inner Tol. $\varepsilon = 10^{-10} / \ r\ $	Var. Inner Tol. $\varepsilon = 10^{-12} / \ r\ $
3810	17.0 (54)	11.4 (54)	14.7 (54)
9102	82.9 (58)	62.8 (58)	70.7 (58)
14880	198.4 (54)	156.5 (54)	170.1 (54)

Structural Dynamics

$$(\mathcal{A} + \sigma\mathcal{B})x = b$$

Solve for many σ 's simultaneously $\Rightarrow (\mathcal{A}\mathcal{B}^{-1} + \sigma I)\hat{x} = b$

(Perotti & Simoncini 2002)

Inexact solutions with \mathcal{B} at each iteration:

	Prec. Fill-in 5		Prec. Fill-in 10	
	e-time [s]	# outer its	e-time [s]	# outer its
Tol 10^{-6}	14066	296	13344	289
Dynamic Tol	11579	301	11365	293

20 % enhancement with tiny change in the code

(see also van den Eshof, Sleijpen and van Gijzen, JCAM 2005)

Inexactness when A symmetric

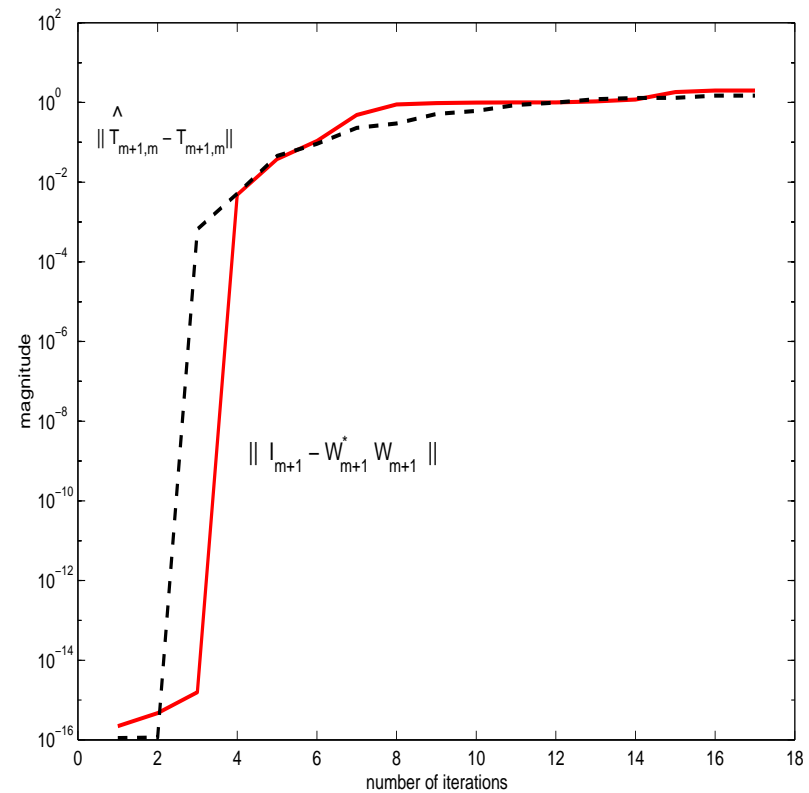
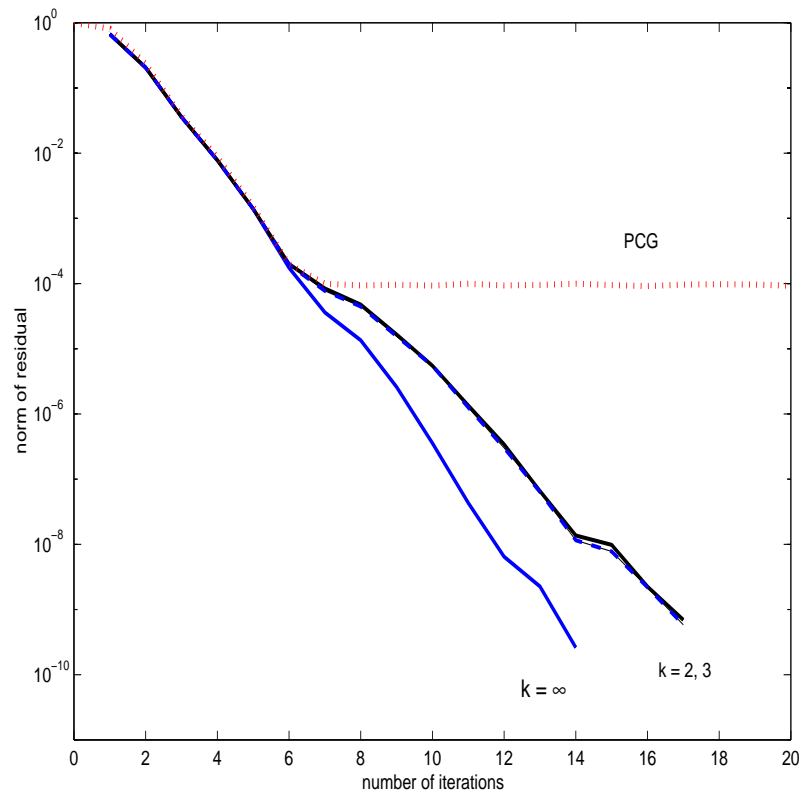
A symmetric $\Rightarrow A + E_i$ nonsymmetric

- Assume $V_m^T V_m = I \rightarrow H_m$ upper Hessenberg
- Wise implementation of short-term recurr. /truncated methods
(V_m non-orth. $\rightarrow W_m$, H_m tridiag./banded $\rightarrow T_m$)
 - **Inexact short-term recurrence system solvers**
(Golub-Overton '88, Golub-Ye '99, Notay '00, Sleijpen-van den Eshof '04, ...)
 - **Inexact symmetric eigensolvers**
(Lai-Lin-Lin 1997, Golub-Ye 2000, Golub-Zhang-Zha 2000, Notay 2002, ...)
 - **Truncated methods** (Simoncini - Szyld, Num. Math. To appear)

$$Ax = b \quad A \text{ sym. (2D Laplacian)}$$

Preconditioner:

\mathcal{P} nonsymmetric perturbation (10^{-5}) of Incomplete Cholesky



One more application: Approximation of the exponential

A symmetric negative semidefinite (large dimension), v s.t. $\|v\| = 1$,

$$\exp(A)v \approx x_m = V_m y_m, \quad y_m = \exp(H_m)e_1$$

Problem: Find preconditioner for A to speed up convergence

Hochbruck & van den Eshof (SISC, to appear):

Determine $x_m \approx \exp(A)v$ as

$$x_m = V_m y_m \in K_m((\gamma I - A)^{-1}, v) \quad \text{for scalar } \gamma$$

$\Rightarrow y_m = \exp(H_m)e_1$ has a structured decreasing pattern

(Lopez & Simoncini, tr. 2005)

Conclusions

- \mathcal{A} may be replaced by \mathcal{A}_{ϵ_i} with increasing ϵ_i and still converge
- Stable procedure for not too ill-conditioned problems

Property inherent of Krylov approximation



Many more applications for this general setting

References

1. [V. Simoncini and D. B. Szyld](#). Theory of Inexact Krylov Subspace Methods and Applications to Scientific Computing. *SIAM J. Scientific Comput.* v.25, n.2 (2003), pp. 454-477.
2. [F. Perotti and V. Simoncini](#). Analytical and Numerical Techniques in frequency domain response computation. *Recent Research Developments in Structural Dynamics*, A. Luongo Ed. Research Signpost Pub., 2003, pp.33-54.
3. [V. Simoncini and D. B. Szyld](#). On the occurrence of Superlinear Convergence of Exact and Inexact Krylov Subspace Methods. *SIAM Review* 2005.
4. [V. Simoncini](#). Variable accuracy of matrix-vector products in projection methods for eigencomputation. *SINUM*, *To appear*.
5. [V. Simoncini and D. B. Szyld](#). The effect of non-optimal bases on the convergence of Krylov Subspace Methods. *Num. Math.* *To appear*.
6. [L. Lopez and V. Simoncini](#). Analysis of projection-type methods for approximating the matrix exponential operator. March 2005.