Recent developments in Krylov Subspace Methods for Scientific Computations

V. Simoncini

Dipartimento di Matematica, Bologna

valeria.simoncini@unibo.it

The Problem

$$Ax = b \qquad \text{or} \quad AX = B, \quad B = [b_1, \ldots, b_s]$$

$A \in \mathbb{C}^{n\times n}$, B full column rank, $s \ll n$

- A large and sparse
- A large and structured: blocks, banded, ...
- A functional: $A = CS^{-1}D$, preconditioned, integral, ...
- ....

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The solution approach. Generate sequence of approximate solutions:

$$\{x_0, x_1, x_2, \ldots\}, \qquad x_k \to_{k \to \infty} x$$

Occurrence of the problem

Very broad range of applications in Engineering and Scientific Computing

Original application context:

- Discretization of 2D and 3D PDEs
  (linear steady state, nonlinear, evolutive, etc.)
- Eigenvalue problems
- Approximation of matrix functions
- Workhorses of more advanced techniques
- ...

Relevant Bibliographic Pointer

Iterative methods for sparse linear systems

Yousef Saad

SIAM, Society for Industrial and Applied Mathematics, 2003, 2nd edition.

V. Simoncini and D. B. Szyld

Recent developments in Krylov Subspace Methods for linear systems

Numerical Linear Algebra with Appl., v. 14, n.1 (2007), pp.1-59.

"Projection" methods (or, reduction methods)

- Approximation vector space K_m. At each iteration m

$$\{u_m\} \text{ such that } u_m \in K_m$$

K_m: dimension[a] m, with the "expansion" property:

$$K_m \subseteq K_{m+1}$$

- Computation of iterate. Galerkin condition:

$$\text{residual} \quad r_m := f - Au_m \quad \perp \quad K_m$$

$\Rightarrow$ This condition uniquely defines $u_m \in K_m$

[a] At most

Optimality property of Galerkin projection method

A symmetric and positive definite. Let $u^\star$ be the true solution.
Galerkin property:

$$\text{residual} \quad r_m := f - Au_m \quad \perp \quad K_m$$

is equivalent to:

$$u_m \quad \text{solution to} \quad \min_{u \in K_m} \|u^\star - u\|_A$$

where $\|\cdot\|_A$ is the energy norm, namely $\|x\|_A^2 := \langle x, Ax \rangle$

Convergence and spectral properties

- In exact arithmetic (i.e., in theory), finite termination property
- A-priori bound for energy norm of the error:

  If $K_m = \mathrm{span}\{f, Af, \ldots, A^{m-1}f\}$, then

$$\|u^\star - u_m\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m \|u^\star - u_0\|_A$$

  where $\kappa = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$

(Conjugate Gradients, Hestenes & Stiefel, '52)

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Consequences:

- Convergence: The closer κ to 1 the faster
- Convergence depends on spectral properties, not directly on problem size!

A well established code

Classical Conjugate Gradient:

Given x_0. Set $r_0 = b - Ax_0$, $p_0 = r_0$

for $i = 0, 1, \ldots$

$$\alpha_i = \frac{r_i^* r_i}{p_i^* A p_i}$$

$$x_{i+1} = x_i + p_i \alpha_i$$

$$r_{i+1} = r_i - A p_i \alpha_i$$

$$\beta_{i+1} = \frac{r_{i+1}^* A p_i}{p_i^* A p_i}$$

$$p_{i+1} = r_i + p_i \beta_{i+1}$$

end

The **Block** Conjugate Gradient

$R_0 = B - AX_0,\ P_0 = R_0 \in \mathbb{C}^{n\times s}$

for $k = 0, 1, \ldots$

$\boldsymbol{\alpha}_k = (P_k^* A P_k)^{-1}(R_k^* R_k) \in \mathbb{C}^{s\times s}$

$X_{k+1} = X_k + P_k \boldsymbol{\alpha}_k$

$R_{k+1} = R_k - A P_k \boldsymbol{\alpha}_k$

$\boldsymbol{\beta}_{k+1} = (P_k^* A P_k)^{-1}(R_{k+1}^* A P_k) \in \mathbb{C}^{s\times s}$

$P_{k+1} = R_k + P_k \boldsymbol{\beta}_{k+1}$

end

A more general picture. Nonsymmetric problems

- A normal, $AA^* = A^*A$
- A (highly) non-normal, $\|AA^* - A^*A\| \gg 0$
- A "Hermitian" in disguise:

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  - ⋆ There exists nonsing. Herm. $H \in \mathbb{C}^{n\times n}$ such that $HA = A^*H$, e.g. M, C Hermitian

$$A = \begin{bmatrix} M & B \\ -B^* & C \end{bmatrix}, \quad H = \begin{bmatrix} I & \\ & -I \end{bmatrix},$$

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$$A = \begin{bmatrix} M & B \\ -B^* & C \end{bmatrix}, \quad H = \begin{bmatrix} I & \\ & -I \end{bmatrix},$$

  - ⋆ $Ax = b \quad \Leftrightarrow \quad A^*Ax = A^*b$ (not recommended in general...)

Outline

- What is the problem with A non-Hermitian ?
- How to handle "Symmetry in disguise"
- Non-normal (non-Hermitian) case
  - ⋆ Long-term recurrences and their problems
  - ⋆ Coping with them $\Rightarrow$ Restarted, truncated, flexible
  - ⋆ Making it without $\Rightarrow$ short-term recurrences
- Tricks for all trades

What goes “wrong” with A non-Hermitian. I

$$\{x_k\}, \quad \text{with} \quad x_k \in x_0 + K_k(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}$$

Let $V_k = [v_1, \ldots, v_k]$ be a (orthogonal) basis of $K_k(A, r_0)$. Then

$$x_k = x_0 + V_k y_k, \qquad y_k \in \mathbb{C}^k$$

A condition is required to specify y_k.

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$$r_k := b - Ax_k = r_0 - AV_k y_k \quad \perp \quad K_k(A, r_0) \qquad V_k^* r_k = 0$$

so that

$$0 = V_k^* r_k = V_k^* r_0 - V_k^* A V_k y_k \quad \Leftrightarrow \quad y_k \ s.t. \ (V_k^* A V_k) y_k = V_k^* r_0$$

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Hence

$$x_k = x_0 + V_k (V_k^* A V_k)^{-1} V_k^* r_0 \qquad \text{with} \quad V_k^* r_0 = e_1 \|r_0\|$$

And: $V_k^* A V_k$ upper Hessenberg (Gram-Schmidt procedure to build V_k)

What goes "wrong" with A non-Hermitian. II

If A were Hpd $\Rightarrow$ $V_k^* A V_k$ also Hpd $\Rightarrow$ tridiagonal

$$V_k^* A V_k = L_k L_k^* \qquad L_k \text{ bidiagonal}$$

$$\begin{aligned} x_k &= x_0 + V_k L_k^{-*} L_k^{-1} e_1 \|r_0\| \\ &= x_0 + V_{k-1} L_{k-1}^{-*} L_{k-1}^{-1} e_1 \|r_0\| + p_k \alpha_k \\ &= x_{k-1} + p_k \alpha_k \end{aligned}$$

with $p_k \in \text{span}\{v_{k-1}, v_k\}$

(development underlying Conjugate Gradient)

What goes "wrong" with A non-Hermitian. II

If A were Hpd $\quad\Rightarrow\quad V_k^* A V_k$ also Hpd $\quad\Rightarrow\quad$ tridiagonal

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with $p_k \in \text{span}\{v_{k-1}, v_k\}$

(development underlying Conjugate Gradient)

A non-Hermitian $\Rightarrow V_k^* A V_k$ only upper Hessenberg

$$p_k \in \text{span}\{v_1, \ldots, v_k\}$$

What goes “wrong” with A non-Hermitian. III

$p_k \in \text{span}\{v_1, \ldots, v_k\}$, with $\{v_1, \ldots, v_k\}$ orthogonal basis

Alternatives

- Give up orthogonal basis, $V_k^* V_k = I_k$
- Give up optimality condition, e.g. $r_k \perp K_k(A, r_0)$
- Resume symmetry

Symmetry in disguise. Shifted systems.

Case 1: $A = M + \sigma I, \quad M \in \mathbb{R}^{n\times n}, \sigma \in \mathbb{C}$

Trick: replace $*$ (conj. transp.) with $\top$ (transp.)

$$A = A^\top \qquad \text{complex symmetric}$$

Apply CG with $\top$

Given x_0. Set $r_0 = b - Ax_0$, $p_0 = r_0$

for $i = 0, 1, \ldots$

$$\alpha_i = \frac{r_i^\top r_i}{p_i^\top A p_i}$$

$$x_{i+1} = x_i + p_i \alpha_i$$

$$r_{i+1} = r_i - A p_i \alpha_i$$

$$\beta_{i+1} = \frac{r_{i+1}^\top A p_i}{p_i^\top A p_i}$$

$$p_{i+1} = r_i + p_i \beta_{i+1}$$

end

...and Complex Symmetric Matrices

$A = M + \sigma I$:   Apply CG with $\top$

Properties:

- V_k real: $K_k(A, r_0) = K_k(A + \sigma I, r_0)$
- $\top$ does not define an inner product!
- $V_k^\top A V_k = V_k^\top M V_k + \sigma I$

  If $\Im(\sigma) \neq 0$ then $V_k^\top A V_k$ is nonsingular $\Rightarrow$ No breakdown

The same code applies in case of any A complex symmetric ($A = A^\top$)

H-symmetry

A is H-Hermitian if there exists $H \in \mathbb{C}^{n\times n}$ Hermitian, nonsingular s.t.

$$HA = A^* H$$

(H-symmetric if $HA = A^\top H$ with H is symmetric)

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If H is Hpd (and HA is also Hpd), use CG in the H-inner product:

Given x_0. Set $r_0 = b - Ax_0$, $p_0 = r_0$

for $i = 0, 1, \ldots$

$$\alpha_i = \frac{r_i^* H r_i}{p_i^* H A p_i}$$

$$x_{i+1} = x_i + p_i \alpha_i$$

$$r_{i+1} = r_i - A p_i \alpha_i$$

$$\beta_{i+1} = \frac{r_{i+1}^* H A p_i}{p_i^* H A p_i}$$

$$p_{i+1} = r_i + p_i \beta_{i+1}$$

end

(H not Hpd $\Rightarrow$ see later)

First Summary

Symmetry in disguise:

- Shifted matrices, $A = M + \sigma I$, M real symmetric
- Complex symmetric matrices
- H-symmetric or H-Hermitian matrices

Long-term recurrences

$$K_k(A, r_0) = \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}, \quad V_k \text{ orth. basis}$$

1. Arnoldi process : $v_{k+1} \leftarrow Av_k - \sum_{j=1}^{k} v_j h_{j,k}$, that is

$$AV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^* = V_{k+1} \underline{H}_k \qquad (H_k = V_k^* A V_k)$$

2. $x_k = x_0 + V_k y_k$

Long-term recurrences

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2. $x_k = x_0 + V_k y_k$

- GMRES. Particular Petrov-Galerkin condition:

$$r_k \perp AK_k \Rightarrow \quad y_k \text{ s.t. } \min_y \|r_0 - AV_k y\|$$

- FOM. Galerkin condition: (H_k nonsingular)

$$r_k \perp K_k \Rightarrow \quad y_k \text{ s.t. } H_k y = e_1 \|r_0\|$$

GMRES

$AV_k = V_{k+1}\underline{H}_k, \qquad r_0 = V_{k+1}e_1\beta_0$

Crucial property:

$$\begin{aligned}\min_y \|r_0 - AV_k y\| &= \\ &= \min_y \|V_{k+1}(e_1\beta_0 - \underline{H}_k y)\| \\ &= \min_y \|e_1\beta_0 - \underline{H}_k y\|\end{aligned}$$

Least squares problem expands at each iteration.

QR decomposition of $\underline{H}_k$ only updated, not recomputed from scratch.

Block GMRES

$$R_0 = B - AX_0, \qquad K_k(A, R_0) = \text{span}\{R_0, AR_0, \ldots, A^{k-1}R_0\},$$

$\mathcal{U}_k$ orth. basis, $\mathcal{U}_k = [U_1, U_2, \ldots, U_k] \in \mathbb{C}^{n\times ks}$

Block Arnoldi process (s MxV + Gram-Schmidt)

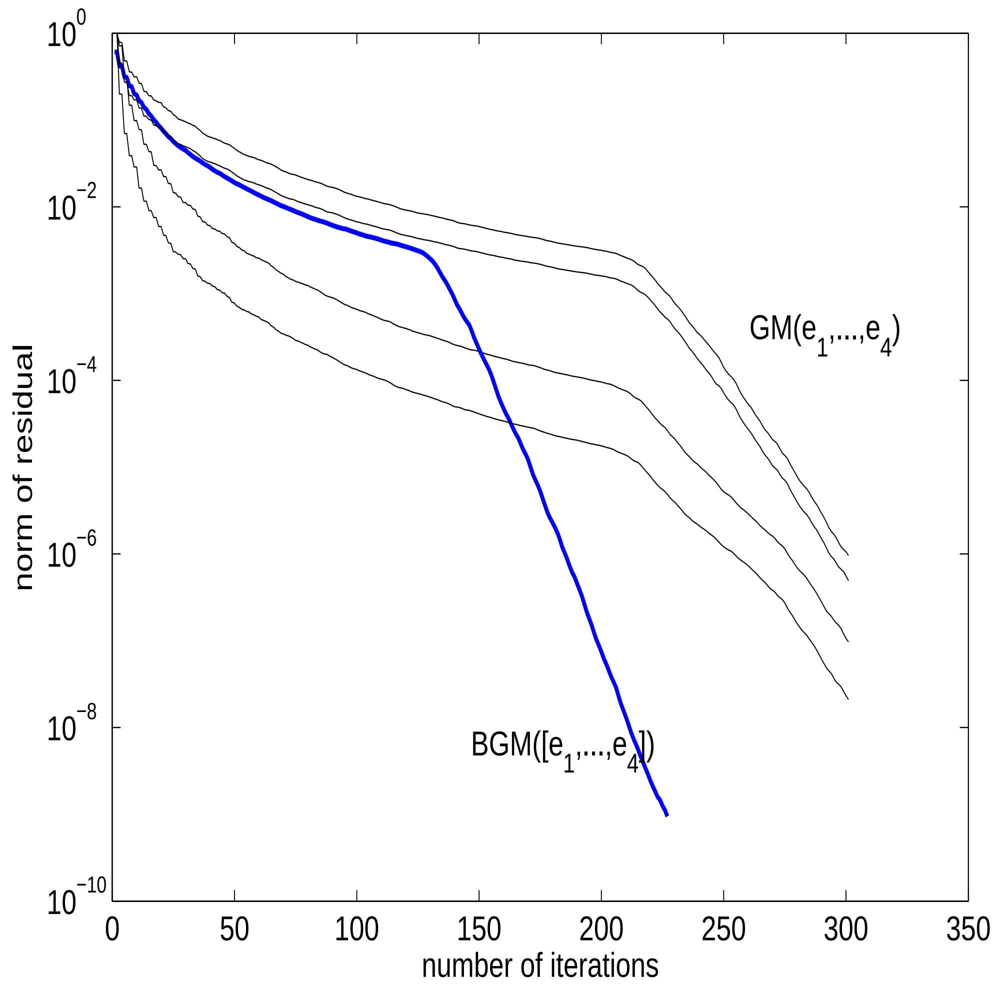
$$\Rightarrow \quad A\mathcal{U}_k = \mathcal{U}_k\mathcal{H}_k + U_{k+1}\chi_{k+1,k}E_k^* = \mathcal{U}_{k+1}\underline{\mathcal{H}}_k \qquad (\mathcal{H}_k = \mathcal{U}_k^* A\mathcal{U}_k)$$

$$\min_Y \|R_0 - A\mathcal{U}_k Y\| = \min_Y \| E_1\boldsymbol{\rho} - \underline{\mathcal{H}}_k Y \| \quad R_0 = U_1\boldsymbol{\rho}$$

$$\underline{\mathcal{H}}_k = \begin{bmatrix} \square & \square & \cdots & \square \\ \square & \square & \cdots & \square \\ O & \square & \cdots & \square \\ O & O & \ddots & \square \\ O & O & O & \square \end{bmatrix}$$

Block GMRES

$A \in \mathbb{R}^{6400\times6400}$: FD discretiz. of $\mathcal{L}(u) = -\Delta u + \frac{1000}{x+y}u_x$ in $[-1,1]^2$



Coping with long-term recurrences

Restarted, Truncated, Flexible variants.

Coping with long-term recurrences

Restarted, Truncated, Flexible variants.

Restarted: Choose $m_{\max}$.

Set $x = x_0$, $r_0 = b - Ax_0$

for $i = 1, 2, \ldots$

$z \leftarrow$ GMRES($A, r_0, m_{\max}$) (or other method)

$x \leftarrow x + z, \quad r_0 = b - Ax$

Check Convergence

Pros and Cons

Pros:

- Shorter dependencies
- Lower and fixed memory requirements

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- Shorter dependencies
- Lower and fixed memory requirements

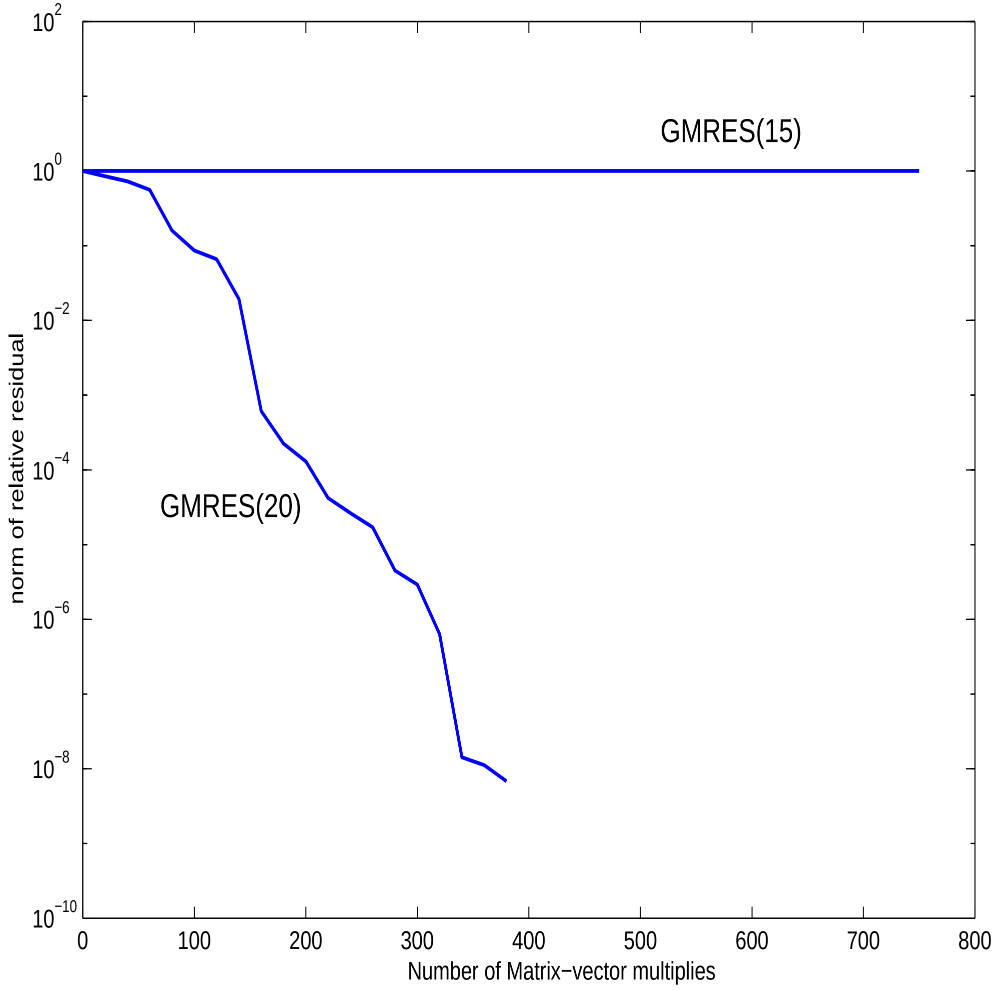
Cons:

- All optimality properties are lost

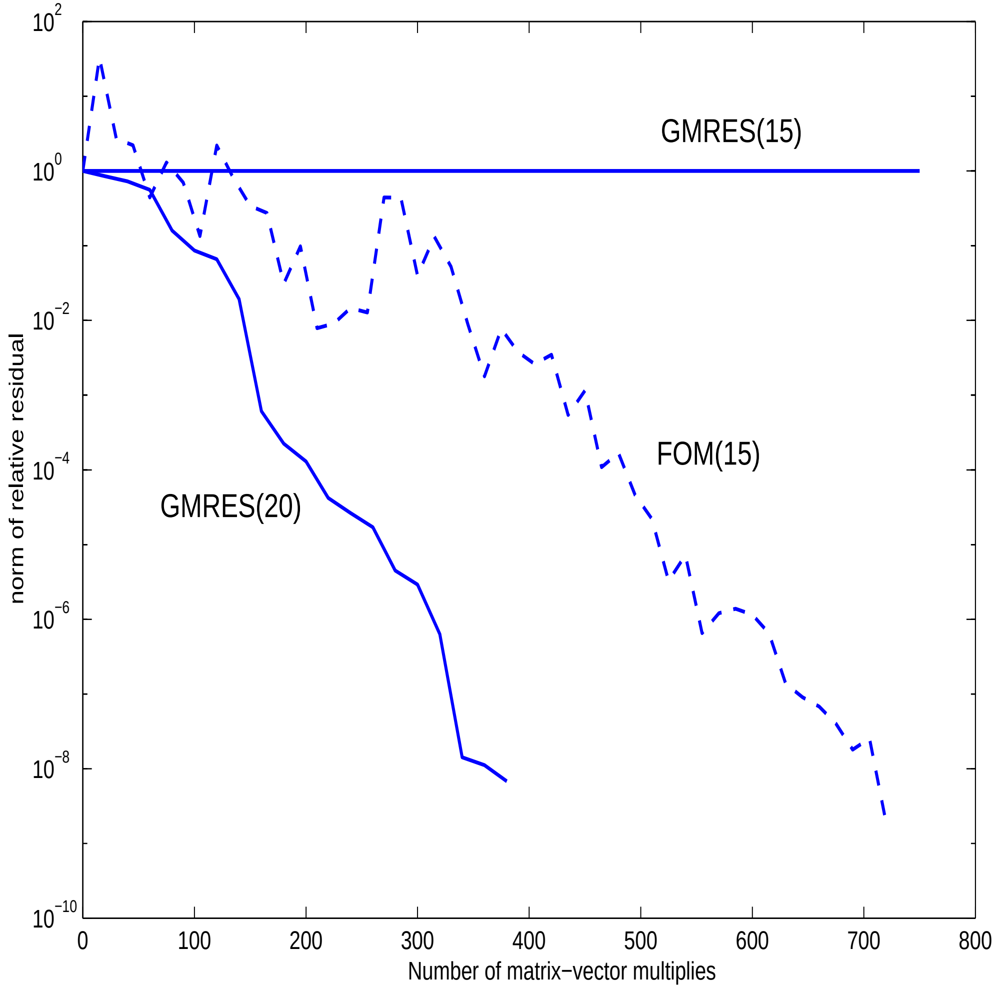
$$K_{m_{\max}}(A, r_0^{(0)}) + K_{m_{\max}}(A, r_0^{(1)}) + \ldots K_{m_{\max}}(A, r_0^{(k)}) + \ldots$$

- Additional parameter. What value for $m_{\max}$??

A problem with the restarting parameter? ...



A problem with the restarting parameter? ... or with the method?



Explanation

$$K_{m_{\max}}(A, r_0^{(0)}) + K_{m_{\max}}(A, r_0^{(1)}) + \ldots K_{m_{\max}}(A, r_0^{(k)}) + \ldots$$

GMRES: $r_0^{(k)} \in \mathrm{range}(V_{m_{\max}+1}^{(k-1)})$. Almost stagnation: $\rightarrow r_0^{(k)} \propto v_1^{(k-1)}$

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GMRES: $r_0^{(k)} \in \mathrm{range}(V_{m_{\max}+1}^{(k-1)})$. Almost stagnation: $\rightarrow r_0^{(k)} \propto v_1^{(k-1)}$

FOM: $r_0^{(k)} \propto v_{m_{\max}+1}^{(k-1)}$ Subspace keeps growing

Truncating

Only local orthogonalization (k-term recurrence, H_m banded)

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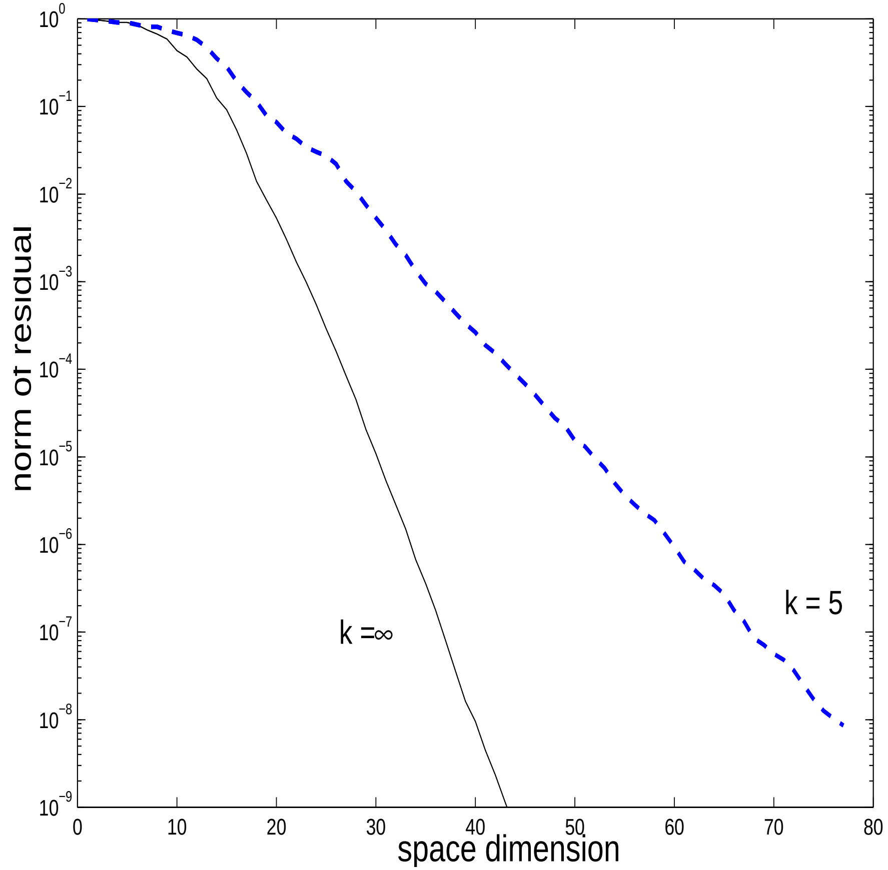
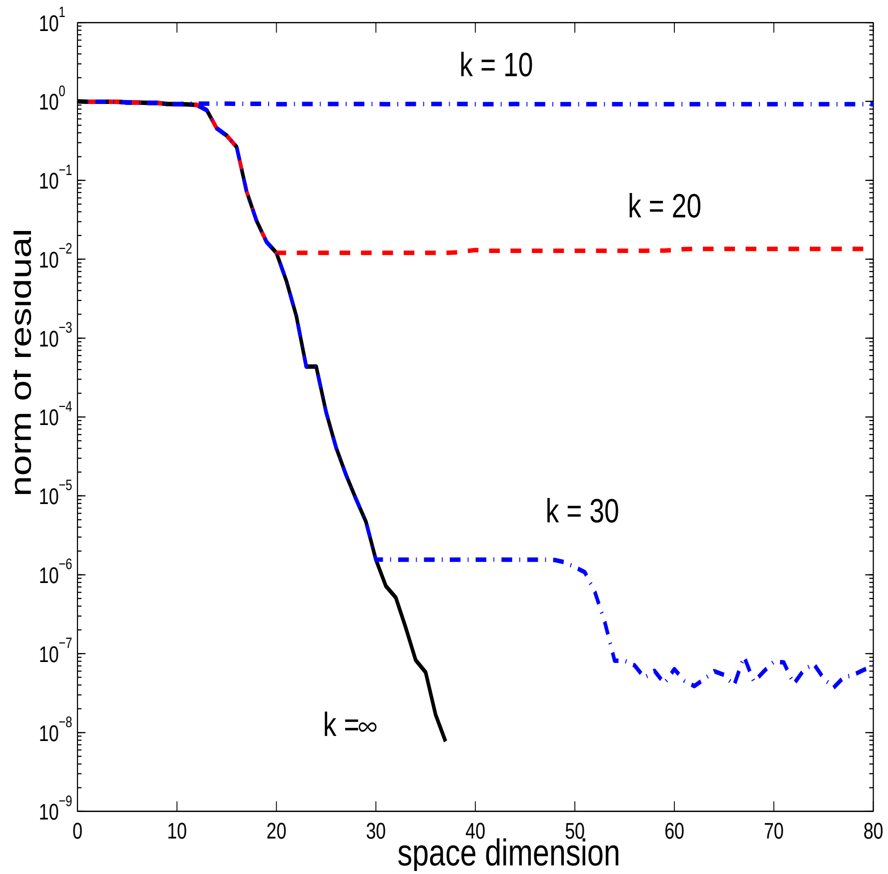


a reasonable strategy

Truncating

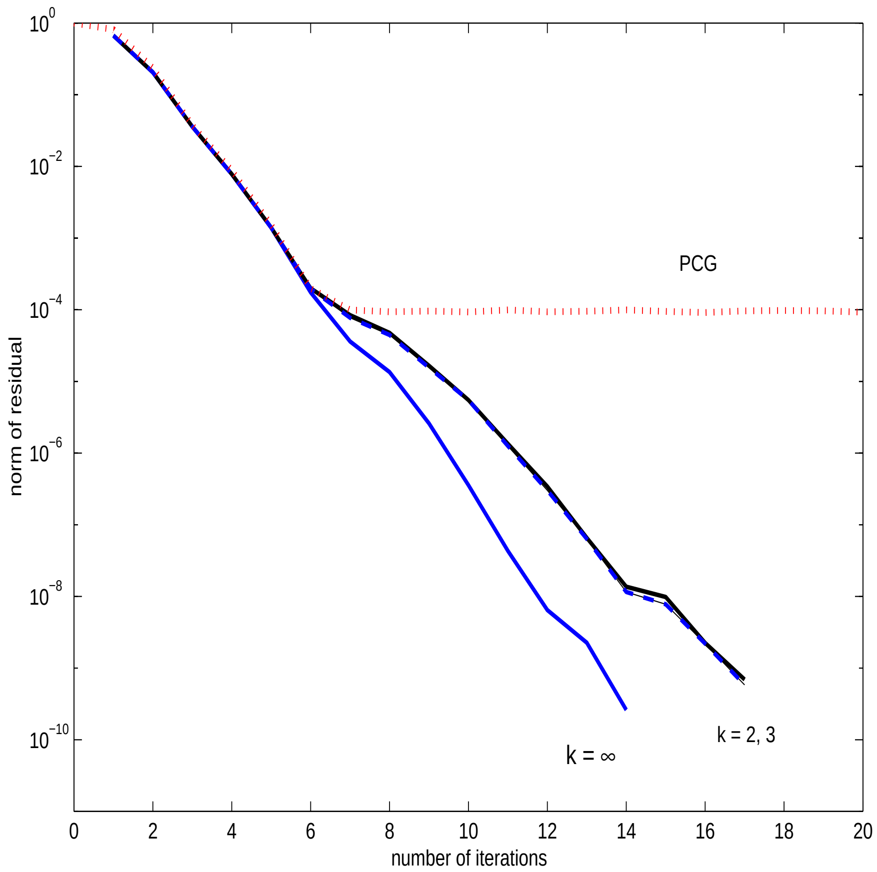
...but not always good



Truncating

A good strategy for P-CG with A symmetric and P inexact precond

$$w = P^{-1}Av + \epsilon\mathbf{1}, \quad \epsilon = 10^{-5}$$



Changing K_k. Flexible methods

Original problem

$$AP^{-1}\hat{x} = b \qquad x = P^{-1}\hat{x}, \qquad P \text{ preconditioner}$$

$$\mathcal{K}_k(AP^{-1}, r_0) = \text{span}\{r_0, AP^{-1}r_0, \ldots, (AP^{-1})^{k-1}r_0\}$$

at each iteration i: $\qquad z_i = P^{-1}v_i$

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Flexible variant:

Iteration i: $\qquad z_i = P^{-1}v_i \qquad \Rightarrow \qquad z_i = P_i^{-1}v_i$

$$\widetilde{x}_m \in \text{span}\{r_0, z_1, z_2, \ldots, z_{m-1}\} \neq \mathcal{K}_k(AP^{-1}, r_0)$$

Flexible and Truncated method. An example

$z = P^{-1}v \quad \Leftrightarrow z \approx A^{-1}v$ span$\{r_0, z_1, z_2, \ldots, z_{m-1}\}$

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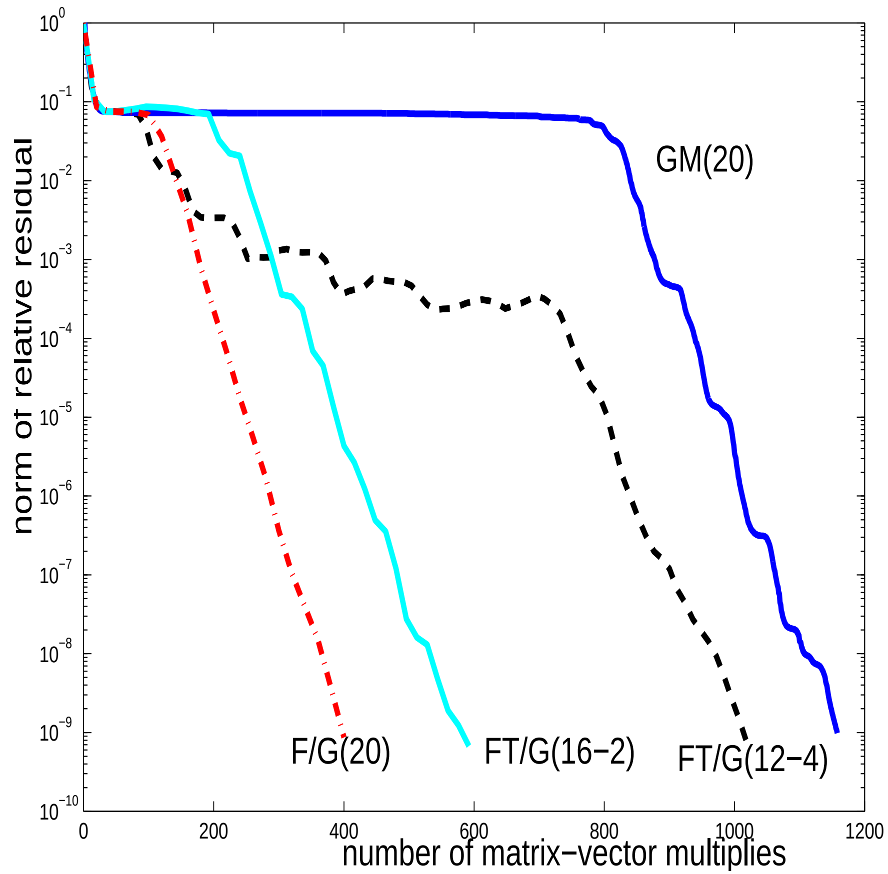
$z = P^{-1}v \quad \Leftrightarrow z \approx A^{-1}v$ span$\{r_0, z_1, z_2, \ldots, z_{m-1}\}$

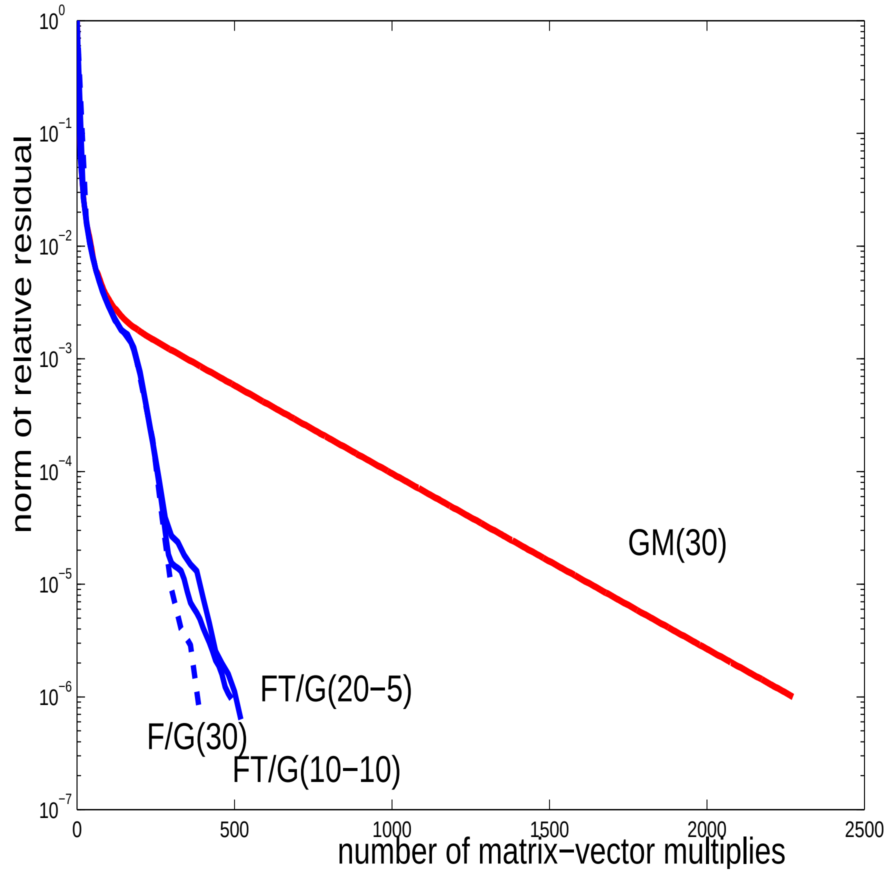
A from $L(u) = -\Delta u + 1000 x u_x$ $n = 900$



Flexible and Truncated method. A second example

$z = P^{-1}v \quad \Leftrightarrow z \approx A^{-1}v$ span$\{r_0, z_1, z_2, \ldots, z_{m-1}\}$

$$L(u) = -1000\Delta u + 2e^{4(x^2+y^2)}u_x - 2e^{4(x^2+y^2)}u_y \qquad n = 40\,000$$



Second Summary

Long-term recurrences:

- Optimal methods (e.g. GMRES), single and multiple right-hand sides
- Restarted, truncated, flexible (and combinations thereof)

Making it without: short-term recurrences for A non-Hermitian

Change optimality condition: Non-Hermitian Lanczos

$$r_k \perp K_k(A^\top, \tilde{r}_0), \qquad \tilde{r}_0 \text{ freely chosen}$$

Range(V_k)$= K_k(A, r_0)$, Range(W_k)$= K_k(A^\top, \tilde{r}_0)$ and s.t.

$$W_k^\top V_k \text{ diagonal}$$

$$AV_k = V_k T_k + v_{k+1} t_{k+1,k} e_k^\top, \quad A^\top W_k = W_k T_k^\top + w_{k+1} t_{k,k+1} e_k^\top,$$

Bi-orthogonal recurrence, T_k tridiagonal $\Rightarrow$ 3-term recurrence

Making it without: short-term recurrences for A non-Hermitian

Change optimality condition: Non-Hermitian Lanczos

$$r_k \perp K_k(A^\top, \tilde{r}_0), \qquad \tilde{r}_0 \text{ freely chosen}$$

Range(V_k)$= K_k(A, r_0)$, Range(W_k)$= K_k(A^\top, \tilde{r}_0)$ and s.t.

$$W_k^\top V_k \text{ diagonal}$$

$$AV_k = V_k T_k + v_{k+1} t_{k+1,k} e_k^\top, \quad A^\top W_k = W_k T_k^\top + w_{k+1} t_{k,k+1} e_k^\top,$$

Bi-orthogonal recurrence, T_k tridiagonal $\Rightarrow$ 3-term recurrence

$*$ Requires $A^\top$

$*$ Robustness problems

$\Rightarrow$ Special case: Simplified Lanczos

Simplified Lanczos

The typical problem

$$AH^{-1}x = b, \quad A, H \text{ symmetric},$$

Range(V_k)$= K_k(AH^{-1}, r_0)$, Range(W_k)$= K_k(H^{-1}A, \tilde{r}_0)$ and s.t.

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$\star$ If $\tilde{r}_0 = H^{-1}r_0$ then $W_k = H^{-1}V_k$

$\Rightarrow$ W_k obtained for free

- Short-term recurrence (cost similar to that of CG)
- Used for A, H indefinite (e.g. Saddle point problems)

An example: $AP^{-1}x = b$

$$A = \begin{bmatrix} M & B^\top \\ B & -C \end{bmatrix} \text{ symmetric} \qquad P = \begin{bmatrix} \widetilde{M} & B^\top \\ B & -\widetilde{C} \end{bmatrix} \text{ symmetric}$$

P: Constraint Preconditioner - used in (cheaper!) factored form

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Apply Simplified Lanczos-type method: Quasi Minimal Residual

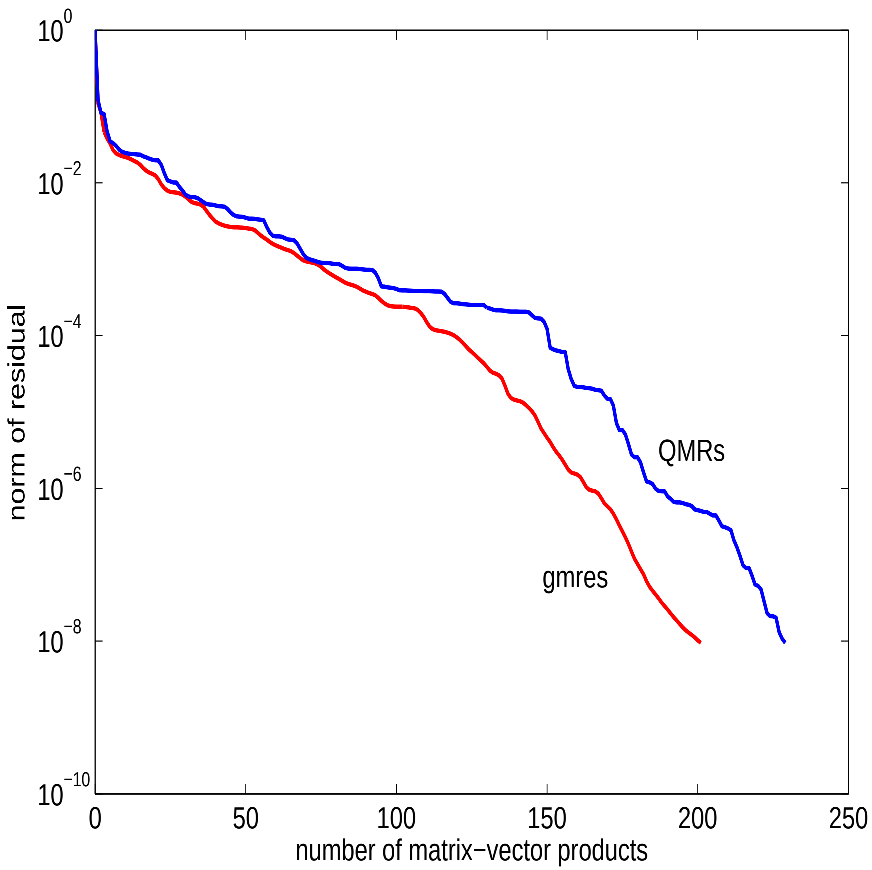
$$\|b - Ax_k\| = \|V_{k+1}\,(e_1\,\|r_0\| - \underline{T}_k y)\,\|$$

$$\min_y \|e_1\,\|r_0\| - \underline{T}_k y\|$$

V_{k+1} not orthogonal

An example: Stokes problem

Lid Driven Cavity problem from IFISS. Default params. A of size 49666



CPU Time: GMRES $=$ 51.66 secs, QMRs $=$ 6.26 secs

(my own GMRES code)

Short-term recurrences

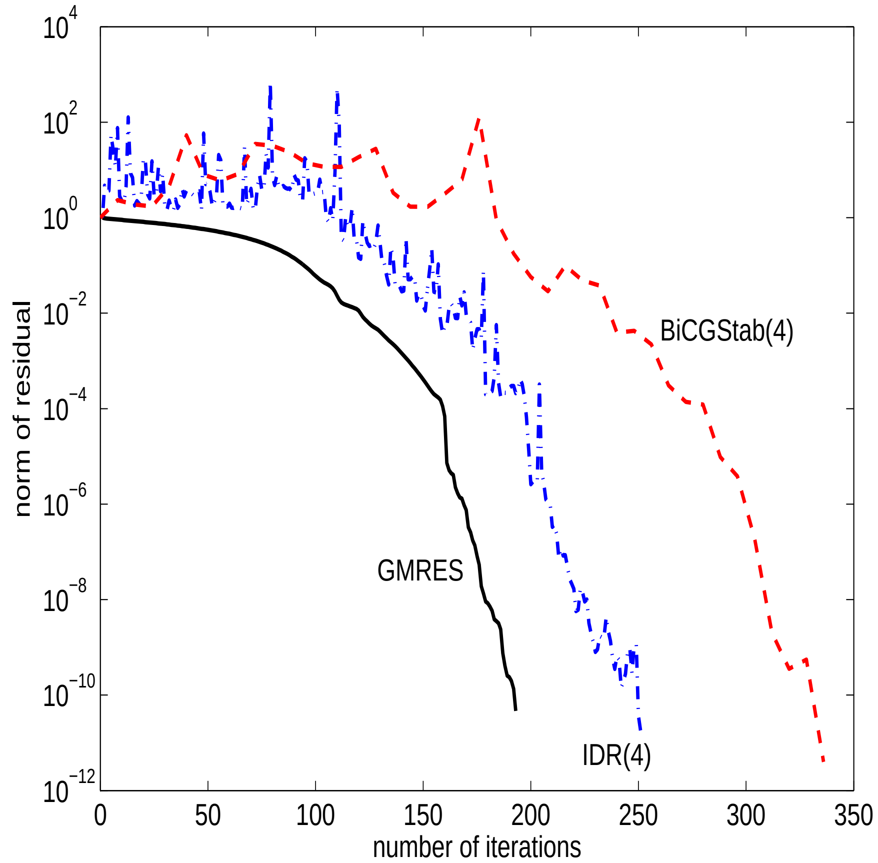
Local optimality conditions:

Polynomial methods, like CG:

- BiCGStab(ℓ): ℓ iterations of GMRES at every step
- IDR(s): $r_k \in \mathcal{G}_k$, where $\mathcal{G}_{k+1} \subset \mathcal{G}_k$

$$\mathcal{G}_{k+1} = (\mu_{k+1} I - A)(\mathcal{G}_k \cap \widetilde{R}_0^{\perp}), \quad \widetilde{R}_0 \in \mathbb{C}^{n \times s},\ \mathcal{G}_0 = \mathbb{C}.$$

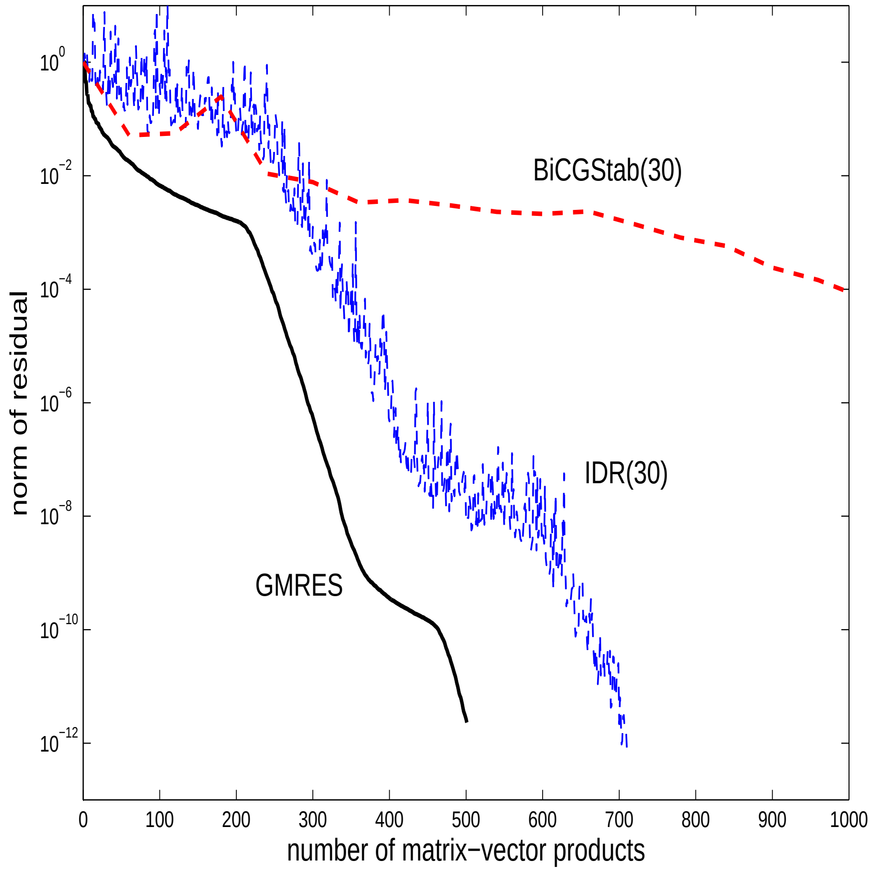
An Example: $L(u) = -\Delta u + 50(x+y)(u_x + u_y)$ $\qquad n = 6\,400$



CPU Time: GMRES = 3.65 secs, IDR(4) = 0.22 secs, BiCGStab(4) = 0.32 secs

(Matlab version of GMRES)

An Example: $L(u) = -\Delta u + 1000/(x+y)u_x$ $\qquad n = 6\,400$



CPU Time: GMRES = 24 secs, IDR(30) = 2.58 secs, BiCGStab(30) = 20 secs

(Matlab version of GMRES)

Tricks for all trades

- Stopping criterion
- Operator inexactness

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Stopping criterion:

- Problem dependent
- Matrix dependent

Stopping criterion within Rayleigh Quotient Iteration

Problem: Compute smallest eigenvalue(s) of A

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Rayleigh Quotient iteration:

Given y_0, compute $\theta_0 = y_0^* A y_0, \quad s_0 = A y_0 - y_0 \theta_0$

for $k = 0, 1, 2, \ldots$

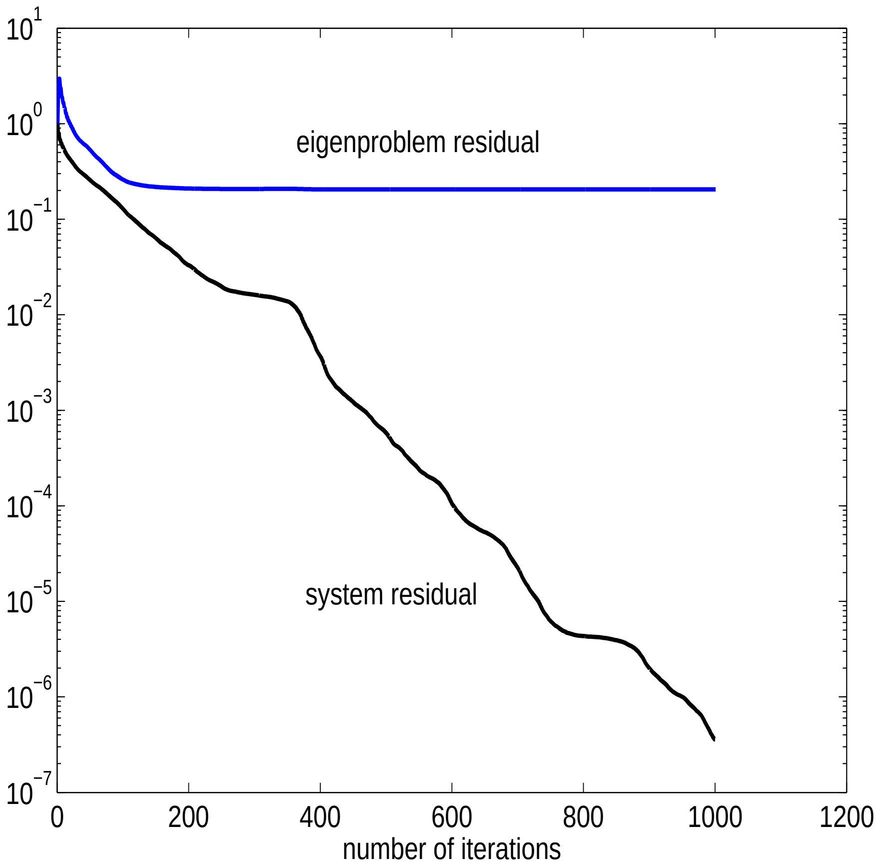
Solve $(A - \theta_k I)t = y_k$

Set $y_{k+1} = t/\|t\|, \;\; \theta_{k+1} = y_{k+1}^* A y_{k+1}$

$s_{k+1} = A y_{k+1} - y_{k+1} \theta_{k+1}$

$\theta_k \to \lambda$, $y_k \to x$ with (λ, x) eigenpair of A

An Example: A 2D Laplace operator



Generic kth RQI iteration. System to be solved: $(A - \theta_k I)t = y_k$

Stopping criterion: Problem dependence

Choice of tolerance:

- Direct method accurate up to machine precision (likely)
- Iterative method accurate up to what is wanted (hopefully)

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Algebraic problem: Discretization of PDEs

$$\text{error} \quad \to O(h)$$

h discretization parameter...

Stopping criterion: Problem dependence

Choice of criterion and norm:

$$\|b - Ax_k\|_2 \qquad \text{vs.} \qquad \|b - Ax_k\|_*$$

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For instance, CG optimal: $(\|x\|_A^2 = x^* A x)$

$$\min_{x_k \in x_0 + K_k(A, r_0)} \|b - Ax_k\|_{A^{-1}} = \min_{x_k \in x_0 + K_k(A, r_0)} \|x - x_k\|_A$$

Available: Cheap, reliable estimates of $\|x - x_k\|_A$

Stopping criterion: Problem dependence

Choice of criterion and norm:

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For instance, matrix G associated with FE error measure:

$$\min_{x_k} \|b - Ax_k\|_G$$

Matrix dependence

A may be very ill-conditioned

$\Rightarrow$ small residual does not necessarily imply small error

Well-known fact, but often not used

$$\frac{\|b - Ax_k\|}{\|b\|} \quad \text{vs} \quad \frac{\|b - Ax_k\|}{\|b\| + \|A\|_\star \|x_k\|}$$

(here $x_0 = 0$)

Matrix dependence

Inner-outer methods. e.g. Solve

$$BM^{-1}B^\top x = b$$

Each multiplication with $A = BM^{-1}B^\top$ requires solving a system with M

$$u = Av \quad \Leftrightarrow \quad \begin{aligned} &\tilde{u} = B^\top v \\ &\tilde{\tilde{u}} \text{ solves } M\tilde{\tilde{u}} = \tilde{u} \\ &u = B\tilde{\tilde{u}} \end{aligned}$$

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Note: True residual $r_k = b - BM^{-1}B^\top x_k$ not available!

How accurately should one solve with M?

Typically: Inner tolerance $<$ Outer tolerance

But: if optimal Krylov method is used to solve $BM^{-1}B^{\top}x = b$ then:

$$\text{Inner tolerance} = \text{c} \cdot \frac{\text{Outer tolerance}}{\text{current outer residual}}$$

The inexact key relation

$$A_{\epsilon_j} v = Av + f_j \qquad \|f_j\| = O(\epsilon_j), \quad j = 1, 2, \ldots$$

$$AV_m = V_{m+1}\underline{H}_m + \underbrace{F_m}_{[f_1, f_2, \ldots, f_m]} \qquad F_m \text{ error matrix}$$

How large is F_m allowed to be?

Claim: the perturbation induced by ϵ_j may be far less devastating for $x_m \to x$ than $|\epsilon_j|$ would predict

$$Ax_m = AV_m y_m = V_{m+1}\underline{H}_m y_m + F_m y_m$$

$$\|F_m y_m\| \quad \text{small then} \quad V_{m+1}\underline{H}_m y_m \approx Ax_m$$

A dynamic setting

$$Ax_m = AV_m y_m = V_{m+1} \underline{H}_m y_m + F_m y_m$$

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

◇ 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 $|\eta_i|$ small $\quad \Rightarrow \quad \|f_i\|$ is allowed to be large

⋆ In several problems it can be shown that $\quad |\eta_i| \le \gamma_m \|r_{i-1}\|$

Relaxing the accuracy in linear systems

$A \cdot v_i$ not performed exactly $\quad \Rightarrow \quad (A + E_i)v_i = Av_i + f_i$

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

E.g., for GMRES: If $\|E_i\| \le \frac{\gamma}{m} \frac{1}{\|\tilde{r}_{i-1}\|}\varepsilon \quad i = 1, \ldots, m$ $(\gamma = \gamma(A))$, then

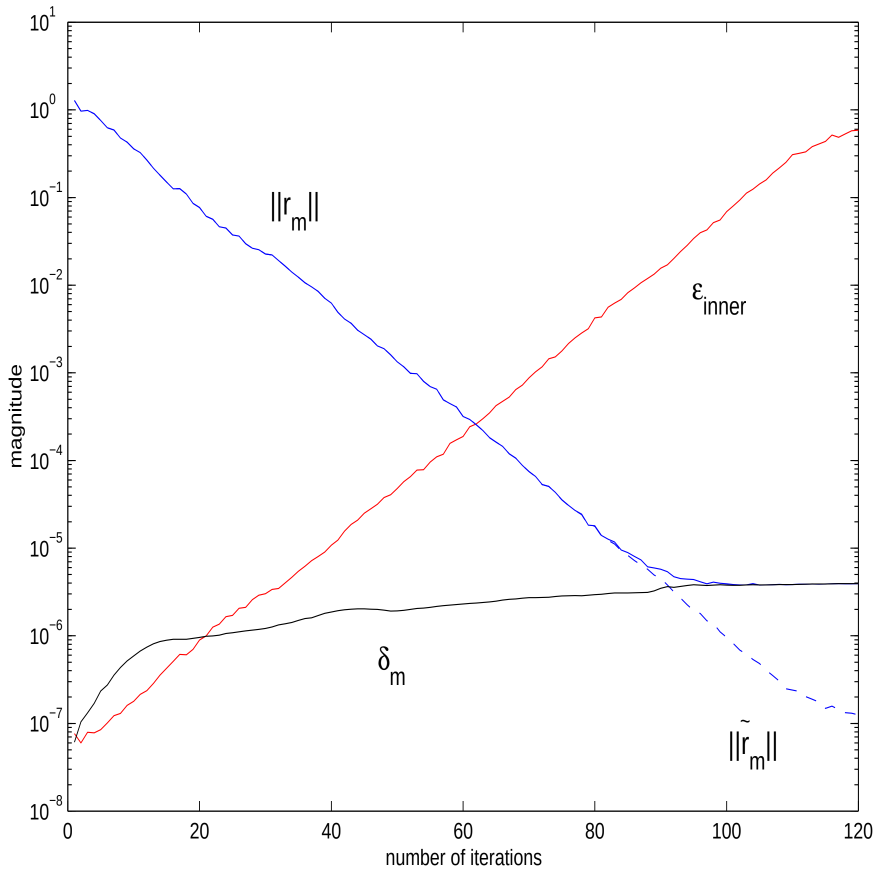
$\|F_m y_m\| \le \sum_{i=1}^{m} \|E_i\||\eta_i| \le \varepsilon$ so that

$$\|(b - Ax_m) - V_{m+1}(e_1\beta - \underline{H}_m y_m)\| \le \varepsilon$$

Note: $\|b - Ax_m\| \le \varepsilon$ final attainable residual norm

An example. GMRES

$$\varepsilon_{\text{inner}} = \frac{10^{-8}}{\|\tilde{r}_m\|}$$



$$r_m := \|b - Ax_m\|, \quad \tilde{r}_m := \|e_1 \|r_0\| - \underline{H}_m y_m\|, \quad \delta_m := \|r_m - \tilde{r}_m\|$$

Relaxed iteration

- Less and less accurate solution of inner system and still converge
- General procedure for any inexact/expensive A
- Save up to 30% computational time

Conclusions

- Computational issues for Krylov solvers well understood
- Other tricks can be used (but not usually in black-box routines)
- Many ideas have wider applicability
- Theory is still under development

http://www.dm.unibo.it/~simoncin
valeria.simoncini@unibo.it