A stable variant of Simpler GMRES and GCR

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joint work with Pavel Jiránek and Martin H. Gutknecht

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Minimum residual methods for $Ax = b$

We consider a nonsingular linear system

$$Ax = b, \qquad A \in \mathbb{R}^{N \times N},\ b \in \mathbb{R}^N.$$

Krylov subspace methods: initial guess x_0, compute $\{x_n\}$ such that

$$x_n \in x_0 + \mathcal{K}_n \quad \Rightarrow \quad r_n \equiv b - Ax_0 \in r_0 + A\mathcal{K}_n,$$

$\mathcal{K}_n \equiv \mathrm{span}(r_0, Ar_0, \ldots, A^{n-1}r_0)$ is the n-th *Krylov subspace* generated by A and r_0.

Minimum residual approach: minimizing the residual $r_n = b - Ax_n = r_0 - d_n$

$$\|r_n\| = \min_{d \in A\mathcal{K}_n} \|r_0 - d\| \quad \Leftrightarrow \quad r_n \perp A\mathcal{K}_n.$$

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Minimum residual methods for $Ax = b$

GMRES by Saad and Schultz [1986]:

- Arnoldi process: $AQ_n = Q_{n+1}H_{n+1,n}$,
- $x_n = x_0 + Q_n y_n$, where y_n solves $\min_y \|\varrho_0 e_1 - H_{n+1,n}y\|$, $\varrho_0 \equiv \|r_0\|$.

Numerical stability of GMRES: Drkošová, Greenbaum, R, and Strakoš [1995], Arioli and Fassino [1996], Greenbaum, R, and Strakoš [1997], Paige, R, and Strakoš [2006].

Other implementations:

- Simpler GMRES: Walker and Zhou [1994],
- ORTHODIR, ORTHOMIN(∞)$\equiv$ GCR: Young and Jea [1980], Vinsome [1976], Eisenstat, Elman, and Schultz [1983].

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Sketch of Simpler GMRES and GCR

- $Z_n \equiv [z_1, \dots, z_n]$ a (normalized) basis of $\mathcal{K}_n$.
- $V_n \equiv [v_1, \dots, v_n]$ an orthonormal basis of $A\mathcal{K}_n$:

$$AZ_n = V_n U_n, \qquad U_n \text{ is upper triangular.}$$

- Residual $r_n \in r_0 + A\mathcal{K}_n = r_0 + \mathcal{R}(V_n)$, $r_n \perp \mathcal{R}(V_n)$ satisfies

$$r_n = (I - V_n V_n^T) r_0 = (I - v_n v_n^T) r_{n-1} = r_{n-1} - \alpha_n v_n, \quad \alpha_n \equiv v_n^T r_{n-1},$$

whereas $x_n \in x_0 + \mathcal{K}_n = x_0 + \mathcal{R}(Z_n)$ satisfes

$$x_n = x_0 + Z_n t_n, \qquad U_n t_n = V_n^T r_0 = [\alpha_1, \dots, \alpha_n]^T.$$

- Approximate solution can be updated at each step

$$P_n \equiv [p_1, \dots, p_n] = A^{-1} V_n, \qquad Z_n = P_n U_n$$

$$\Rightarrow \qquad x_n = x_{n-1} + \alpha_n p_n.$$

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Backward and forward errors

Assume stable computation of U_n (e.g., using modified Gram-Schmidt orthogonalization or Householder reflections), $c\,\varepsilon\kappa(A)\kappa(Z_n) < 1$, and $r_n \to 0$.

Solution of a triangular system

$$\frac{\|b - Ax_n\|}{\|A\|\|x_n\| + \|b\|} \leq c\,\varepsilon\kappa(Z_n)\left(1 + \frac{\|x_0\|}{\|x_n\|}\right),$$

$$\frac{\|x - x_n\|}{\|x_n\|} \leq \frac{c\,\varepsilon\kappa(A)\kappa(Z_n)}{1 - c\,\varepsilon\kappa(A)\kappa(Z_n)}\left(1 + \frac{\|x_0\|}{\|x_n\|}\right).$$

Updated approximate solutions

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Choice of Z_n

1. $Z_n = [r_0/\|r_0\|, V_{n-1}]$ (Simpler GMRES, ORTHODIR)
   Robust, but numerically less stable (Liesen, R, and Strakoš [2002]):

$$\frac{\|r_0\|}{\|r_{n-1}\|} \leq \kappa([\frac{r_0}{\|r_0\|}, V_{n-1}]) \leq 2\frac{\|r_0\|}{\|r_{n-1}\|}.$$

2. $Z_n = R_n$, $R_n \equiv [r_0/\|r_0\|, \ldots, r_{n-1}/\|r_{n-1}\|]$ (ORTHOMIN(∞), GCR)
   Residuals are linearly independent iff the residual norms decrease, but R_n is well conditioned:

$$\max_{k=1,\ldots,n-1} \left(\frac{\|r_{k-1}\|^2 + \|r_k\|^2}{\|r_{k-1}\|^2 - \|r_k\|^2}\right)^{\frac{1}{2}} \leq \kappa(R_n) \leq (n+1)^{\frac{1}{2}} \left(1 + \sum_{k=1}^{n-1} \frac{\|r_{k-1}\|^2 + \|r_k\|^2}{\|r_{k-1}\|^2 - \|r_k\|^2}\right)^{\frac{1}{2}}$$

3. Can we benefit from advantages of both bases without suffering from disadvantages?
   Adaptive choice of the direction z_n: introduce $\nu \in [0, 1)$ and compute z_n as

$$z_n = \begin{cases} r_0/\|r_0\| & \text{if } n = 1, \\ r_{n-1}/\|r_{n-1}\| & \text{if } n > 1 \ \& \ \|r_{n-1}\| \leq \nu\|r_{n-2}\|, \\ v_{n-1} & \text{otherwise.} \end{cases}$$

   PCR algorithm of Ramage and Wathen [1994]: "hybridization of the fast ORTHOMIN and robust ORTHODIR"

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Conditioning of the adaptive Z_n

Assume a *near stagnation* in the initial phase and a *fast convergence* in the subsequent steps:

- $\|r_{k-1}\| > \nu \|r_{k-2}\|$ for $k = 2, \ldots, q$ (Simpler GMRES basis),
- $\|r_{k-1}\| \leq \nu \|r_{k-2}\|$ for $k = q+1, \ldots, n$ (residual basis).

Then

$$\max\left\{1, \frac{1}{2}\underline{\gamma}_{n,q}\frac{\|r_{q-1}\|}{\|r_0\|}, \overline{\gamma}_{n,q}^{-1}\frac{\|r_0\|}{\|r_{q-1}\|}\right\} \leq \kappa(Z_n) \leq 2\overline{\gamma}_{n,q}\frac{\|r_0\|}{\|r_{q-1}\|},$$

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Similar estimates for general case (for multiple "switches" between bases).

Moreover,

$$\kappa(Z_n) \leq \frac{2\sqrt{2}}{\nu^{q-1}}\frac{1+\nu}{1-\nu}.$$

Quasi-optimal choice $\nu_{\rm opt} = (\sqrt{1+n^2} - 1)/n$ leads to

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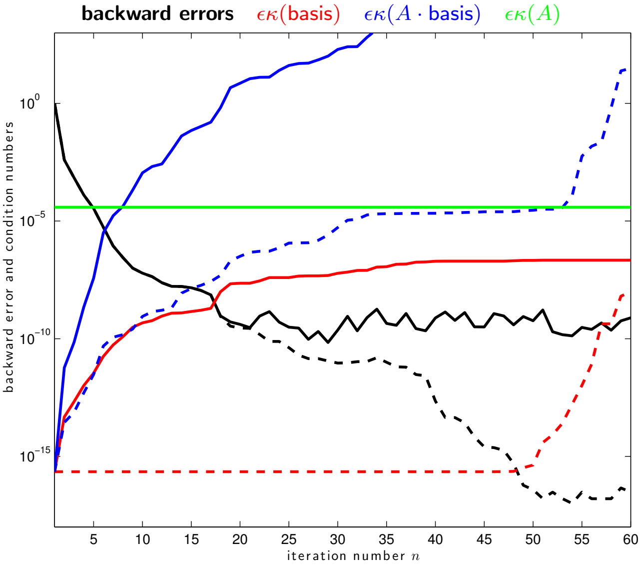
FS1836, $b = A(1, \dots, 1)^T$: Simpler GMRES fails, adaptive wins



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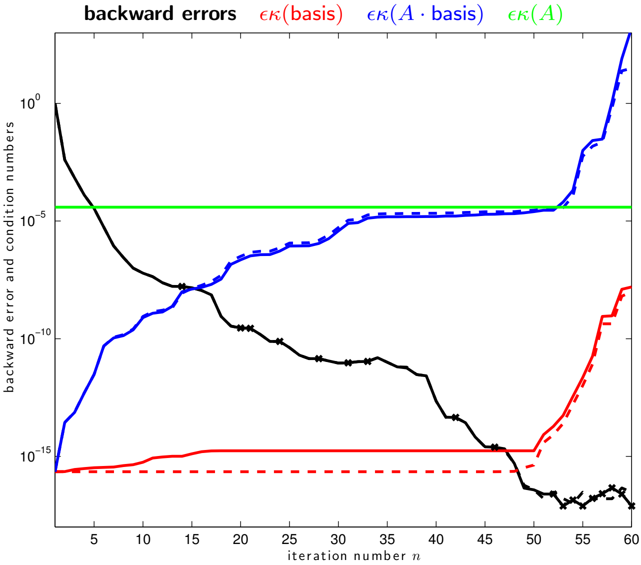

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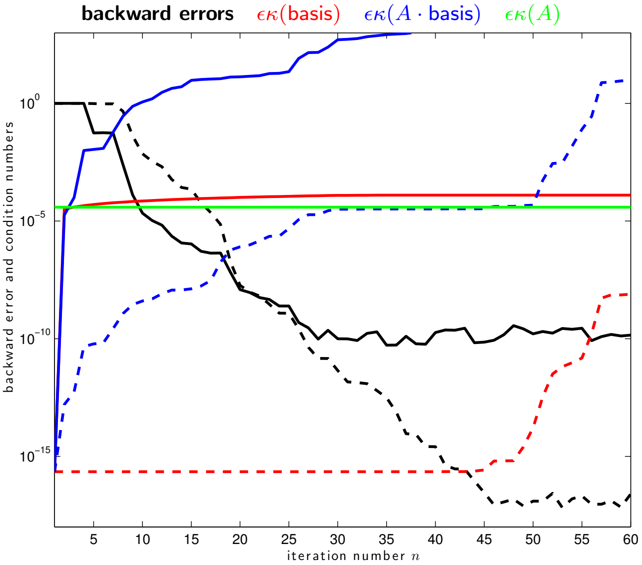

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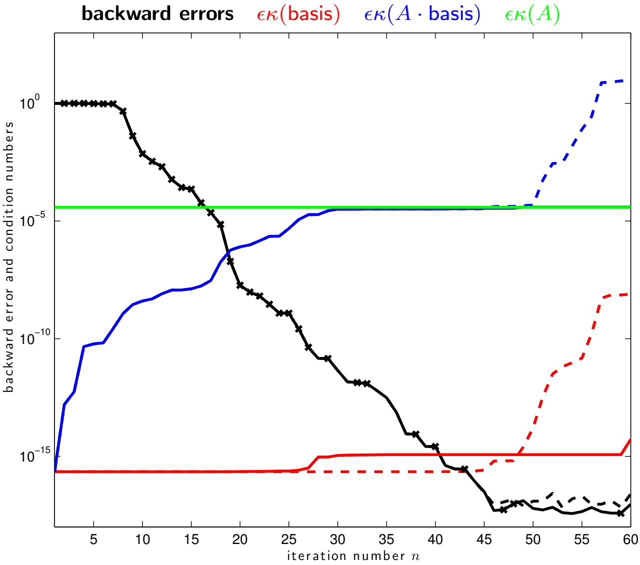
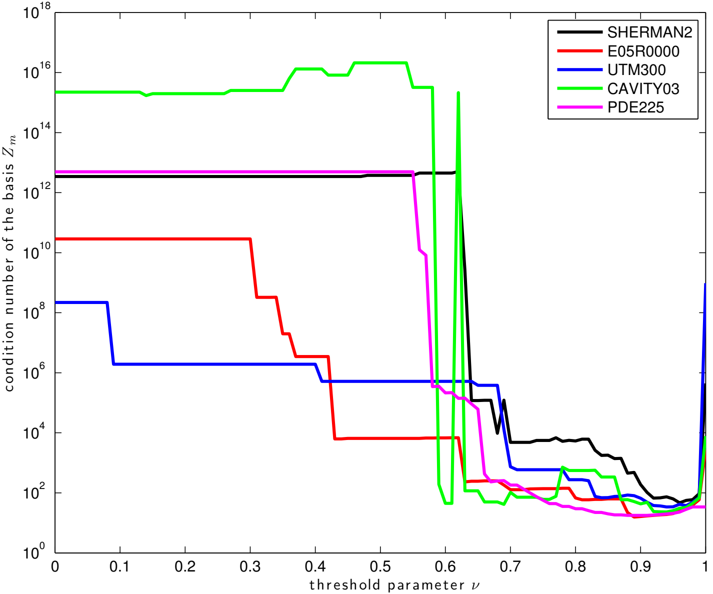


Dependence of $\kappa(Z_n)$ on ν



Conclusions and references

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- Simpler GMRES with residuals and ORTHOMIN(∞)/GCR can break down, but already moderate convergence implies good conditioning of the basis.
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- P. Jiránek, R, M. H. Gutknecht, How to make Simpler GMRES and GCR more stable, *SIAM J. Matrix Anal. Appl.*, 30 (2008), pp. 1483–1499.
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