# NUMERICAL BEHAVIOR OF GMRES

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joint work with
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# OUTLINE

1. ROUNDING ERROR EFFECTS: DELAY OF CONVERGENCE AND MAXIMUM ATTAINABLE ACCURACY

2. BACKWARD ERROR AND BACKWARD STABILITY

3. LOSS OF ORTHOGONALITY AND NUMERICAL BEHAVIOR OF GMRES: HOUSEHOLDER GMRES, MGS AND CGS GMRES

4. HOW TO MAKE SIMPLER GMRES AND GCR MORE STABLE: ADAPTIVE SIMPLER GMRES

## ITERATIVE METHODS IN EXACT ARITHMETIC

generate approximate solutions to the solution of $Ax = b$

$$x_0, x_1, \ldots, x_n \longrightarrow x$$

with residual vectors $r_0 = b - Ax_0, \ldots, r_n = b - Ax_n \to 0$

## METHODS IN FINITE PRECISION ARITHMETIC

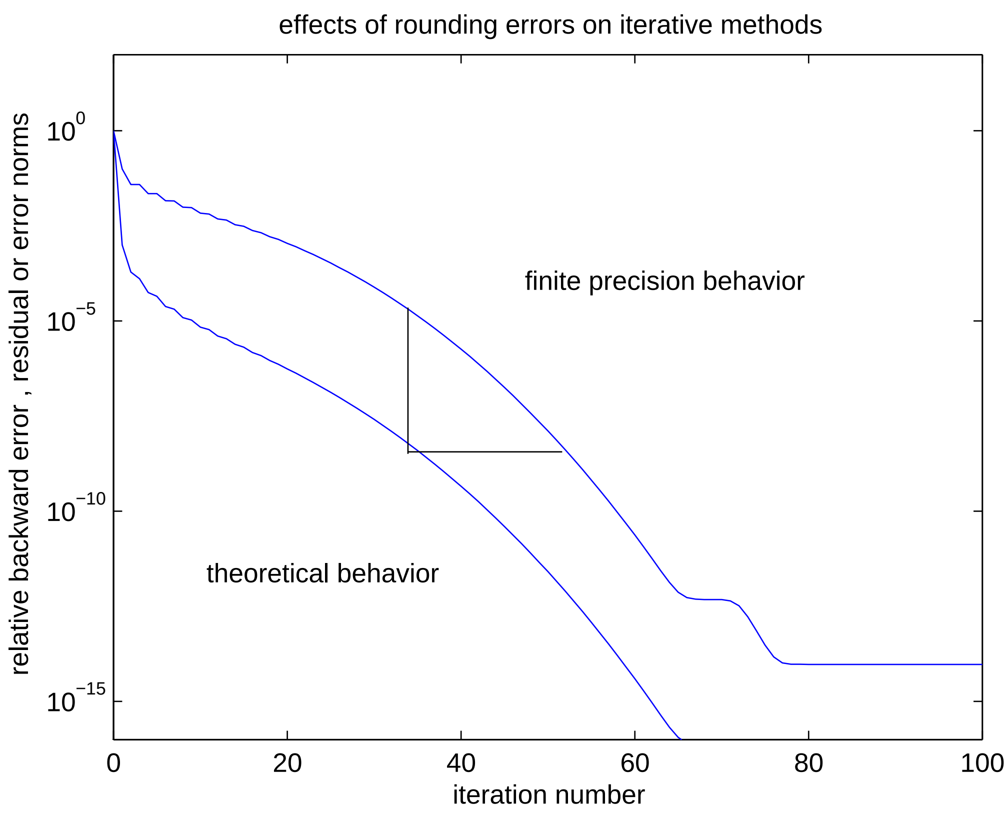
compute approximations $x_0, \bar{x}_1, \ldots, \bar{x}_n$ and updated residual vectors $\bar{r}_0, \bar{r}_1, \ldots, \bar{r}_n$ which are usually close to (but different from) the true residuals $b - A\bar{x}_n$

## TWO MAIN QUESTIONS

- How good is the computed approximate solution $\bar{x}_n$? How many (extra) steps do we need to reach the same accuracy as one can get in the exact method?

- How well the computed vector $\bar{r}_n$ approximates the (true) residual $b - A\bar{x}_n$? Is there a limitation on the accuracy of the computed approximate solution?

## TWO EFFECTS OF ROUNDING ERRORS: DELAY OF CONVERGENCE AND LIMITING (MAXIMUM ATTAINABLE) ACCURACY



effects of rounding errors on iterative methods
relative backward error , residual or error norms
$10^{0}$
$10^{-5}$
$10^{-10}$
$10^{-15}$
finite precision behavior
theoretical behavior
0
20
40
60
80
100
iteration number

# THE CONCEPT OF BACKWARD STABILITY

A backward stable algorithm eventually computes the exact answer to a nearby problem, i.e. the vector $\bar{x}_n$ satisfying

$$(A + \Delta A_n)\bar{x}_n = b + \Delta b_n$$

$$\|\Delta A_n\|_{(F)} / \|A\|_{(F)} \leq O(\varepsilon), \; \|\Delta b_n\| / \|b\| \leq O(\varepsilon)$$

$\Longleftrightarrow$ The normwise backward error associated with the approximate solution $\bar{x}_n$ satisfies

$$\frac{\|b - A\bar{x}_n\|}{\|b\| + \|A\|_{(F)}\|\bar{x}_n\|} \leq O(\varepsilon)$$

Prager, Oettli, 1964; Rigal, Gaches, 1967

see also Higham, 2nd ed. 2002; Stewart, Sun, 1990; Meurant 1999

# THE LEVEL OF MAXIMUM ATTAINABLE ACCURACY

We are looking for the difference between the updated $\bar{r}_n$ and true residual $b - A\bar{x}_n$ (divided by $\|A\|\|\bar{x}_n\| + \|b\|$ or $\|A\|_F\|\bar{x}_n\| + \|b\|$)

$$\frac{\|b - A\bar{x}_n - \bar{r}_n\|}{\|A\|\|\bar{x}_n\| + \|b\|} \leq ?$$

$$\|\bar{r}_n\| \longrightarrow 0 \Longrightarrow \lim_{n\to\infty} \frac{\|b - A\bar{x}_n\|}{\|A\|\|\bar{x}_n\| + \|b\|} \leq ?$$

In the optimal case the bound is of $O(\varepsilon)$; then we have a backward stable solution

Chris Paige, R, Strakoš, 2006

# MOTIVATION: SYMMETRIC LANCZOS PROCESS AND CONJUGATE GRADIENT METHOD

## THE CONCEPT OF CONVERGENCE DELAY

Greenbaum, 1989; Strakoš, Greenbaum, 1991

Paige, Strakoš, 1999

Meurant, Strakoš, Acta Numerica 2006

Strakoš, Liesen, ZAMM 2006

Delay in convergence of the conjugate gradient method (due to rounding errors) is given by the rank-deficiency of the computed Lanczos basis!

# NONSYMMETRIC ARNOLDI PROCESS AND THE GMRES METHOD

Saad, Schultz 1986

# THE CORRECTED PRINCIPLE OF CONVERGENCE DELAY:

Once the rank-deficiency occurs in the Arnoldi process the GMRES method stagnates on its final accuracy level

# THEORETICAL JUSTIFICATION?

## BASIC QUESTION:

How important is the orthogonality of computed basis vectors in the GMRES method?

## ANSWER:

For solving the system accurately we **do not** need fully orthogonal vectors - we need their **linear independence**! The crucial thing is a **complete loss** of their orthogonality!

$$Ax = b$$

$A \in R^{N,N}$, $A$ nonsingular, $b \in R^N$

## THE GMRES METHOD:

$$x_0, r_0 = b - Ax_0,$$
$$K_n(A, r_0) = span\ \{r_0, Ar_0, \ldots, A^{n-1}r_0\}$$

$$x_n \in x_0 + K_n(A, r_0)$$

$$\|b - Ax_n\| = \min_{u \in x_0 + K_n(A, r_0)} \|b - Au\|$$

## IMPLEMENTATION OF GMRES

$$\bar{x}_n = fl(x_0 + \bar{V}_n \bar{y}_n)$$

**Arnoldi (orthogonalization) process:**

The loss of orthogonality (loss of rank) in $\bar{V}_n = [\bar{v}_1, \bar{v}_2, \ldots, \bar{v}_n]$
$\|I - \bar{V}_n^T \bar{V}_n\| \leq ?$ , $\sigma_n(\bar{V}_n) \leq ?$

**Upper-Hessenberg least squares problem:**

The (in)accurate $\bar{y}_n = fl(\arg\min_y \| \|r_0\| e_1 - \bar{H}_{n+1,n} y \|)$
$\kappa(\bar{H}_{n+1,n}) \leq ?$

# THE NONSYMMETRIC ARNOLDI PROCESS

$$V_n = [v_1, v_2, \ldots, v_n]$$

**Arnoldi process is a (recursive) column-oriented QR decomposition of** $[r_0, AV_n]$**!**

$$[r_0, AV_n] = V_{n+1}[\|r_0\|e_1, H_{n+1,n}]$$

$H_{n+1,n}$ **is an upper Hessenberg matrix**

# WELL-PRESERVED ORTHOGONALITY $\Rightarrow$ BACKWARD STABILITY

## HOUSEHOLDER GMRES:

$$\|I - \bar{V}_N^T \bar{V}_N\| \leq O(\varepsilon)$$

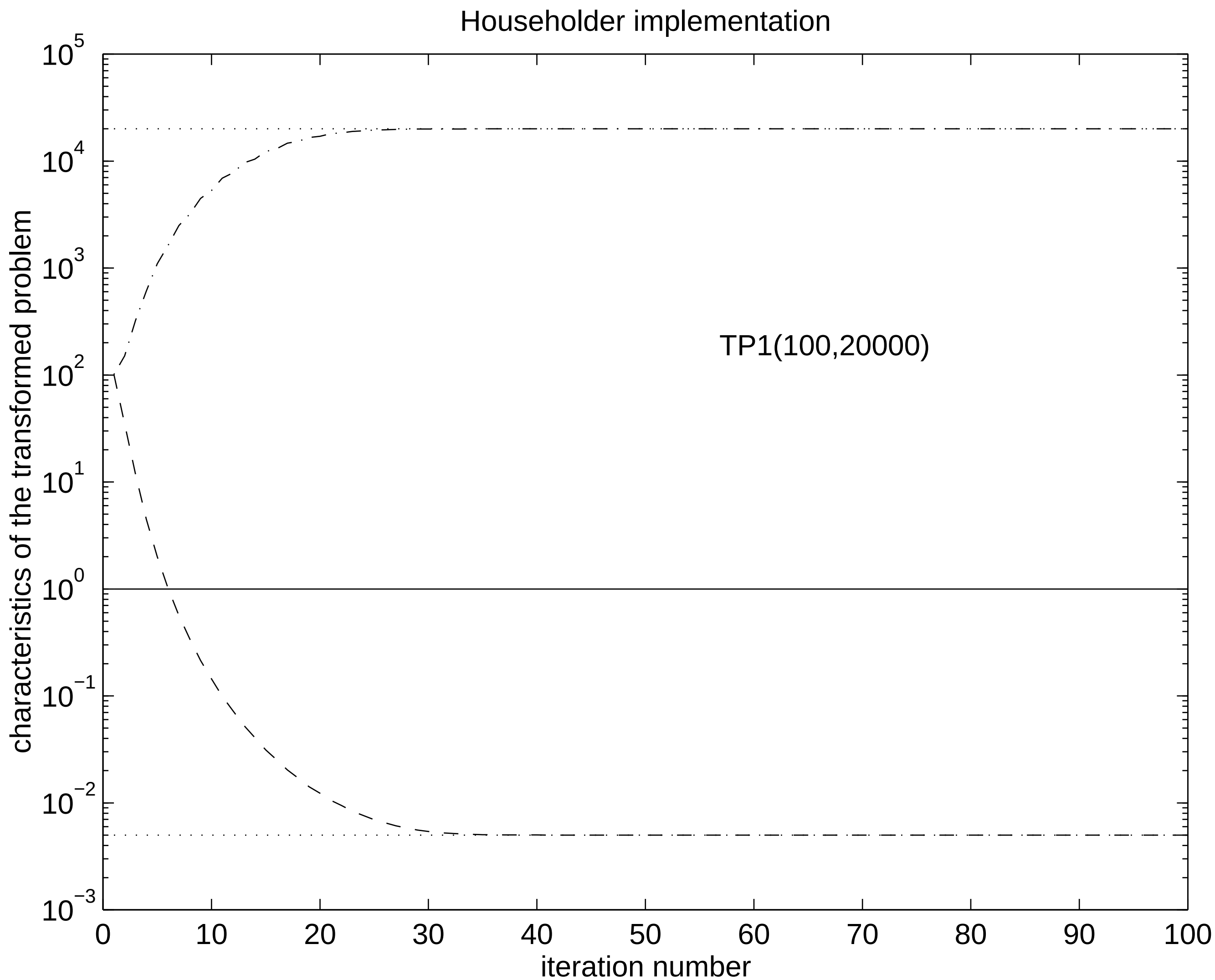
Wilkinson 1967, Walker 1988, 1989

$$\frac{\|b - A\bar{x}_N\|}{\|A\|\|\bar{x}_N\| + \|b\|} \leq O(\varepsilon)$$

$\bar{x}_N$ represents an exact solution to the nearby problem

$$(A + \Delta A)\bar{x}_N = b + \Delta b$$

Greenbaum, Drkošová, R, Strakoš, 1995


Householder implementation
characteristics of the transformed problem
iteration number
TP1(100,20000)
$10^5$
$10^4$
$10^3$
$10^2$
$10^1$
$10^0$
$10^{-1}$
$10^{-2}$
$10^{-3}$
0
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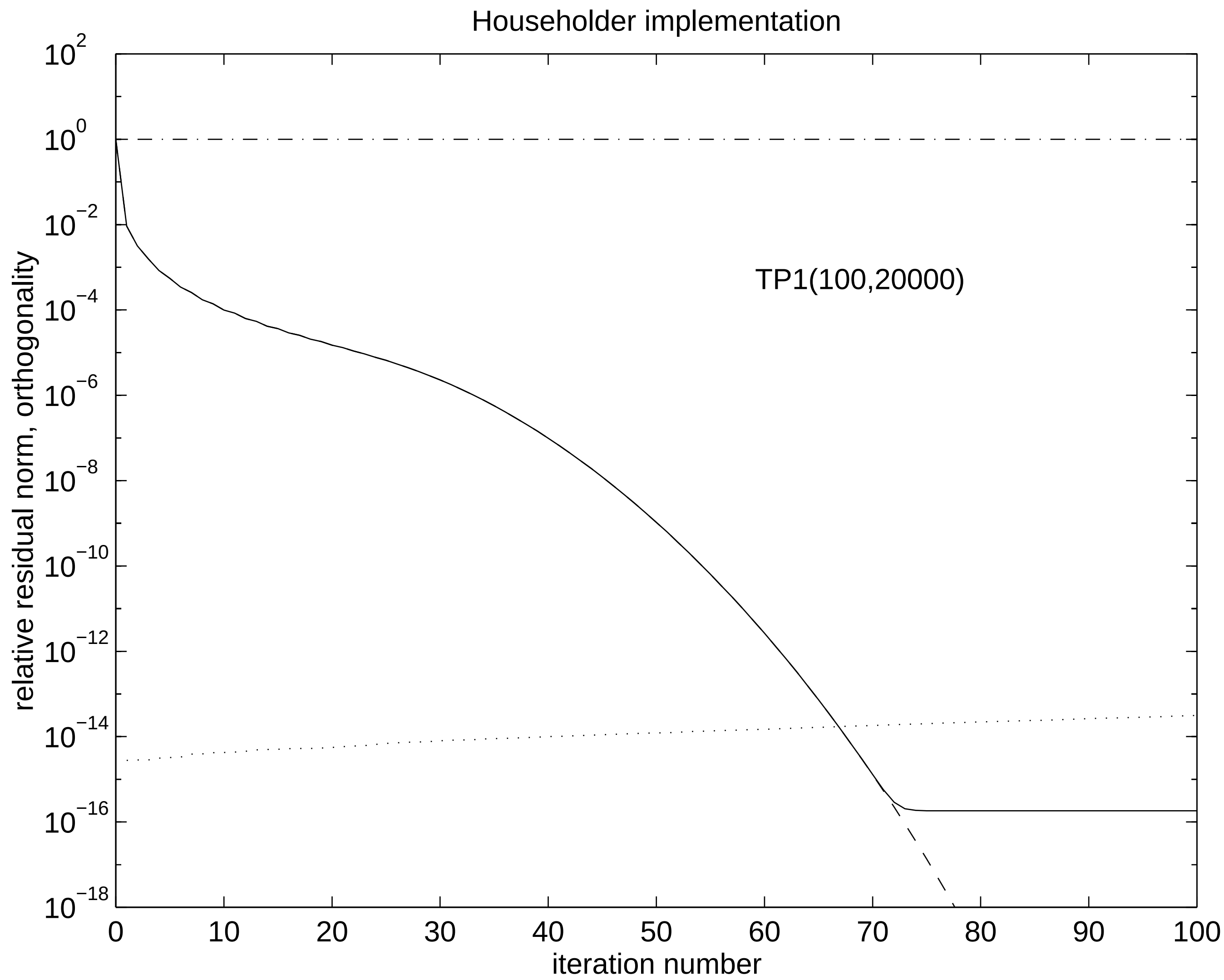
100


Householder implementation
TP1(100,20000)
relative residual norm, orthogonality
iteration number
10^2
10^0
10^−2
10^−4
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10^−10
10^−12
10^−14
10^−16
10^−18
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100

# GRAM-SCHMIDT GMRES

## MODIFIED GRAM-SCHMIDT:

$$\|I - \bar{V}_n^T \bar{V}_n\| \leq O(\varepsilon)\kappa([r_0, A\bar{V}_n])$$

Björck, 1967

Björck, Paige, 19992

## CLASSICAL GRAM-SCHMIDT:

$$\|I - \bar{V}_n^T \bar{V}_n\| \leq O(\varepsilon)\kappa^2([r_0, A\bar{V}_n])$$

van den Eshof, Giraud, Langou, R, 2005

Smoktunowicz, Barlow, Langou, 2006

## The GRAM-SCHMIDT GMRES IMPLEMENTATION

The (modified) Gram-Schmidt version of GMRES (MGS-GMRES) is efficient, but looses orthogonality.

The rank-deficiency (total loss of orthogonality $\equiv$ loss of linear independence of computed basis vectors) in the Arnoldi process with (modified) Gram-Schmidt can occur **only after** GMRES reaches its final accuracy level!

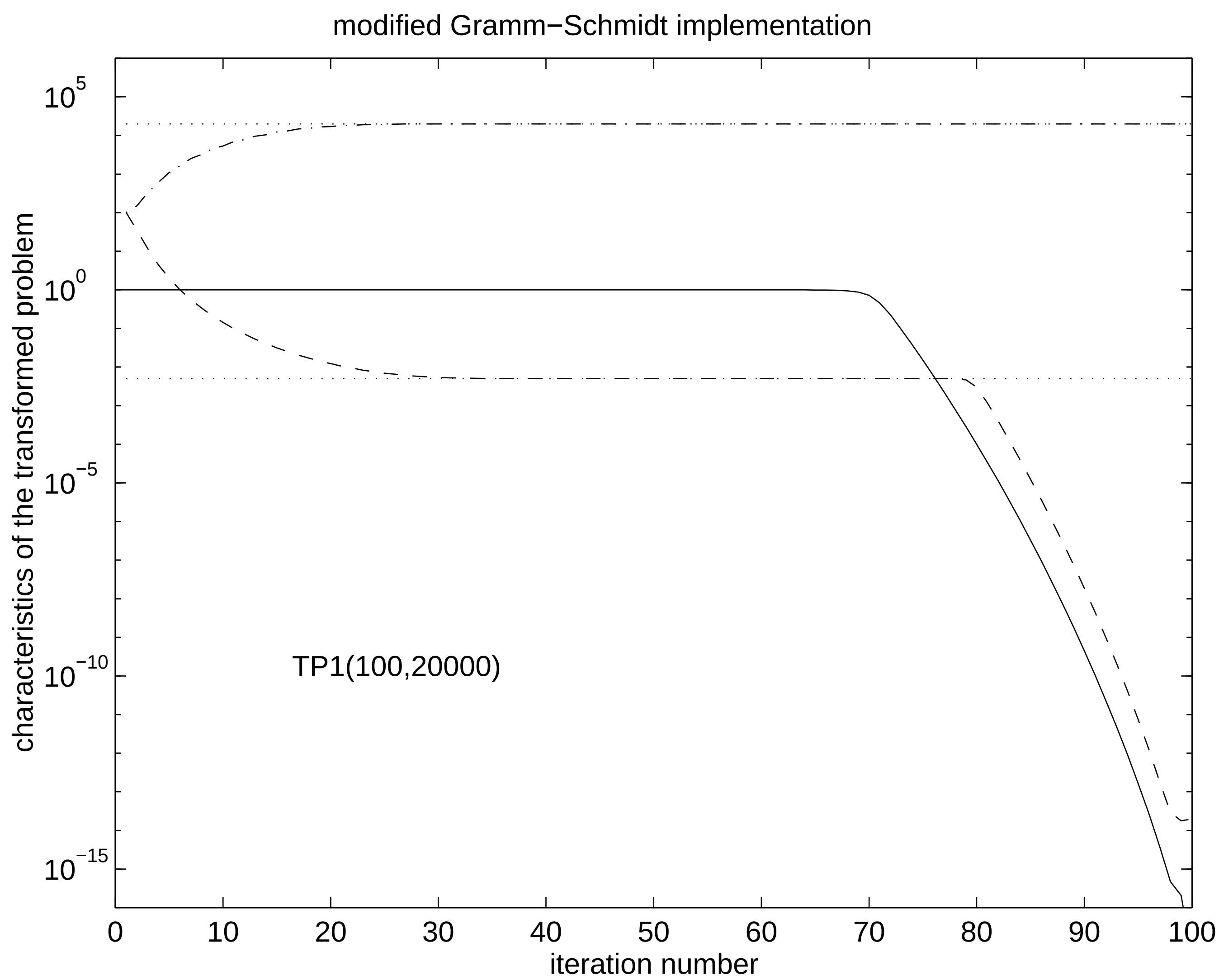
Greenbaum, R, Strakoš, 1997

Paige, R, Strakoš, 2006

## GMRES WITH CGS ARNOLDI PROCESS

van den Eshof, Giraud, Langou, R, 2005

Smoktunowicz, Barlow, Langou, 2006



modified Gramm−Schmidt implementation
characteristics of the transformed problem
iteration number
TP1(100,20000)
$10^{5}$
$10^{0}$
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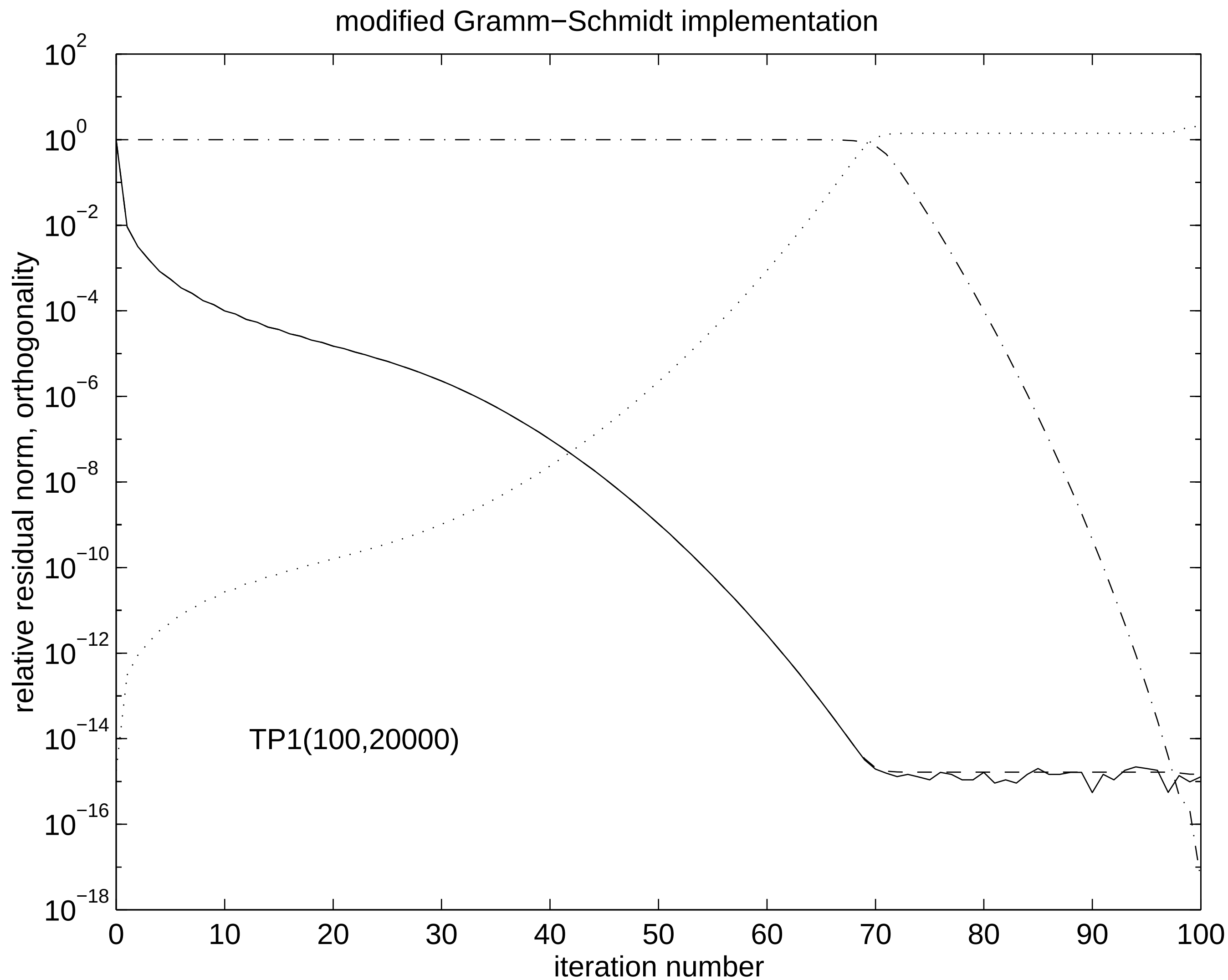

modified Gramm−Schmidt implementation
relative residual norm, orthogonality
iteration number
TP1(100,20000)
$10^{2}$
$10^{0}$
$10^{-2}$
$10^{-4}$
$10^{-6}$
$10^{-8}$
$10^{-10}$
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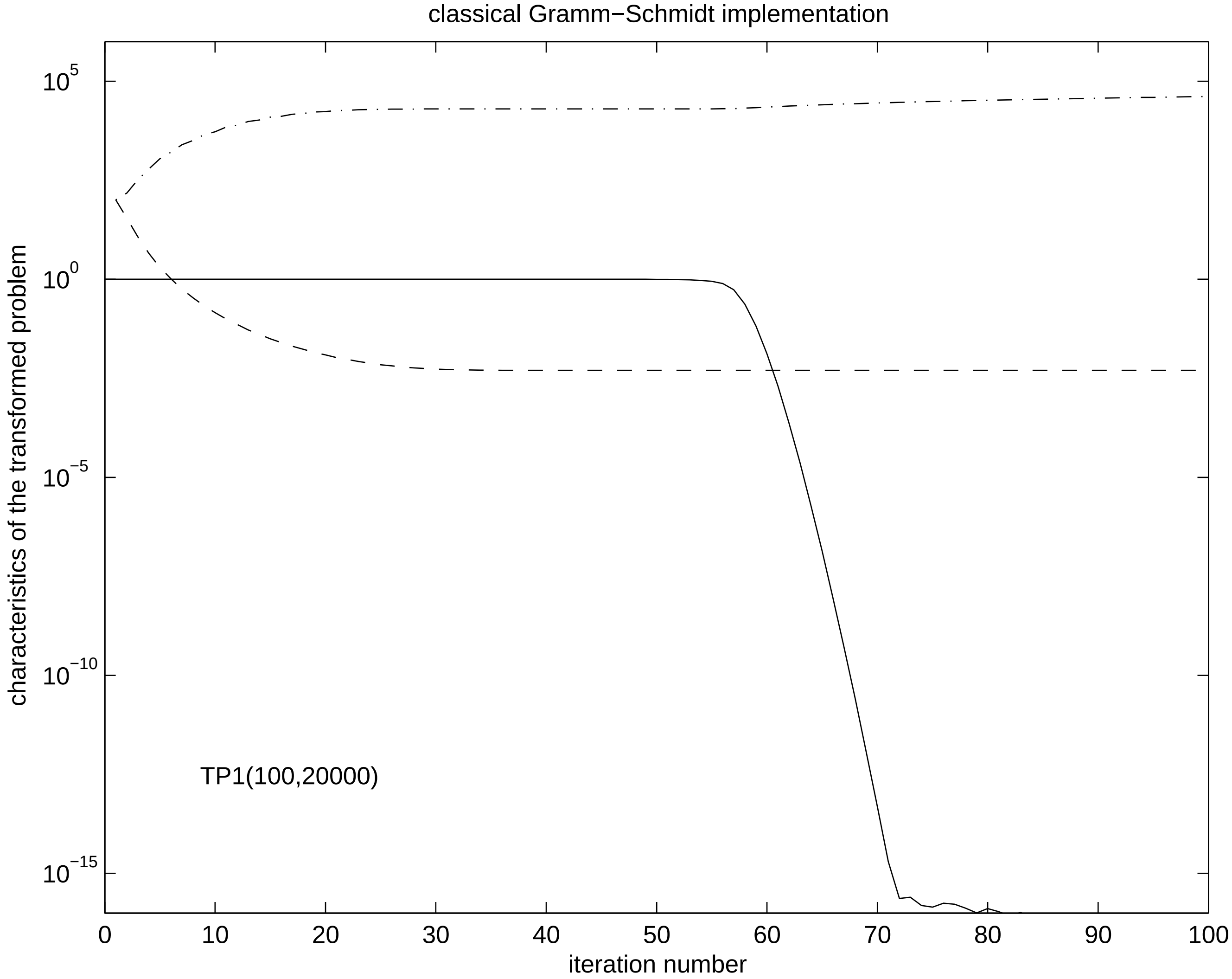

classical Gramm−Schmidt implementation
characteristics of the transformed problem
$10^{5}$
$10^{0}$
$10^{-5}$
$10^{-10}$
$10^{-15}$
TP1(100,20000)
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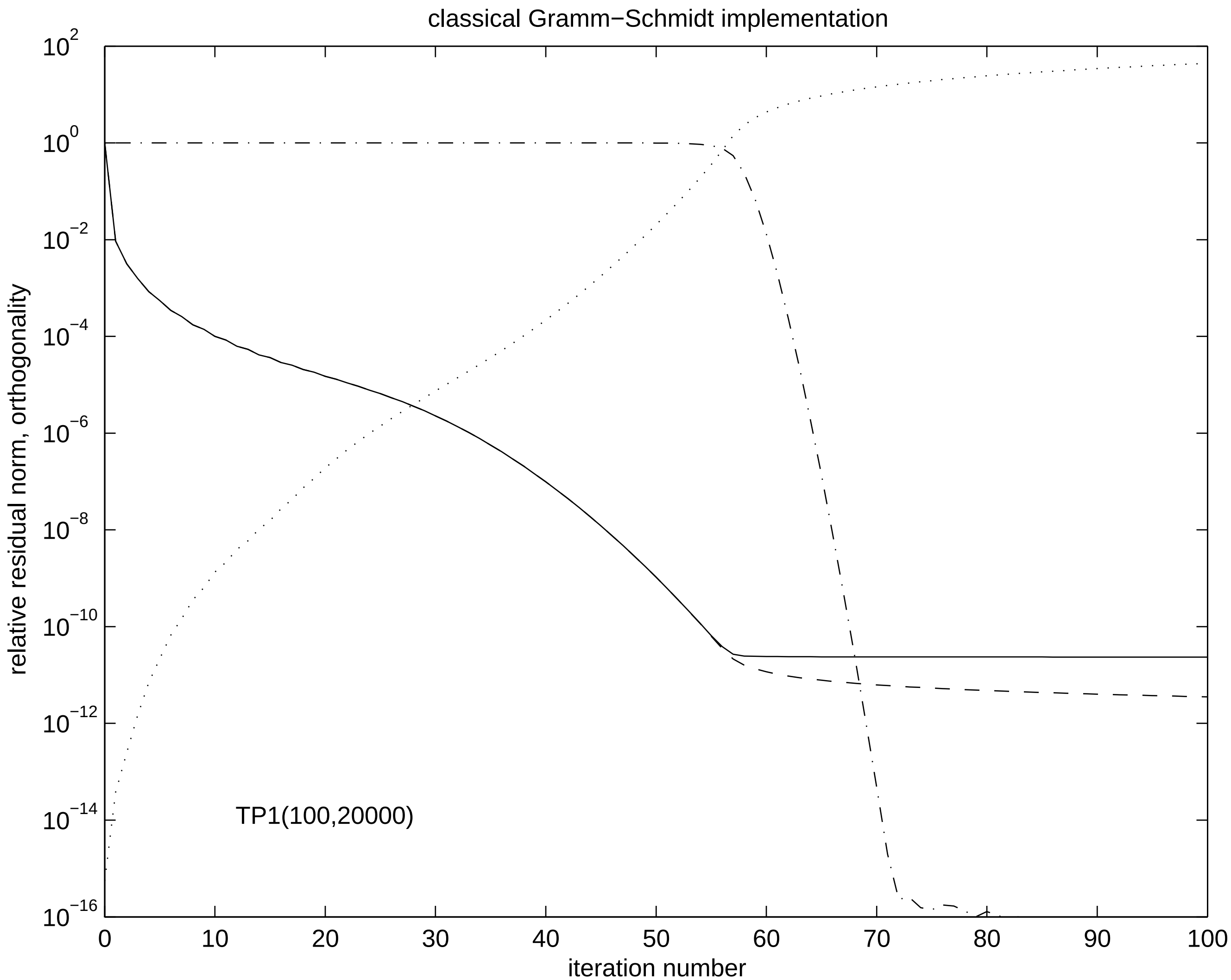
iteration number



classical Gramm−Schmidt implementation
relative residual norm, orthogonality
iteration number
TP1(100,20000)
$10^{2}$
$10^{0}$
$10^{-2}$
$10^{-4}$
$10^{-6}$
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# GMRES WITH MGS ARNOLDI PROCESS

The MGS-GMRES implementation is a **backward stable** iterative method.

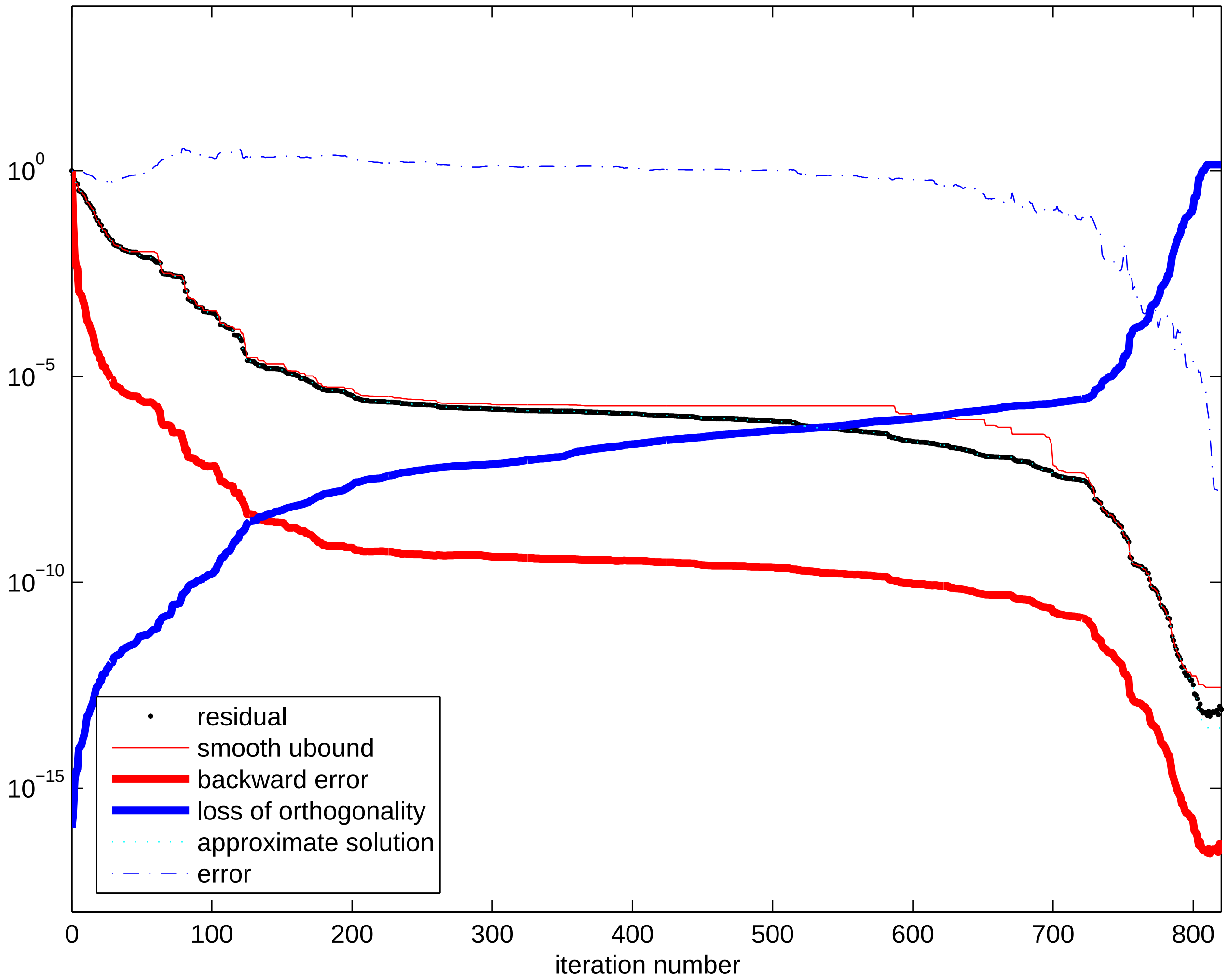
## STATEMENT:

For some iteration step $n \leq N$ the computed approximate solution $\bar{x}_n$ satisfies

$$(A + \Delta A_n)\bar{x}_n = b + \Delta b_n$$

$$\|\Delta A_n\|/\|A\| \leq O(\varepsilon), \; \|\Delta b_n\|/\|b\| \leq O(\varepsilon)$$

Paige, R, Strakoš, 2006



$10^{0}$
$10^{-5}$
$10^{-10}$
$10^{-15}$
0
100
200
300
400
500
600
700
800
iteration number
residual
smooth ubound
backward error
loss of orthogonality
approximate solution
error

# HOW TO MAKE SIMPLER GMRES AND GCR MORE STABLE

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## MINIMUM RESIDUAL METHODS

$$x_n \in x_0 + K_n(A, r_0), \qquad r_n \equiv b - Ax_n$$

$$K_n(A, r_0) \equiv \mathrm{span}\{r_0, Ar_0, \ldots, A^{n-1}r_0\}$$

$$\|r_n\| = \min_{u \in x_0 + K_n(A, r_0)} \|b - Au\|$$

$$\Leftrightarrow$$

$$r_n \perp AK_n(A, r_0)$$

# THE SIMPLER GMRES APPROACH

$[q_1, Z_{n-1}]$: a basis of $K_n(A, r_0)$, $q_1 \equiv r_0/\|r_0\|$, $\|Z_{n-1}e_k\| = 1$

$V_n$: an orthonormal basis of $AK_n(A, r_0)$, $V_n^T V_n = I$

$$A[q_1, Z_{n-1}] = V_n U_n, \quad V_n \equiv [v_1, \ldots, v_n]$$

$$r_n \perp AK_n(A, r_0) = \mathcal{R}(V_n)$$

$$\Updownarrow$$

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

$$x_n = x_0 + [q_1, Z_{n-1}] t_n, \quad U_n t_n = V_n^T r_0 = (\alpha_1, \ldots, \alpha_n)^T.$$

Walker, Zhou, 1994

# ROUNDING ERROR ANALYSIS

- The QR decomposition:
  $A[q_1, Z_{n-1}] = V_n U_n + F_n, \ \|F_n\| \leq O(\varepsilon)\|A\|\|[q_1, Z_{n-1}]\|$

  Wilkinson, 1963, Björck, 1967

- Solution of the triangular system:
  $(U_n + \Delta U_n)\widehat{t}_n = (\alpha_1, \ldots, \alpha_n)^T, \ |\Delta U_n| \leq O(\varepsilon)|U_n|$

  Wilkinson, 1963

## MAXIMUM ATTAINABLE ACCURACY: THE BACKWARD AND FORWARD ERROR

$$\frac{\|b - A\widehat{x}_n - r_n\|}{\|A\|\|\widehat{x}_n\|} \leq O(\varepsilon)\kappa([q_1, Z_{n-1}])\left(1 + \frac{\|x_0\|}{\|\widehat{x}_n\|}\right).$$

$$\frac{\|x_n - \widehat{x}_n\|}{\|x\|} \leq O(\varepsilon)\kappa(A)\kappa([q_1, Z_{n-1}])\frac{\|\widehat{x}_n\| + \|x_0\|}{\|x\|}.$$

# THE CHOICE $[q_1, Z_{n-1}] = [q_1, V_{n-1}]$

The **simpler** approach $\equiv$ Simpler GMRES of Walker and Zhou,1994.

$[q_1, V_{n-1}]$ is of full column rank if $r_0 \notin A\mathcal{K}_{n-1}(A, r_0)$.

Conditioning of $[q_1, V_{n-1}]$ related to the convergence of residuals, Walker and Zhou, 1994, Liesen,R, Strakoš 2002

$$\frac{\|r_0\|}{\|r_{n-1}\|} \leq \kappa([q_1, V_{n-1}]) \leq 2\frac{\|r_0\|}{\|r_{n-1}\|}.$$

## THE CHOICE $[q_1, Z_{n-1}] = \tilde{R}_n \equiv [\frac{r_0}{\|r_0\|}, \ldots, \frac{r_{n-1}}{\|r_{n-1}\|}]$

The **simpler** approach $\equiv$ SGMRES (new implementation)

$\tilde{R}_n$ is of full-column rank if
$r_0 \notin AK_{n-1}(A, r_0)$ and $\|r_0\| > \cdots > \|r_{n-1}\|$.

Conditioning of $\tilde{R}_n$ related to the stagnation of residuals:

$$\kappa(\tilde{R}_n) \leq n^{1/2}\gamma_n, \quad \gamma_n \equiv \sqrt{1 + \sum_{i=1}^{n-1} \frac{\|r_{i-1}\|^2 + \|r_i\|^2}{\|r_{i-1}\|^2 - \|r_i\|^2}}$$

THANK YOU FOR YOUR ATTENTION!

# THE UPDATE APPROACH: ORTHODIR, ORTHOMIN, GCR, GMRESR

$V_n$: an orthonormal basis of $AK_n(A, r_0)$, $V_n^T V_n = I$

$$A[q_1, Z_{n-1}] = V_n U_n, \quad V_n \equiv [v_1, \ldots, v_n]$$

$P_n \equiv A^{-1} V_n$: $A^T A$-orthonormal basis of $K_n(A, r_0)$

$$[q_1, Z_{n-1}] = P_n U_n, \quad P_n \equiv [p_1, \ldots, p_n]$$

$$\Downarrow$$

$$\left.\begin{aligned} x_n &= x_{n-1} + \alpha_n p_n, \\ r_n &= r_{n-1} - \alpha_n v_n, \end{aligned}\right\} \quad \alpha_n = \langle r_{n-1}, v_n \rangle$$

/insome,1976, Young, Jea, 1980, Elman et al. 1983, van der Vorst, Vuik, 1990