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Theoretical and Numerical Comparisons of GMRES and WZ-GMRES

GUIZHI CHEN
Department of Mathematics, Xiamen University
Xiamen 361005, P.R. China

ZHONG XIAO JIA
Department of Mathematical Sciences, Tsinghua University
Beijing 100084, P.R. China
zjia@math.tsinghua.edu.cn

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Abstract—WZ-GMRES, 'a simpler GMRES' proposed by Walker and Zhou, is mathematically equivalent to the generalized minimal residual method (GMRES) for solving large unsymmetric linear systems of equations. In this paper, relationships are established between two bases of an m-dimensional Krylov subspace $\mathcal{K}_m(A, r_0)$, and the condition number of the transition matrix between two bases is studied. Some relationships are derived between the condition numbers of the small matrices R_G and R_{WZ} resulting from GMRES and WZ-GMRES, respectively. A detailed analysis shows that generally R_{WZ} is worse conditioned than R_G, and in particular, R_{WZ} is definitely ill conditioned when the method is near convergence. Furthermore, numerical behavior of WZ-GMRES is analyzed. It turns out that WZ-GMRES is not numerically equivalent to GMRES when the method is near convergence, and WZ-GMRES is numerically less stable than GMRES and can be numerically unstable. Numerical examples confirm the theoretical results.

Keywords—GMRES, WZ-GMRES, Arnoldi's process, Krylov subspace, Finite precision.

1. INTRODUCTION

GMRES proposed by Saad and Schultz [1] is one of the most popular iterative solvers for the large unsymmetric (non-Hermitian) linear system of equations

$$Ax = b, \tag{1}$$

where $A \in C^{N\times N}$ is an $N \times N$ matrix and $b \in C^N$ is a vector of dimension N. The method takes an initial vector x_0 and initial residual $r_0 = b - Ax_0$, and computes an approximate solution $xm = x_0 + z_m$ at step m, where z_m is the solution of the least squares problem

$$\min_{z\in\mathcal{K}_m(A,r_0)} \|b - A(x_0 + z)\| = \min_{z\in\mathcal{K}_m(A,r_0)} \|r_0 - Az\|. \tag{2}$$

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Here $\|\cdot\|$ denotes the usual Euclidean norm of a vector and the induced matrix norm, and $\mathcal{K}_m(A, r_0)$ is the Krylov subspace generated by $r_0, Ar_0, \ldots, A^{m-1}r_0$.

There have been numerous theoretical and numerical studies of GMRES and its variants. For example, Saad and Schultz [1] and Jia [2] have established *a priori* upper error bounds for $\|r_m\| = \|b - Ax_m\|$ when A is diagonalizable and defective, respectively. Liesen [3] derives new computable convergence bounds for GMRES. His bounds depend on the initial guess and can be approximated from the information generated by the run of a certain GMRES implementation. Brown [4] and Greenbaum and Trefethen [5] have compared GMRES with other Krylov subspace methods such as Arnoldi's method. Their results have shown that under certain circumstances, GMRES can stagnate and Arnoldi's method will break down when this happens. There are many other interesting results and progress on the variants of GMRES; see, e.g., [6–9].

Walker and Zhou [6] have proposed a so-called simpler GMRES, i.e., WZ-GMRES, which is mathematically equivalent to the original GMRES. GMRES and WZ-GMRES first use the Arnoldi process [1] to generate an orthonormal basis of $\mathcal{K}_m(A, r_0)$ and of $A\mathcal{K}_{m-1}(A, r_0) = \mathrm{span}\{Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}$, respectively, and then apply the principle of GMRES to derive the corresponding small triangular linear systems $R_G y = b_G$ for GMRES and $R_{WZ} y = b_{WZ}$ for WZ-GMRES. With these, they solve for each y by back substitution and give the approximate solution x_m.

Drkošová *et al.* [7] analyze the numerical stability of GMRES. They prove that if the dimension of the Krylov subspace $\mathcal{K}_m(A, r_0)$ is m and its orthonormal basis is computed by a Householder variant of the Arnoldi algorithm [8], then GMRES is backward stable in the normwise sense. That is, the backward error $\|b - Ax_m\|/(\|A\|\,\|x_m\| + \|b\|)$ for the approximation x_m is proportional to the machine precision ϵ. Using general theoretical results about least square residual, Liesen *et al.* [10] show that there is a potential weakness of WZ-GMRES which may negatively affect its computational behavior in comparison with GMRES, and GMRES has numerical advantages over WZ-GMRES.

In this paper, we take a different approach to study the numerical stability of WZ-GMRES and compare it with that of the original GMRES. Note that it is well known that for R_G, we have $\kappa(R_G) \leq \kappa(A)$, where $\kappa(A)$ is the spectral condition number of A. For the nonsingular A, $\kappa(R_G)$ can be much smaller than $\kappa(A)$. Therefore, the small R_G is better and can be much better conditioned than A, which means that in finite precision, the computed solution of $R_G y = b_G$ by back substitution has relatively high accuracy. In this paper, we are led to consider the conditioning of R_{WZ} as it has a strong effect on the computed accuracy of x_m for WZ-GMRES in finite precision. We give the upper and lower bounds of $\kappa(R_{WZ})$. Furthermore, we establish an upper bound of the residual norm $\|b - Ax_m\|$ for WZ-GMRES in finite precision and analyze the numerical behavior of WZ-GMRES. We attempt to compare WZ-GMRES with GMRES and discuss their connections and differences theoretically and numerically. We show that WZ-GMRES is not numerically equivalent to GMRES and explain why WZ-GMRES is numerically certainly unstable when the method is near convergence. These constitute the tasks of the current paper.

The paper is organized as follows. In Section 2, we briefly describe GMRES and WZ-GMRES. In Section 3, we study some relationships between two bases generated by GMRES and WZ-GMRES, and we determine the structure of the transition matrix between the two bases and obtain an explicit expression of its condition number. A detailed analysis shows that the transition matrix is definitely very ill conditioned when WZ-GMRES is near convergence. In Section 4, we derive some relationships between $\kappa(R_G)$, $\kappa(R_{WZ})$, and $\kappa(A)$. In Section 5, we analyze the numerical behavior of WZ-GMRES. The remarks in Sections 4 and 5 imply that x_m computed by WZ-GMRES may have very poor accuracy in finite precision and deviate from the exact x_m in exact arithmetic considerably when WZ-GMRES is near convergence, so WZ-GMRES is numerically unstable.

Finally, we run numerical experiments in Section 6, which confirm the theoretical results.

Throughout the paper, denote by $\kappa(B) = \sqrt{(\lambda_{\max}(B^*B))/(\lambda_{\min}(B^*B))}$ the condition number of a matrix B, by the superscripts $*$ and $\top$ the conjugate transpose and the transpose, respectively, by C^m the complex space of dimension m, and by I_N the identity matrix of order N.

2. GMRES AND WZ-GMRES

2.1. GMRES

Let $v_1 = r_0/\|r_0\|$. Then, Arnoldi's process [1] can be used to successively generate an orthonormal basis $\{v_i\}_{i=1}^m$ of the m-dimensional Krylov subspace $\mathcal{K}_m(A, r_0)$. Define $V_m = [v_1, v_2, \dots, v_m]$ and $V_{m+1} = [V_m, v_{m+1}]$. Then, Arnoldi's process can be written in matrix form

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^* \tag{3}$$

or

$$AV_m = V_{m+1} \tilde{H}_m, \tag{4}$$

where $H_m = (h_{ij})_{m\times m}$ and $\tilde{H}_m = (h_{ij})_{(m+1)\times m} = \left(\begin{smallmatrix} H_m \\ h_{m+1,m} e_m^* \end{smallmatrix}\right)$ are upper Hessenberg matrices.

Relation (2) is equivalent to

$$\begin{aligned} \|r_m\| &= \min_{y \in C^m} \|r_0 - AV_m y\| = \min_{y\in C^m} \left\| \|r_0\| V_{m+1} e_1 - V_{m+1} \tilde{H}_m y \right\| \\ &= \min_{y \in C^m} \left\| \|r_0\| e_1 - \tilde{H}_m y \right\|. \end{aligned} \tag{5}$$

Let

$$\tilde{H}_m = Q \begin{pmatrix} R_G \\ 0 \end{pmatrix} \tag{6}$$

be the QR decomposition of $\tilde{H}_m$, where Q is orthogonal (unitary) and R_G is an invertible upper triangular matrix. Substituting (6) into (5) gives

$$\|r_m\| = \min_{y\in C^m} \left\| \|r_0\| Q^* e_1 - \begin{pmatrix} R_G \\ 0 \end{pmatrix} y \right\|. \tag{7}$$

Solve

$$R_G y = \|r_0\| (I_m, 0) Q^* e_1, \tag{8}$$

for y_m. Then, we obtain the GMRES iterative solution to (1)

$$x_m = x_0 + V_m y_m.$$

2.2. WZ-GMRES

Let $R_m = b - Ax_m$. Then, (2) can be written as [3]

$$\|r_m\| = \min_{r \in r_0 + A\mathcal{K}_m(A, r_0)} \|r\|, \tag{9}$$

which is equivalent to

$$r_m \perp A\mathcal{K}_m(A, r_0). \tag{10}$$

If $w_1 = (Ar_0)/\|Ar_0\|$, we can use Arnoldi's process to generate an orthonormal basis $\{w_i\}_{i=1}^{m-1}$ of the Krylov subspace $A\mathcal{K}_{m-1}(A, r_0) = \text{span}\{Ar_0, A^2 r_0, \dots, A^{m-1} r_0\}$. Define $W_{m-1} = [w_1, w_2, \dots, w_{m-1}]$ and $W_m = [W_{m-1}, w_m]$. Then, the above Arnoldi process can be written in matrix form

$$AW_{m-1} = W_{m-1} G_{m-1} + g_{m,m-1} w_m e_{m-1}^* \tag{11}$$

or

$$AW_{m-1} = W_m \tilde{G}_{m-1}, \tag{12}$$

where $G_{m-1} = (g_{ij})_{(m-1)\times(m-1)}$ and $\tilde{G}_{m-1} = (g_{ij})_{m\times(m-1)} = \binom{G}{g_{m,m-1}e^*_{m-1}}$ are upper Hessenberg matrices.

Since

$$\mathcal{K}_m(A, r_0) = \text{span}\{r_0\} \oplus A\mathcal{K}_{m-1}(A, r_0) = \text{span}\{v_1, w_1, \dots, w_{m-1}\},$$

$v_1, w_1, \dots, w_{m-1}$ form a basis of $\mathcal{K}_m(A, r_0)$, where the symbol $\oplus$ denotes the direct sum.

Write

$$F = \left[\frac{r_0}{\|r_0\|}, w_1, \dots, w_{m-1}\right] = [v_1, W_{m-1}].$$

Then, it satisfies

$$AF = \left(\frac{Ar_0}{\|r_0\|}, AW_{m-1}\right) = \left(\frac{\|Ar_0\|}{\|r_0\|}w_1, W_m\tilde{G}_{m-1}\right).$$

Let

$$R_{WZ} = \begin{pmatrix} \frac{\|Ar_0\|}{\|r_0\|} & \tilde{G}_{m-1} \\ 0 & \end{pmatrix}.$$

Obviously, R_{WZ} is upper triangular and

$$AF = W_m R_{WZ}. \tag{13}$$

Let

$$x_m = x_0 + Fy_m. \tag{14}$$

It then follows from (10) that y_m satisfies

$$0 = W_m^* r_m = W_m^* r_0 - W_m^* AFy_m.$$

Noting (13), we get

$$R_{WZ} y_m = W_m^* r_0, \tag{15}$$

which is easily solved for y by back substitution. We then get x_m in (14).

This procedure is proposed by Walker and Zhou [6], originally called a "simpler GMRES". We name it WZ-GMRES in this paper.

It is easily seen that

$$r_m = b - Ax_m = (I_N - W_m W_m^*) r_0, \tag{16}$$

which yields

$$\|r_m\| = \|r_0\| \sin\theta(v_1, A\mathcal{K}_m(A, r_0)). \tag{17}$$

3. RELATIONSHIPS BETWEEN TWO BASES OF $\mathcal{K}_m(A, r_0)$

3.1. Basic Relationship and Properties on Transition Matrix

We can prove the following results.

THEOREM 1. *Let two bases $v_1, v_2, \dots, v_m$ and $v_1, w_1, \dots, w_{m-1}$ of $\mathcal{K}_m(A, r_0)$ satisfy*

$$[v_1, v_2, \dots, v_m] = [v_1, w_1, w_2, \dots, w_{m-1}]T, \qquad \text{i.e., } V_m = FT. \tag{18}$$

Then, the transition matrix

$$T = \begin{pmatrix} 1 & p_{11} & \cdots & p_{1m-1} \\ 0 & p_{21} & \cdots & p_{2m-1} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & p_{mm-1} \end{pmatrix} = \begin{pmatrix} 1 & h^* \\ 0 & P \end{pmatrix},$$

where $h^* = (p_{11}, \dots, p_{1m-1})$. *We have*

$$P^*P - hh^* = I_{m-1}, \tag{19}$$

$$\kappa(T) = \kappa(F) = \|h\| + \sqrt{\|h\|^2 + 1}. \tag{20}$$

PROOF. Clearly, $v_1 = 1v_1 + 0w_1 + \cdots + 0w_{m-1}$. For $j = 1, 2, \dots, m-1$, since $\mathcal{K}_{j+1}(A, r_0) = \operatorname{span}\{v_1, v_2, \dots, v_{j+1}\} = \operatorname{span}\{v_1, w_1, \dots, w_j\}$, we have

$$v_{j+1} = p_{1j}v_1 + p_{2j}w_1 + \cdots + p_{j+1j}w_j, \qquad j = 1, 2, \dots, m-1,$$

which means that T is upper triangular.

Since V_m is orthonormal, we obtain from (18)

$$I_m = V_m^* V_m = \begin{pmatrix} 1 & h^* + v_1^* W_{m-1} P \\ h + P^* W_{m-1}^* v_1 & hh^* + P^* W_{m-1}^* v_1 h^* + h v_1^* W_{m-1}^* P + P^* P \end{pmatrix}.$$

Hence,

$$\begin{aligned} h^* + v_1^* W_{m-1} P &= 0, \\ hh^* + P^* W_{m-1}^* v_1 h^* + h v_1^* W_{m-1} P + P^* P &= I_{m-1}. \end{aligned} \tag{21}$$

Combining the above two relations gives

$$P^*P - hh^* = I_{m-1},$$

which proves (19). We now proceed to prove (20). Form the matrix

$$T^*T = \begin{pmatrix} 1 & 0 \\ h & P^* \end{pmatrix} \begin{pmatrix} 1 & h^* \\ 0 & P \end{pmatrix} = I_m + B,$$

where

$$B = \begin{pmatrix} 0 & h^* \\ h & 2hh^* \end{pmatrix} = \begin{pmatrix} 0 \\ h \end{pmatrix} (1, h^*) + \begin{pmatrix} 1 \\ h \end{pmatrix} (0, h^*)$$

is a symmetric (Hermitian) matrix of rank at most two and thus has at most two nonzero eigenvalues. For $\lambda \neq 0$, we obtain from

$$\begin{pmatrix} 1 & 0 \\ \dfrac{h}{\lambda} & 1 \end{pmatrix} \begin{pmatrix} \lambda & -h^* \\ -h & \lambda I_{m-1} - 2hh^* \end{pmatrix} = \begin{pmatrix} \lambda & -h^* \\ 0 & -\dfrac{hh^*}{\lambda} + \lambda I_{m-1} - 2hh^* \end{pmatrix}$$

that

$$|\lambda I - B| = \begin{vmatrix} \lambda & -h^* \\ 0 & -\dfrac{hh^*}{\lambda} + \lambda I_{m-1} - 2hh^* \end{vmatrix} = \frac{(1+2\lambda)^{m-1}}{\lambda^{m-2}} \left| \frac{\lambda^2}{1+2\lambda} I_{m-1} - hh^* \right|.$$

Therefore, $\lambda^2/(1+2\lambda)$ is the only nonzero eigenvalue of the rank one matrix hh^*. Noting that the nonzero eigenvalue of hh^* is equal to $h^*h = \|h\|^2$, we have the equality

$$\frac{\lambda^2}{1+2\lambda} = \|h\|^2,$$

from which we get two nonzero eigenvalues

$$\lambda_1 = \|h\|^2 + \|h\|\sqrt{\|h\|^2+1}, \qquad \lambda_2 = \|h\|^2 - \|h\|\sqrt{\|h\|^2+1}.$$

They are the largest and smallest eigenvalues of B, respectively. We then get the largest and smallest eigenvalues of T^*T

$$\lambda_{\max}(T^*T) = 1 + \|h\|^2 + \|h\|\sqrt{\|h\|^2+1}, \qquad \lambda_{\min}(T^*T) = 1 + \|h\|^2 - \|h\|\sqrt{\|h\|^2+1}.$$

Therefore, we obtain the condition number

$$\begin{aligned} \kappa(T) &= \sqrt{\frac{\lambda_{\max}(T^*T)}{\lambda_{\min}(T^*T)}} = \sqrt{\frac{1 + \|h\|^2 + \|h\|\sqrt{\|h\|^2+1}}{1 + \|h\|^2 - \|h\|\sqrt{\|h\|^2+1}}} = \sqrt{\frac{\sqrt{1+\|h\|^2} + \|h\|}{\sqrt{1+\|h\|^2} - \|h\|}} \\ &= \|h\| + \sqrt{\|h\|^2+1}. \end{aligned} \tag{22}$$

Making use of (18) and the nonsingularity of T leads to

$$\kappa(F) = \kappa\left(V_m T^{-1}\right) = \kappa(T). \qquad \blacksquare$$

3.2. More Properties on $\kappa(T)$

3.2.1. When $\kappa(T) = 1$?

We present the following results.

THEOREM 2.

(1) $\kappa(T) = 1$ *if and only if* $W_{m-1}^* v_1 = 0$, *i.e.,* $r_0 \perp A\mathcal{K}_{m-1}(A, r_0)$.

(2) $r_0 \perp A\mathcal{K}_{m-1}(A, r_0)$ *if and only if* $\|r_{m-1}\| = \|r_0\|$.

PROOF.

PART 1. It follows from Theorem 1 that $\kappa(T) = 1$ if and only if $h = 0$. So, we have from (21) that $\kappa(T) = 1$ if and only if $v_1^* W_{m-1} P = 0$. Noting from (19) that $P^*P = I_{m-1}$, we know that P is unitary and thus nonsingular. Therefore, $\kappa(T) = 1$ if and only if $W_{m-1}^* v_1 = 0$.

PART 2. It is a fairly basic fact. ∎

According to a basic face of GMRES, i.e., $r_0 \perp A\mathcal{K}_{m-1}(A, r_0)$ if and only if $\|r_{m-1}\| = \|r_0\|$, we see that $\kappa(T) = 1$ if and only if $\|r_{m-1}\| = \|r_0\|$, which amounts to saying that GMRES stagnates when applied to $\mathcal{K}_{m-1}(A, r_0)$. Therefore, $\kappa(T) = 1$ implies that GMRES and WZ-GMRES stagnate from step one to step $m-1$. We should be aware that such a situation is rare in practice for GMRES. So, generally we have $\kappa(T) > 1$.

3.2.2. When is T ill conditioned?

As has been seen previously, we usually have $W_{m-1}^* v_1 \neq 0$, i.e., $\theta(v_1, A\mathcal{K}_{m-1}(A, r_0)) \neq \pi/2$. Now, we give an explicit expression on sine of the acute angle between r_0 and $A\mathcal{K}_{m-1}(A, r_0)$, and we then analyze the expression and reveal how GMRES and WZ-GMRES will behave.

THEOREM 3. *We have*

$$\sin\theta\left(v_1, A\mathcal{K}_{m-1}(A, r_0)\right) = \begin{cases} 0, & \dim \mathcal{K}_m(A, r_0) = \dim A\mathcal{K}_{m-1}(A, r_0) \leq m-1, \\ \sqrt{\left(1 + h^* P^{-1} W_{m-1}^* v_1\right)^2 + \left\|P^{-1} W_{m-1}^* v_1\right\|^2}, & \\ & \dim \mathcal{K}_m(A, r_0) = m. \end{cases} \tag{23}$$

PROOF. If $\dim \mathcal{K}_m(A, r_0) = \dim A\mathcal{K}_{m-1}(A, r_0) \leq m-1$, then $r_0 \in A\mathcal{K}_{m-1}(A, r_0)$. Therefore,

$$\sin\theta(v_1, A\mathcal{K}_{m-1}(A, r_0)) = 0.$$

If $\mathcal{K}_m(A, r_0) = m$, then

$$\begin{aligned} \sin\theta(v_1, A\mathcal{K}_{m-1}(A, r_0)) &= \|(I_N - W_{m-1} W_{m-1}^*) v_1\| = \left\|(v_1 W_{m-1}) \begin{pmatrix} 1 \\ -W_{m-1}^* v_1 \end{pmatrix}\right\| \\ &= \left\|V_m T^{-1} \begin{pmatrix} 1 \\ -W_{m-1}^* v_1 \end{pmatrix}\right\| = \left\|T^{-1} \begin{pmatrix} 1 \\ -W_{m-1}^* v_1 \end{pmatrix}\right\|. \end{aligned} \tag{24}$$

Since

$$T^{-1} = \begin{pmatrix} 1 & -h^* P^{-1} \\ 0 & P^{-1} \end{pmatrix},$$

we obtain

$$\begin{aligned} \sin\theta(v_1, A\mathcal{K}_{m-1}(A, r_0)) &= \left\|\begin{pmatrix} 1 + h^* P^{-1} W_{m-1}^* v_1 \\ -P^{-1} W_{m-1}^* v_1 \end{pmatrix}\right\| \\ &= \sqrt{\left(1 + h^* P^{-1} W_{m-1}^* v_1\right)^2 + \left\|P^{-1} W_{m-1}^* v_1\right\|^2}. \end{aligned} \tag{25}$$ ∎

REMARKS.

- Suppose $\|r_{m-1}\| = 0$, i.e., GMRES and WZ-GMRES find exact solution at step $m-1$. It is seen from (17) that this happens if and only if $r_0 \in A\mathcal{K}_{m-1}(A, r_0)$. By the definition of F, it is known that F is column rank deficient. Therefore, $\kappa(T) = \kappa(F)$ must be infinite.
- If $\|r_{m-1}\|/\|r_0\| = \epsilon_1$ is small, we see from (17) that

$$\sin\theta(v_1, A\mathcal{K}_{m-1}(A, r_0)) = \epsilon_1.$$

It follows from Theorem 3 that

$$1 + h^* P^{-1} W_{m-1}^* v_1 = \epsilon_2, \tag{26}$$

$$\left\|P^{-1} W_{m-1}^* v_1\right\| = \epsilon_3, \tag{27}$$

where $\epsilon_3 \le \epsilon_1$. By definition and (26), we have

$$\|h\| \left\|P^{-1} W_{m-1}^* v_1\right\| \cos\theta\left(h, P^{-1} W_{m-1}^* v_1\right) = \epsilon_2 - 1, \tag{28}$$

from which and (27) it follows that

$$\|h\| \left|\cos\theta\left(h, P^{-1} W_{m-1}^* v_1\right)\right| = \frac{1-\epsilon_2}{\epsilon_3} = O\left(\frac{1}{\epsilon_3}\right). \tag{29}$$

Since $|\cos\theta(h, P^{-1} W_{m-1}^* v_1)| \le 1$, (29) means that if GMRES is near convergence at step $m-1$, then $\|h\|$ is at least of the same order as $1/\epsilon_3 \ge 1/\epsilon_1$. So, we know from Theorem 1 that T and F are definitely ill conditioned.

4. ON $\kappa(R_G)$ AND $\kappa(R_{WZ})$

4.1. Relationships between $\kappa(R_G)$, $\kappa(R_{WZ})$, and $\kappa(A)$

It is easy to prove the following results.

THEOREM 4. *It holds that*

$$\kappa(R_G) \le \kappa(A), \tag{30}$$

$$\kappa(R_{WZ}) \le \kappa(A)\kappa(T). \tag{31}$$

PROOF. Inequality (30) is obvious. It follows from (13) and the definition of condition number that

$$\begin{aligned}
\kappa(R_{WZ}) = \kappa(AF) &= \frac{\max_{\forall x \in C^m, x \ne 0} (\|AFx\|/\|x\|)}{\min_{\forall x \in C^m, x \ne 0} (\|AFx\|/\|x\|)} \\
&= \frac{\max_{\forall x \in C^m, x \ne 0} (\|AFx\|/\|Fx\|)\ (\|Fx\|/\|x\|)}{\min_{\forall x \in C^m, x \ne 0} (\|AFx\|/\|Fx\|)\ (\|Fx\|/\|x\|)} \\
&\le \frac{\max_{\forall x \in \mathcal{K}_m(A, r_0), x \ne 0} (\|Ax\|/\|x\|)}{\min_{\forall x \in \mathcal{K}_m(A, r_0), x \ne 0} (\|Ax\|/\|x\|)} \times \frac{\max_{\forall x \in C^m, x \ne 0} (\|Fx\|/\|x\|)}{\min_{\forall x \in C^m, x \ne 0} (\|Fx\|/\|x\|)} \\
&\le \kappa(A)\kappa(F) = \kappa(A)\kappa(T),
\end{aligned}$$

which proves (31). ∎

4.2. Relationship between $\kappa(R_G)$ and $\kappa(R_{WZ})$

Relation (31) can be refined by replacing $\kappa(A)$ with a smaller $\kappa(R_G)$, as shown below.

THEOREM 5. *We have*

$$\frac{\kappa(T)}{\kappa(R_G)} \le \kappa(R_{WZ}) \le \kappa(R_G)\kappa(T). \tag{32}$$

PROOF. Recall from Theorem 1 that $V_m = FT$. Left multiplying both sides by A gives

$$AV_m = AFT.$$

Making use of (4) and (13) leads to

$$V_{m+1}\tilde{H}_m = W_m R_{WZ} T.$$

Based on the QR decomposition of $\tilde{H}_m$ and letting $Q = (\tilde{Q}, q_{m+1})$, we get

$$V_{m+1}\hat{Q}R_G = W_m R_{WZ} T.$$

Since R_G and R_{WZ} are invertible and $V_{m+1}\hat{Q}$ and W_m are orthonormal, we get

$$\kappa(R_{WZ}) = \kappa\left(R_G T^{-1}\right) \le \kappa(R_G)\kappa(T).$$

On the other hand,

$$\begin{aligned}\sigma_{\max}(R_{WZ}) &= \max_{x\neq 0}\frac{\left\|R_G T^{-1}x\right\|}{\|x\|} = \max_{x\neq 0}\left\{\frac{\left\|R_G T^{-1}x\right\|}{\left\|T^{-1}x\right\|}\,\frac{\left\|T^{-1}x\right\|}{\|x\|}\right\}\\ &\ge \max_{x\neq 0}\frac{\left\|T^{-1}x\right\|}{\|x\|}\min_{x\neq 0}\frac{\left\|R_G T^{-1}x\right\|}{\left\|T^{-1}x\right\|} = \frac{\sigma_{\min}(T_G)}{\sigma_{\min}(T)}.\end{aligned} \tag{33}$$

Similarly, we have

$$\begin{aligned}\sigma_{\min}(R_{WZ}) &= \min_{x\neq 0}\frac{\left\|R_G T^{-1}x\right\|}{\|x\|} = \min_{x\neq 0}\left\{\frac{\left\|R_G T^{-1}x\right\|}{\left\|T^{-1}x\right\|}\,\frac{\left\|T^{-1}x\right\|}{\|x\|}\right\}\\ &\le \min_{x\neq 0}\frac{\left\|T^{-1}x\right\|}{\|x\|}\max_{x\neq 0}\frac{\left\|R_G T^{-1}x\right\|}{\left\|T^{-1}x\right\|} = \frac{\sigma_{\max}(T_G)}{\sigma_{\max}(T)}.\end{aligned} \tag{34}$$

Combining (33) with (34), we obtain (32).

Let us make some remarks on the implications of Theorems 4 and 5.

- Theorem 4 states that the condition number of R_G is always smaller than that of A.
- Theorem 4 indicates that $\kappa(A)$ is not an upper bound on $\kappa(R_{WZ})$. However, (31) may give a large overestimate of $\kappa(R_{WZ})$. The bound in Theorem 5 can be much smaller than (31). It is seen from Theorems 2 and 3 that if GMRES stagnates from step one to step $m-1$, then T and thus R_{WZ} must be well conditioned. On the other hand, according to the remarks in Section 3.2.2, if GMRES and WZ-GMRES are near convergence at step $m-1$, then the matrix T must be ill conditioned and Theorem 5 shows that the matrix R_{WZ} must be very ill conditioned. Numerical experiments later will indicate that generally $\kappa(R_{WZ})$ is quite ill conditioned, and the larger the dimension m of the Krylov subspace $\mathcal{K}_m(A, r_0)$ is, the worse conditioned the matrix R_{WZ} is.

In finite precision, using the conclusion similar to Theorem 4, Liesen *et al.* [10] showed that decreasing $\|r_{m-1}\|$ may lead to ill-conditioning of the triangular matrix R_{WZ}, and thus to a potentially large error in solving the upper triangular system (15), independent of the (well-)conditioning of the matrix A. Obviously, we here give a tighter estimate for the conditioning of matrix R_{WZ}. Particularly, the lower bound in Theorem 5 means that decreasing $\|r_{m-1}\|$ must lead to ill-conditioning of the triangular matrix R_{WZ}.

5. NUMERICAL BEHAVIOR OF WZ-GMRES

Hereafter, we will assume that the finite precision arithmetic satisfies the following assumption. Let $\mathrm{fl}(\cdot)$ denote the result of a floating point computation. We assume the following model of floating point arithmetic on a machine with the machine precision ϵ:

$$\mathrm{fl}(a \odot b) = (a \odot b)(1+\delta), \qquad |\delta| \le \epsilon,$$

where $\odot$ is one of $+$, $-$, $*$, $/$. Under this model, we have the following standard results for operations involving an $N \times N$ matrix A, N-vectors x and y, and a number α [9]:

$$\|\alpha x - \mathrm{fl}(\alpha x)\| \le \epsilon \|\alpha x\|, \tag{35}$$

$$\|x + y - \mathrm{fl}(x+y)\| \le \epsilon(\|x\| + \|y\|), \tag{36}$$

$$|\langle x, y\rangle - \mathrm{fl}(\langle x, y\rangle)| \le N\left(\epsilon + O\left(\epsilon^2\right)\right) \|x\|\, \|y\|, \tag{37}$$

$$\|\mathrm{fl}(Ax) - Ax\| \le N^{3/2} \epsilon \|A\|\, \|x\|. \tag{38}$$

5.1. Finite Precision Arnoldi Recurrence

Because of rounding errors, the computed quantities do not satisfy the exact recurrence. Here, we denote by bars the quantities computed in finite precision arithmetic with the machine precision ϵ. The following results are presented in [7,10].

LEMMA 1.

(1) *Assume that the Householder orthogonalization was used for computing the Arnoldi basis vectors $\bar{w}_1, \bar{w}_2, \dots, \bar{w}_n$. Then, the computed quantities satisfy*

$$A\left[\bar{v}_1, \bar{W}_{m-1}\right] = \bar{W}_m \bar{R}_{WZ} + E_1, \tag{39}$$

where

$$\|E_1\| \le \zeta_1' m N^{3/2} \epsilon \|A\|\, \left\|\left[\bar{v}_1, \bar{W}_{m-1}\right]\right\|,$$

for some positive constants ζ_1', and there exists an exactly orthonormal matrix $\hat{W}_m$ such that

$$\left\|\bar{W}_m - \hat{W}_m\right\| \le \zeta_2 m^{3/2} N \epsilon, \tag{40}$$

with some positive constant ζ_2.

(2)

$$\|\bar{r}_0 - (b - Ax_0)\| \le \zeta_3 N^{3/2} \epsilon (\|A\|\, \|x_0\| + \|b\|),$$

with some positive constant ζ_3.

(3)

$$\left\|\bar{v}_1 - \frac{\bar{r}_0}{\|\bar{r}_0\|}\right\| \le (N+4)\epsilon.$$

Using Lemma 1, we have the following.

THEOREM 6.

(1) *Suppose that W_m is computed by the HHA. Then, we have*

$$A\bar{F} = \bar{W}_m \bar{R}_{WZ} + E_2, \tag{41}$$

where

$$\|E_2\| \le \zeta_1 m^2 N^{3/2} \epsilon \|A\|,$$

with some positive constant ζ_1.

(2)
$$1 - \zeta_2 m^{3/2} N\epsilon \le \sigma_k\left(\bar{W}_m\right) \le 1 + \zeta_2 m^{3/2} N\epsilon, \qquad k = 1, 2, \ldots, m.$$

(3) *For any N-vector z, we have*
$$\left\|z - \bar{W}_m \bar{W}_m^* z\right\| \le \left(\sin\theta\left(z, \operatorname{span}\left\{\hat{W}_m\right\}\right) + \zeta_4 m^{3/2} N\epsilon\right) \|z\|,$$
where $\operatorname{span}\{\hat{W}_n\}$ *is the subspace spanned by the columns of the matrix* $\hat{W}_m$ *and* ζ_4 *is some positive constant.*

PROOF. Obviously,
$$\|[\bar{v}_1, \bar{w}_1, \ldots, \bar{w}_{m-1}]\| \le \|[\bar{v}_1, \bar{w}_1, \ldots, \bar{w}_{m-1}]\|_F = m + O(\epsilon), \tag{42}$$
where $\|\cdot\|_F$ is the Frobenius norm, and $\bar{F} = [\bar{r}_0/\|\bar{r}_0\|, \bar{w}_1, \ldots, \bar{w}_{m-1}]$. Using Lemma 1 and (38), we have
$$\left\|A\left[\bar{v}_1, \bar{W}_{m-1}\right] - A\bar{F}\right\| \le N^{5/2}\epsilon^2\|A\|. \tag{43}$$
Relation (41) follows immediately from combining (42),(43) with (39).

From (40) and perturbation theory of singular values [11], it follows that
$$\left|\sigma_k\left(\bar{W}_m\right) - \sigma_k\left(\hat{W}_m\right)\right| \le \zeta_2 m^{3/2} N\epsilon, \qquad k = 1, 2, \ldots, m.$$
Assertion (2) follows immediately from $\sigma_k(\hat{W}_m) = 1$.

Let $E_3 = \bar{W}_m - \hat{W}_m$. Then,
$$\bar{W}_m \bar{W}_m^* = \hat{W}_m \hat{W}_m^* + \hat{W}_m E_3^* + E_3 \hat{W}_m^* + E_3 E_3^*.$$
Hence, for any N-vector z,
$$\left\|z - \bar{W}_m \bar{W}_m^* z\right\| \le \left\|z - \hat{W}_m \hat{W}_m^* z\right\| + (2 + \|E_3\|)\|E_3\|\,\|z\|.$$
Note that $\|E_3\| \le \zeta_2 m^{3/2} N\epsilon$ and $\|z - \hat{W}_m \hat{W}_m^* z\| = \|z\| \sin\theta(z, \operatorname{span}\{\hat{W}_m\})$. Conclusion (3) follows. ∎

5.2. An Upper Bound on the Residual Norm $\|b - A\bar{x}_m\|$

The approximate solution $\bar{y}_m$ in (15) is computed by back substitution. Using the backward error analysis for back substitution [12], we have the following.

LEMMA 2. *The back substitution is backward stable in the sense that the computed solution $\bar{y}_m$ satisfies*
$$\left(\bar{R}_{WZ} + E_4\right)\bar{y}_m = \bar{W}_m^* \bar{r}_0, \tag{44}$$
where
$$\|E_1\| \le \zeta_5 m\epsilon \left\|\bar{R}_{WZ}\right\|.$$

For WZ-GMRES, the computed m^{th} approximate solution $\bar{x}_m$ in (14) is given by
$$\bar{x}_m = \mathrm{fl}\left(x_0 + \mathrm{fl}\left(\bar{F}\bar{y}_m\right)\right).$$
Using (38), (36), and $\|\bar{F}\| = m + O(\epsilon)$, we have
$$\bar{x}_m = x_0 + \bar{F}\bar{y}_m + d_m,$$
where $\|d_m\| \le \zeta_6 m N^{3/2}\epsilon\|\bar{y}_m\| + \epsilon\|x_0\|$.

THEOREM 7. *The residual norm* $\|b - A\bar{x}_m\|$ *satisfies*

$$\begin{aligned}\|b - A\bar{x}_m\| \le \sin\theta\left(\bar{r}_0, \operatorname{span}\left\{\hat{W}_n\right\}\right)\|\bar{r}_0\| + \nu_1(m,N)\epsilon\left\|\bar{R}_{WZ}\right\|\|\bar{y}_m\| \\ +\nu_2(m,N)\epsilon\|A\|\|\bar{y}_m\| + \nu_3(m,N)\epsilon(\|A\|\|x_0\| + \|b\|),\end{aligned} \tag{45}$$

with $\nu_1(m,N) = (1+\zeta_2 m^{3/2}N\epsilon)\zeta_5 m$, $\nu_2(m,N) = (\zeta_1 m + \zeta_6)mN^{3/2}$, $\nu_3(m,N) = \zeta_4 m^{3/2}N + \zeta_3 N^{3/2}$.

PROOF. Using Lemma 2 and Theorem 6 gives

$$\begin{aligned}b - A\bar{x}_m &= b - Ax_0 - A\bar{F}\bar{y}_m - Ad_m = \bar{r}_0 - \bar{W}_m\bar{R}_{WZ}\bar{y}_m - E_2\bar{y}_m - Ad_m + \tilde{d}_m \\ &= \bar{r}_0 - \bar{W}_m\bar{W}_m^*\bar{r}_0 + \bar{W}_m E_4\bar{y}_m - E_2\bar{y}_m - Ad_m + \tilde{d}_m,\end{aligned}$$

where $\|\tilde{d}_m\| \le \zeta_3 N^{3/2}\epsilon(\|A\|\|x_0\| + \|b\|)$.

Using the bounds for $\|\bar{r}_0 - \bar{W}_m\bar{W}_m^*\bar{r}_0\|$, $\|\bar{W}_m\|$, $\|E_4\|$, $\|E_2\|$, $\|d_m\|$, and $\|\tilde{d}_m\|$, and taking norm in the above relation, we obtain

$$\begin{aligned}\|b - A\bar{x}_m\| &\le \left\|\bar{r}_0 - \bar{W}_m\bar{W}_m^*\bar{r}_0\right\| + \left(\left\|\bar{W}_m\right\|\|E_4\| + \|E_2\|\right)\|\bar{y}_m\| + \|A\|\|d_m\| + \left\|\tilde{d}_m\right\| \\ &\le \left(\sin\theta\left(\bar{r}_0, \operatorname{span}\left\{\hat{W}_m\right\}\right) + \zeta_4 m^{3/2}N\epsilon\right)\|\bar{r}_0\| \\ &\quad + \left(\left(1+\zeta_2 m^{3/2}N\epsilon\right)\zeta_5 m\epsilon\left\|\bar{R}_{WZ}\right\| + \zeta_1 m^2 N^{3/2}\epsilon\|A\|\right)\|\bar{y}_m\| \\ &\quad + \left(\zeta_6 m N^{3/2}\epsilon\|\bar{y}_m\| + \epsilon\|x_0\|\right)\|A\| + \zeta_3 N^{3/2}\epsilon(\|A\|\|x_0\| + \|b\|) \\ &\le \sin\theta\left(\bar{r}_0, \operatorname{span}\left\{\hat{W}_m\right\}\right)\|\bar{r}_0\| + \left(1+\zeta_2 m^{3/2}N\epsilon\right)\zeta_5 m\epsilon\left\|\bar{R}_{WZ}\right\|\|\bar{y}_m\| \\ &\quad + \left(\zeta_1 m^2 N^{3/2} + \zeta_6 N^{3/2}\right)\epsilon\|A\|\|\bar{y}_m\| + \left(\zeta_4 m^{3/2}N + \zeta_3 N^{3/2}\right)\epsilon(\|A\|\|x_0\| + \|b\|),\end{aligned}$$

which proves (45). ∎

Similar to GMRES [7], if $\|x_0\|$ is not extremely large, $\|\bar{r}_0\|$ and $\nu_3(m,N)\epsilon(\|A\|\|x_0\| + \|b\|)$ are not significant. By (17), WZ-GMRES computes the exact solution of (1) in exact arithmetic if and only if $\sin\theta(b - Ax_0, A\mathcal{K}_m(A, b - Ax_0)) = 0$ and $|\sin\theta(b - Ax_0, A\mathcal{K}_m(a, b - Ax_0))| \ll 1$ is the necessary condition that WZ-GMRES is near convergence. In terms of the results due to Arioli and Fassino [13], $\hat{W}_m$ is an orthonormal basis of $A\mathcal{K}_m(A+E, b - Ax_0 + e)$, where $\|E\| \le \sqrt{N}(174N + 3\sqrt{N} + 87)\epsilon\|A\| + O(\epsilon^2)$ and $\|e\| \le 87\epsilon\|r_0\| + O(\epsilon^2)$. So, in finite precision, $\sin\theta(\bar{r}_0, \operatorname{span}\{\hat{W}_m\}) \approx \sin\theta(b - Ax_0, \operatorname{span}\{\hat{W}_m\}) = \sin\theta(b - Ax_0, A\mathcal{K}_m(A+E, b - Ax_0 + e))$ is also very small if WZ-GMRES is near convergence. Note that $\|\bar{R}_{WZ}\| = m\|A\| + O(\epsilon)$. Then, Theorem 7 shows that the bound on the residual norm $\|b - A\bar{x}_m\|$ can become large if and only if $\|\bar{y}_m\|$ becomes large.

So, in what follows, we need to find a bound for $\|\bar{y}_m\|$.

THEOREM 8. *Assume*

$$\sigma_{\min}\left(\bar{R}_{WZ}\right) \ge \zeta_5 m\epsilon\left\|\bar{R}_{WZ}\right\|. \tag{46}$$

Then, the following inequality holds:

$$\|\bar{y}_m\| \le \zeta_6\left(\sigma_{\min}\left(\bar{R}_{WZ}\right)\right)^{-1}\left(1 - \zeta_5 m\epsilon\kappa\left(\bar{R}_{WZ}\right)\right)^{-1}(\|A\|\|x_0\| + \|b\|), \tag{47}$$

with $\zeta_6 = (1+\zeta_2 m^{3/2}N\epsilon)(1+\zeta_3 N^{3/2}\epsilon)$.

PROOF. It follows from Lemma 2 and perturbation theory of singular values [11] that

$$\left|\sigma_{\min}\left(\bar{R}_{WZ} + E_4\right) - \sigma_{\min}\left(\bar{R}_{WZ}\right)\right| \le \zeta_5 m\epsilon\left\|\bar{R}_{WZ}\right\|. \tag{48}$$

Relation (48) and assumption (46) imply

$$\sigma_{\min}\left(\bar{R}_{WZ}+E_4\right) \geq \sigma_{\min}\left(\bar{R}_{WZ}\right) - \zeta_5 m\epsilon \left\|\bar{R}_{WZ}\right\| > 0.$$

Using (44), we have

$$\begin{aligned}\|\bar{y}_m\| &\leq \left\|\left(\bar{R}_{WZ}+E_4\right)^+\right\| \left\|\bar{W}_m^*\right\| \|\bar{r}_0\| = \frac{1}{\sigma_{\min}\left(\bar{R}_{WZ}+E_4\right)} \left\|\bar{W}_m\right\| \|\bar{r}_0\| \\ &\leq \frac{\left(1+\zeta_2 m^{3/2} N\epsilon\right)\left(1+\zeta_3 N^{3/2}\epsilon\right)\left(\|A\|\,\|x_0\|+\|b\|\right)}{\sigma_{\min}\left(\bar{R}_{WZ}\right) - \zeta_5 m\epsilon \left\|\bar{R}_{WZ}\right\|}. \qquad \blacksquare\end{aligned}$$

In summary, we can state the following result.

THEOREM 9. *Under assumption (46), the following inequality holds:*

$$\begin{aligned}\|b - A\bar{x}_m\| &\leq \sin\theta\left(\bar{r}_0, \operatorname{span}\left\{\hat{W}_m\right\}\right)\|\bar{r}_0\| + \mu_1(A,x_0,b)\frac{\epsilon\kappa\left(\bar{R}_{WZ}\right)}{1-\zeta_5 m\epsilon\kappa\left(\bar{R}_{WZ}\right)} \\ &+\mu_2(A,x_0,b)\frac{\epsilon\|A\|}{\sigma_{\min}\left(\bar{R}_{WZ}\right)\left(1-\zeta_5 m\epsilon\kappa\left(\bar{R}_{WZ}\right)\right)} + \nu_3(m,N)\epsilon(\|A\|\,\|x_0\|+\|b\|),\end{aligned} \tag{49}$$

where $\mu_1(A,x_0,b) = \zeta_6\nu_1(m,N)(\|A\|\,\|x_0\|+\|b\|)$, $\mu_2(A,x_0,b) = \zeta_6\nu_2(m,N)(\|A\|\,\|x_0\|+\|b\|)$.

PROOF. Combining (45) with (47) proves the assertion. ∎

Let us now compare WZ-GMRES with GMRES and discuss their numerical differences.

- As was pointed out in the Introduction, Drkošová *et al.* [7] proved that the residual norm $\|b-A\bar{x}_m\|$ computed by the HHA implementation of GMRES in finite precision is bounded like $\epsilon\|A\|$, and the computed solution $\bar{x}_m$ is bounded like $\epsilon\kappa(A)$. Recall that the error of a computed solution to the original large problem (1) by a backward stable direct solver, e.g., the Gaussian elimination with column pivoting, is bounded like $\epsilon\kappa(A)$. So, we should be content with the accuracy of the computed solution $\bar{x}_m$.
- Theorem 9 establishes an estimate of the residual norm $\|b - A\bar{x}_m\|$ computed by the HHA implementation of WZ-GMRES in finite precision. The residual norm $\|b - A\bar{x}_m\|$ reaches a level of order $\epsilon\kappa(\bar{R}_{WZ})$. According to the remarks in Section 4, $\bar{R}_{WZ}$ must be ill conditioned if WZ-GMRES is near convergence at step $m-1$ and Theorem 9 shows that the residual norm $\|b-A\bar{x}_m\|$ would become unbounded. Then, the computed solution $\bar{x}_m$ may be very poor, and WZ-GMRES may be numerically unstable in finite precision. This reminds us that WZ-GMRES is not numerically equivalent to GMRES and WZ-GMRES is usually a poor choice in practice when it is tending to converge.

We should point out that Householder implementation can be replaced by other stable orthogonalization within working precision, e.g., the Gram-Schmidt with refinement. By this, we can achieve the essentially same stability results up to different constants in the bounds of Section 5.

Using general theoretical results about least square residuals and minimal residual methods, Liesen *et al.* [10] also discussed the numerical behavior of WZ-GMRES, but they did not give a complete rounding error analysis of WZ-GMRES.

6. NUMERICAL EXPERIMENTS

We have run numerical experiments on an INTEL PENTIUMII 120/MMX with main memory 48 MB using MATLAB 5.0 with $\epsilon = 2.22 \times 10^{-16}$. We first inspect the behavior of R_G and R_{WZ} for various matrices taken from the Harwell-Boeing test collection [14] and initial vectors x_0

Table 1. $\kappa(\bar{R}_G)$ and $\kappa(\bar{R}_{WZ})$ of LSHP3025.

m	$\kappa(\bar{R}_G)$	$\kappa(\bar{R}_{WZ})$	m	$\kappa(\bar{R}_G)$	$\kappa(\bar{R}_{WZ})$
	6.77	3.7×10^2		11.59	1.3×10^3
	6.71	3.3×10^2		11.58	1.2×10^3
20	6.50	3.4×10^2	30	11.43	1.2×10^3
	6.68	3.4×10^2		11.79	1.2×10^3
	6.58	3.3×10^2		11.46	1.3×10^3
	17.25	3.8×10^3		21.68	8.6×10^3
	16.81	3.6×10^3		22.06	8.8×10^3
40	16.53	3.8×10^3	50	21.59	9.0×10^3
	17.11	4.1×10^3		21.40	9.0×10^3
	16.82	3.9×10^3		22.98	9.9×10^3
	27.54	1.9×10^4		35.04	4.0×10^4
	26.07	1.9×10^4		33.98	4.1×10^4
60	28.03	2.1×10^4	70	33.54	4.2×10^4
	28.22	2.2×10^4		33.14	4.3×10^4
	27.87	2.1×10^4		35.04	4.1×10^4

and m, and further observe the differences between the residual norms $\|b - Ax_m\|$ computed by GMRES and WZ-GMRES in finite precision, respectively.

EXAMPLE 1. We look at how $\kappa(\bar{R}_G)$ and $\kappa(\bar{R}_{WZ})$ behave with an initial vector generated randomly in a uniform distribution and m. Two test matrices come from [14]. They are LSHP3025 of order 3025 with $\kappa(A) = 1757$, which is well conditioned, and SHERMAN2 of order 1080 with $\kappa(A) = 1.42 \times 10^{12}$, which is very ill conditioned. The right-hand side b of (1) was taken to be $A[1, \dots, 1]^\top$. Tables 1 and 2 report the results obtained, in which for each fixed m we computed $\kappa(\bar{R}_G)$ and $\kappa(\bar{R}_{WZ})$ for five random x_0.

Tables 1 and 2 illustrate that for either well-conditioned LSHP3025 or ill-conditioned SHERMAN2, different x_0 and different m has very little effect on $\kappa(\bar{R}_G)$ and $\kappa(\bar{R}_{WZ})$. Table 1 also shows that for the well-conditioned problem (1), all the matrices R_Gs are well conditioned too and $\kappa(\bar{R}_G)$s are smaller than $\kappa(A)$, while the $\bar{R}_{WZ}$s are ill conditioned. Table 2 indicates that for the ill-conditioned SHERMAN2 the matrices $\bar{R}_G$s are well conditioned and $\kappa(\bar{R}_G)$ is much smaller than $\kappa(A)$ but the matrices R_{WZ}s are ill conditioned.

EXAMPLE 2. We now report more tests to show the conditioning of $\bar{R}_G$ and $\bar{R}_{WZ}$. All the matrices come from [14]. In tests, we took $x_0 = 0$, the right-hand sides of $b = A[1, \dots, 1]^\top$, and $m = 50$. Table 3 lists the computed results.

These experiments have illustrated that once A is well conditioned, the $\bar{R}_G$s are all well conditioned too, but the $\bar{R}_{WZ}$s are quite ill conditioned no matter how A is.

EXAMPLE 3. We report some tests to show the differences between the residual norms $\|b - A\bar{x}_m\|$ computed by the HHA implementation of GMRES and WZ-GMRES in finite precision arithmetic, respectively. At the same time, we observe how the condition numbers of $\bar{R}_G$ and $\bar{R}_{WZ}$ vary with the dimension m of the Krylov subspace $\mathcal{K}_m(A, r_0)$. Three test matrices come from [14]. They are PLAT1919 of order 1919 with $\kappa(A) = 490.59$, which is well conditioned, CAN1072 of order 1072 with $\kappa(A) = 3.1 \times 10^5$, which is moderately ill conditioned, and SAYLR3 of order 1000 with $\kappa(A) = \inf$, which is numerically singular matrix. In tests, we took $x_0 = 0$, the right-hand sides of $b = A[1, \dots, 1]^\top$. Figures 1–3 report the results obtained.

We observed a big difference in condition number shown in the plots in the figures. There are a few reasons. First, the condition number of R_G is always smaller than that of A. Second, according to Theorem 5, the matrix R_{WZ} must be very ill conditioned and nearly singular if

Table 2. $\kappa(\bar{R}_G)$ and $\kappa(\bar{R}_{WZ})$ of SHERMAN2.

m	$\kappa(\bar{R}_G)$	$\kappa(\bar{R}_{WZ})$	m	$\kappa(\bar{R}_G)$	$\kappa(\bar{R}_{WZ})$
	1.0×10^3	1.1×10^4		2.0×10^3	4.9×10^4
	8.8×10^2	7.7×10^3		1.9×10^3	3.7×10^4
20	9.0×10^2	1.1×10^4	30	2.0×10^3	5.3×10^4
	9.6×10^2	8.4×10^3		2.1×10^3	4.3×10^4
	9.9×10^2	6.7×10^3		2.1×10^3	3.4×10^4
	7.7×10^3	3.1×10^5		2.9×10^4	1.1×10^6
	7.4×10^3	2.8×10^5		2.5×10^4	1.0×10^6
40	7.4×10^3	3.4×10^5	50	2.9×10^4	1.6×10^6
	7.6×10^3	2.6×10^5		2.9×10^4	1.1×10^6
	8.7×10^3	2.4×10^5		2.8×10^4	7.7×10^5
	3.7×10^4	1.8×10^6		4.3×10^4	2.7×10^6
	3.4×10^4	1.6×10^6		4.4×10^4	2.8×10^6
60	3.8×10^4	2.4×10^6	70	5.8×10^4	4.4×10^6
	3.9×10^4	1.6×10^6		4.3×10^4	2.3×10^6
	4.8×10^4	1.5×10^6		5.3×10^4	2.1×10^6

Table 3. $\kappa(A)$, $\kappa(\bar{R}_G)$, and $\kappa(\bar{R}_{WZ})$.

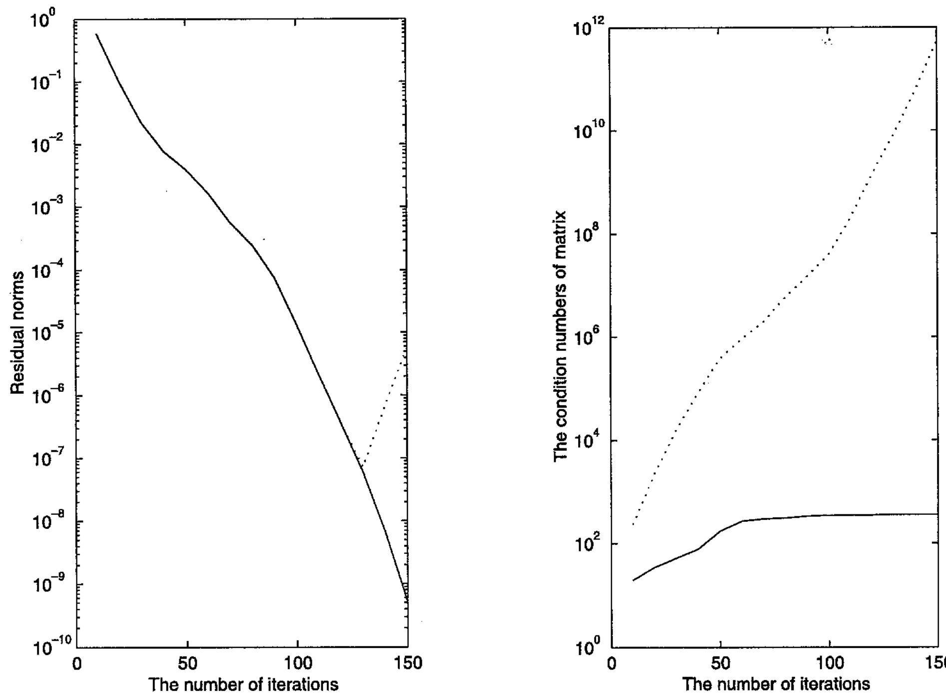
A	n	$\kappa(A)$	$\kappa(\bar{R}_G)$	$\kappa(\bar{R}_{WZ})$
LSHP1009	1009	959	27.26	1.6×10^5
LSHP2233	2233	1491	24.43	6.7×10^4
LSHP3025	3025	1757	23.75	4.4×10^4
LSHP3466	3466	1029	2.414	3.8×10^4
JAGMESH1	936	318	25.32	9.3×10^4
JAGMESH2	1009	959	27.26	1.6×10^5
JAGMESH3	1089	510	25.12	3.5×10^4
JAGMESH4	1440	525	31.13	1.7×10^5
SHERMAN1	1000	2.3×10^4	1.3×10^3	1.0×10^6
SHERMAN2	1080	1.4×10^{12}	3.7×10^4	1.7×10^6
SHERMAN4	1104	7.2×10^3	1.7×10^3	1.1×10^5

WZ-GMRES is near convergence, so that $\kappa(R_{WZ})$ is very large and may even well exceed $1/\epsilon$, where ϵ is machine precision. It is seen from (15) that in finite precision we may get a computed approximate $\bar{y}_m$ with very poor accuracy and very large $\|\bar{y}_m\|$ as (47) shows, so that the computed residual norm $\|b - A\bar{x}_m\|$ is not near zero as (45) shows, and even may be quite big, as the right-hand sides of (47) and (49) reveal.

These experiments indicate that the matrix $\bar{R}_{WZ}$ becomes very ill conditioned as the dimension m of the Krylov subspace $\mathcal{K}_m(A, r_0)$ increases and the residual norms $\|b - A\bar{x}_m\|$ computed by the HHA implementation of WZ-GMRES is not near zero and even is quite big when the method is near convergence. This phenomenon can be explained by Theorems 6 and 8. So, WZ-GMRES is not numerically equivalent to GMRES and is numerically unstable.

7. CONCLUSIONS

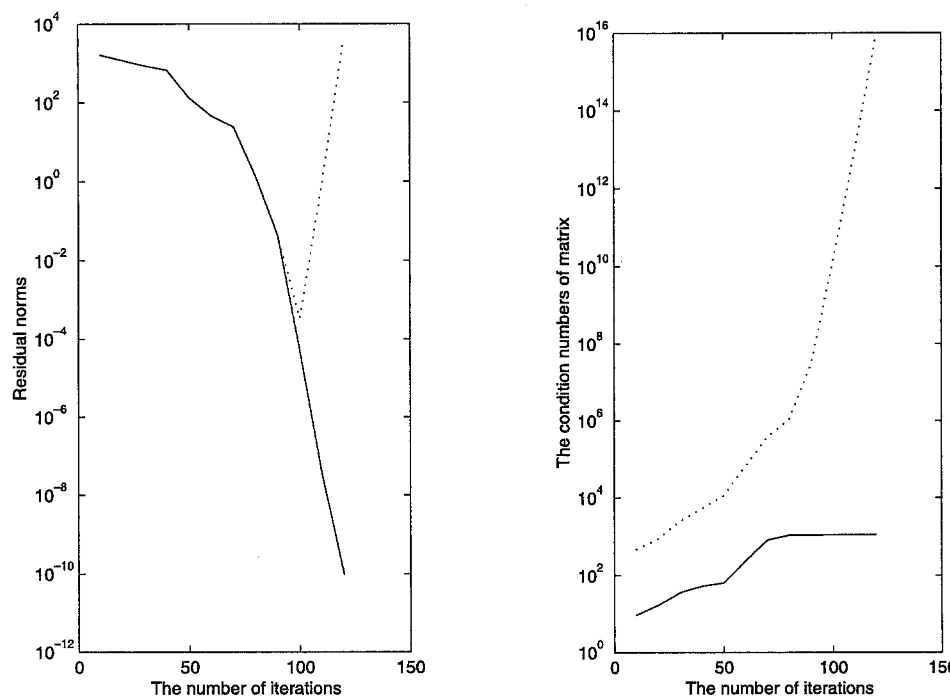
This paper shows that the small matrix R_{WZ} generated by WZ-GMRES must be ill conditioned if WZ-GMRES is near convergence in theory. In finite precision arithmetic, this may deliver a very poor computed approximate solution and make WZ-GMRES numerically unstable if WZ-



(a) The difference between the residual norms. Solid line: the residual norm for GMRES; dash-dot line: the residual norm for WZ-GMRES.

(b) The condition numbers of matrices $\bar{R}_G$ and $\bar{R}_{WZ}$. Solid line: $\kappa(\bar{R}_G)$; dash-dot line: $\kappa(\bar{R}_{WZ})$.

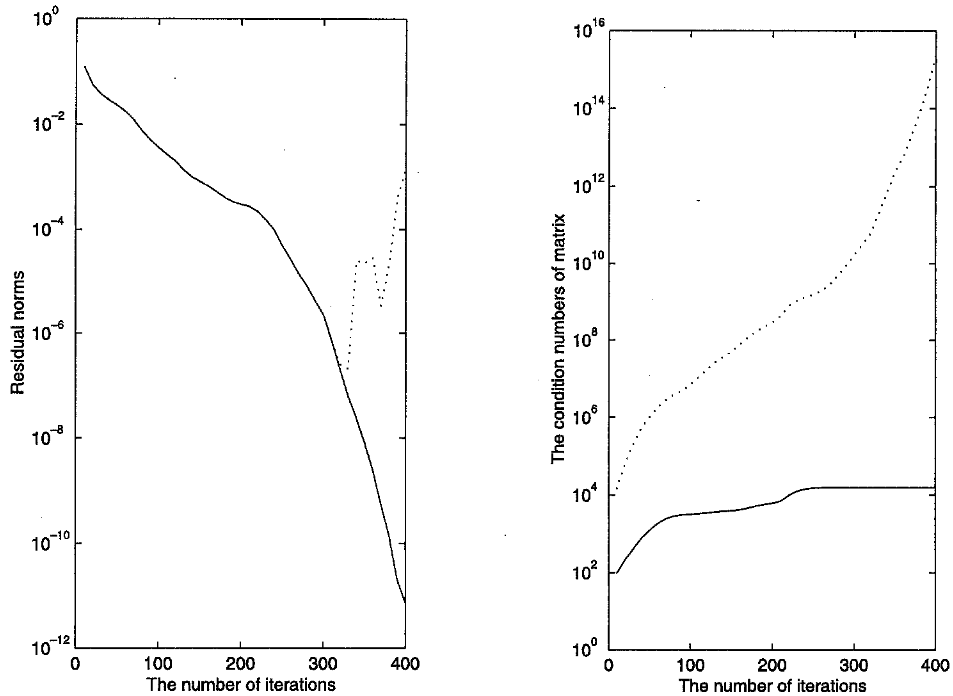
Figure 1. PLAT1919.



(a) The difference between the residual norms. Solid line: the residual norm for GMRES; dash-dot line: the residual norm for WZ-GMRES.

(b) The condition numbers of matrices $\bar{R}_G$ and $\bar{R}_{WZ}$. Solid line: $\kappa(\bar{R}_G)$; dash-dot line: $\kappa(\bar{R}_{WZ})$.

Figure 2. CAN1072.



(a) The difference between the residual norms. Solid line: the residual norm for GMRES; dash-dot line: the residual norm for WZ-GMRES.

(b) The condition numbers of matrices $\bar{R}_G$ and $\bar{R}_{WZ}$. Solid line: $\kappa(\bar{R}_G)$; dash-dot line: $\kappa(\bar{R}_{WZ})$.

Figure 3. SAYLR3.

GMRES is theoretically near convergence. Although WZ-GMRES is mathematically equivalent to GMRES, its poor numerical behavior suggests that it is less preferable and we should use the original GMRES implementation, in particular when GMRES is near convergence.

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