Adaptive version of Simpler GMRES

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Abstract. In this paper we propose a stable variant of Simpler GMRES by Walker and Zhou [15]. It is based on the adaptive choice of the Krylov subspace basis at given iteration step using the intermediate residual norm decrease criterion. The new direction vector is chosen as in the original implementation of Simpler GMRES or it is equal the normalized residual vector as in the GCR method. We show that such adaptive strategy leads to a well-conditioned basis of the Krylov subspace and we support our theoretical results with illustrative numerical examples.

1. Introduction

We consider the solution of a large and sparse system of linear algebraic equations

$$Ax = b, \tag{1.1}$$

where $A \in \mathbb{R}^{N\times N}$ is nonsingular and $b \in \mathbb{R}^N$ is a right-hand side vector. A popular method for solving such system is the GMRES method by Saad and Schultz [12]. It seeks at the nth iteration step the approximate solution x_n in the affine subspace $x_0 + \mathcal{K}_n(A, r_0)$, where

$$\mathcal{K}_n(A, r_0) := \operatorname{span}\{r_0, Ar_0, \ldots, A^{n-1}r_0\}$$

is the nth Krylov subspace generated by the matrix A and the residual vector $r_0 := b - Ax_0$ corresponding to the initial guess x_0. The GMRES method is based on the Arnoldi process [1] generating the orthonormal basis

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Q_n of the Krylov subspace $\mathcal{K}_n(A, r_0)$ and minimizes the Euclidean norm of the residual in $r_0 + A\mathcal{K}_n(A, r_0)$, i.e.,

$$\|b - Ax_n\| = \|b - A(x_0 + d_n)\| = \min_{d \in \mathcal{K}_n(A, r_0)} \|b - A(x_0 + d)\|. \tag{1.2}$$

If a stopping criterion is satisfied at some iteration step m, the coordinates y_m of d_m in the orthogonal basis Q_m are found by solving an $(m+1) \times m$ upper Hessenberg least squares problem and the approximate solution is then computed as $x_m = x_0 + d_m = x_0 + V_m y_m$. The GMRES method with the Householder or modified Gram-Schmidt Arnoldi implementation was proved to be backward stable in [**3, 9**], which means that there is an approximate solution of (1.1) which can be interpreted as an exact solution of a system (1.1) with slightly perturbed initial data A and b. See also the Higham's book [**6**] for details of the backward error concept.

In [**15**] Walker and Zhou proposed another implementation of the GMRES method. We will describe it in a slightly more general way. Let $Z_n := [z_1, \ldots, z_n]$ be a basis of $\mathcal{K}_n(A, r_0)$ such that $\mathcal{R}(Z_k) = \mathcal{K}_k(A, r_0)$ for all $k = 1, \ldots, n$ and, in addition, we assume that its columns are normalized, i.e., $\|z_k\| = 1$ for $k = 1, \ldots, n$. Here $\mathcal{R}(\cdot)$ denotes the range of the matrix. The minimum residual property (1.2) is equivalent to the requirement of the residual vector $r_n := b - Ax_n$ being ortogonal to the subspace $A\mathcal{K}_n(A, r_0)$:

$$\langle r_n, v \rangle = 0 \qquad \forall v \in A\mathcal{K}_n(A, r_0) = \mathcal{R}(AZ_n), \tag{1.3}$$

where $\langle \cdot, \cdot \rangle$ stands for the standard Euclidean inner product. The residual r_n is then easily evaluated provided we have an orthonormal basis $V_n := [v_1, \ldots, v_n]$ of $A\mathcal{K}_n(A, r_0) = \mathcal{R}(AZ_n)$, which can be computed by the QR factorization of the matrix AZ_n:

$$AZ_n = V_n U_n. \tag{1.4}$$

The matrix $U_n \in \mathbb{R}^{n \times n}$ is upper triangular and nonsingular if and only if the dimension of $\mathcal{K}_n(A, r_0)$ is equal to n. The residual $r_n \in r_0 + A\mathcal{K}_n(A, r_0) = r_0 + \mathcal{R}(V_n)$ satisfying the property (1.3) (and (1.2)) can be then computed as the orthogonal projection of the initial residual r_0:

$$r_n = (I - V_n V_n^T) r_0 = (I - v_n v_n^T) r_{n-1} = r_{n-1} - \alpha_n v_n, \; \alpha_n := \langle r_{n-1}, v_n \rangle. \tag{1.5}$$

The approximate solution x_n corresponding to the residual r_n has the form $x_n = x_0 + Z_n t_n$, where t_n is the solution of the upper triangular system

$$U_n t_n = V_n^T r_0 = [\alpha_1, \ldots, \alpha_n]^T. \tag{1.6}$$

In [**15**] the basis Z_n is chosen as $[\widetilde{r}_0, V_{n-1}]$, i.e., the normalized initial residual is extended by the first $n-1$ vectors of the orthonormal basis V_n. We will denote here the normalized residual vectors by $\widetilde{r}_k := r_k / \|r_k\|$. However, it was shown in [**15, 8**] that the conditioning of $[\widetilde{r}_0, V_{n-1}]$ is in fact proportional to the inverse of the relative residual norm, i.e., it grows as the residual norm decreases. Therefore the original implementation of the Simpler GMRES method can suffer from numerical instability due to the ill-conditioning of the basis which moreover leads to the severe ill-conditioning of the upper triangular factor U_n in (1.4) possibly affected also by ill-conditioning of A; see the numerical experiments in [**8, 7**]. On the other hand, if the minimum residual method (nearly) stagnates the Simpler GMRES basis $[\widetilde{r}_0, V_{n-1}]$ remains well-conditioned. As it was shown in [**7**] the basis Z_n consisting of the normalized residuals $[\widetilde{r}_0, \ldots, \widetilde{r}_{n-1}]$ remains well-conditioned provided there is a reasonable residual norm decrease at each iteration. The Simpler GMRES method with such residual basis, called RB-SGMRES in [**7**], was shown to be conditionally backward stable and it is closely related to GCR by Eisenstat, Elman and Schultz [**4**]. See [**7**] and [**11**] for more details.

It was shown in [**7**] that the condition number of Z_n can affect the maximum attainable accuracy of the computed approximation. In Section 2 we propose a variant of the Simpler GMRES method (called the adaptive Simpler GMRES here), which keeps the conditioning of the basis Z_n on a reasonable level by adaptive selection at each iteration a suitable direction vector based on the intermediate residual norm decrease. Whenever the residual norm (nearly) stagnates we use the vector v_{n-1} at the particular iteration step n. Otherwise, when we observe sufficient residual norm decrease, we set the new direction vector equal to the normalized residual vector $\widetilde{r}_{n-1}$. Similar strategy is employed, e.g., in [**10**], where the Orthomin method [**14**] is combined with Orthodir [**16**] for solving saddle point problems in computational fluid dynamics. Here we show that the adaptive choice of direction vectors keeps the basis well-conditioned and that the conditioning grows in a quasi-optimal case at most linearly with the iteration number. Finally, we illustrate our theoretical results on numerical experiments in Section 3.

Throughout the paper, we denote by $\|\cdot\|$ the Euclidean vector norm and the induced matrix norm, and by $\|\cdot\|_F$ the Frobenius norm. For $B \in \mathbb{R}^{N\times n}$ $(N \geq n)$ of rank n, $\sigma_1(B) \geq \sigma_n(B) > 0$ are the extremal singular values of B and $\kappa(B) = \sigma_1(B)/\sigma_n(B)$ is the spectral condition number. By I_n we denote the $n \times n$ unit matrix. If $X_i \in \mathbb{R}^{n_i\times n_i}$ $(i = 1, \ldots, m)$ are square matrices, we denote by $\mathrm{diag}(X_1, \ldots, X_m)$ the block diagonal matrix with blocks $X_1, \ldots, X_m$ of the order $\sum_{i=1}^m n_i$. For a vector $y \in \mathbb{R}^n$ the notation $\mathrm{diag}(y)$ or $\mathrm{diag}(y^T)$ is used in a usual manner and defines the $n\times n$ diagonal matrix with the components of y on the main diagonal and zeros elsewhere.

2. Adaptive Simpler GMRES

In this section we propose an adaptive variant of the Simpler GMRES method, which computes the basis Z_n in (1.4) such that its conditioning is kept on a reasonably small level. This is achieved by adaptive switching between the bases from Simpler GMRES and RB-SGMRES using an intermediate residual decrease criterion. If the residual norm at given step decreases sufficiently the Krylov subspace basis is extended by the normalized residual vector as in RB-SGMRES or GCR; otherwise we use the last available vector of the orthonormal basis as in Simpler GMRES. In order to decide whether the residual norm is reduced sufficiently enough we introduce the threshold parameter $\nu \in [0,1]$ and choose for $n > 1$ either the vector $z_n = \widetilde{r}_{n-1}$ provided that $\|r_{n-1}\| \le \nu \|r_{n-2}\|$ or $z_n = v_{n-1}$ in the latter case. We sketch the algorithm of adaptive Simpler GMRES as follows:

Algorithm 2.1 (Adaptive Simpler GMRES). 1. *choose* x_0 *and the threshold parameter* $\nu \in [0,1]$, *compute* $r_0 := b - Ax_0$

2. *for* $n = 1, \ldots, m$ *(until convergence) do*
   a. *compute* z_n*:*
$$z_n = \begin{cases} \widetilde{r}_0 & \textit{if } n = 1, \\ \widetilde{r}_{n-1} & \textit{if } n > 1 \textit{ and } \|r_{n-1}\| \le \nu \|r_{n-2}\|, \\ v_{n-1} & \textit{otherwise}, \end{cases} \tag{2.1}$$
   b. *update the QR factorization* $AZ_n = V_n U_n$
   c. *compute* $\alpha_n := \langle r_{n-1}, v_n \rangle$
   d. *update* $r_n := r_{n-1} - \alpha_n v_n$
3. *end*
4. *solve* $U_m t_m = [\alpha_1, \ldots, \alpha_m]^T$
5. *compute* $x_m := x_0 + Z_m t_m$

If $\nu = 0$ then $Z_n = [\widetilde{r}_0, V_{n-1}]$ and Algorithm 2.1 is identical to Simpler GMRES [**15**]. The choice $\nu = 1$ results in $Z_n = [\widetilde{r}_0, \ldots, \widetilde{r}_{n-1}]$ which corresponds to RB-SGMRES [**7**].

Theorem 2.2. *Let* A *in* (1.1) *be nonsingular and* n *be such that the dimension of* $\mathcal{K}_n(A, r_0)$ *is equal to* n. *If* $\nu \in [0,1)$ *then* Z_n *computed in Algorithm 2.1 forms a basis of* $\mathcal{K}_n(A, r_0)$ *satisfying* $z_k \in \mathcal{K}_k(A, r_0) \backslash \mathcal{K}_{k-1}(A, r_0)$ *for all* $k = 1, \ldots, n$. *In particular, adaptive Simpler GMRES does not break down unless the exact solution of* (1.1) *is found.*

Proof. We proceed by induction on n. For $n = 1$ the statement is clearly satisfied by setting $\mathcal{K}_0(A, r_0) := \{0\}$. Let $n > 1$ and Z_{n-1} be a basis of $\mathcal{K}_{n-1}(A, r_0)$. From (1.4) the columns of V_{n-1} form an orthonormal basis of $A\mathcal{K}_{n-1}(A, r_0)$. The vector v_{n-1} is computed from the vector $Az_{n-1} \in \mathcal{K}_n(A, r_0) \backslash \mathcal{K}_{n-1}(A, r_0)$ orthogonalizing it against the orthonormal basis V_{n-2} of $A\mathcal{K}_{n-2}(A, r_0)$ and thus belongs to $\mathcal{K}_n(A, r_0) \setminus \mathcal{K}_{n-1}(A, r_0)$. We consider two cases: First let $\|r_{n-1}\| > \nu \|r_{n-2}\|$ and hence by (2.1) $z_n = v_{n-1}$. The vector v_{n-1} extends the basis Z_{n-1} of $\mathcal{K}_{n-1}(A, r_0)$ to the basis of $\mathcal{K}_n(A, r_0)$ as follows from the discussion above. Otherwise, let $\|r_{n-1}\| \le \nu \|r_{n-2}\|$. Since $\|r_{n-1}\| < \|r_{n-2}\|$ and $r_k \in r_0 + A\mathcal{K}_k(A, r_0)$ it follows that $r_{n-1} = r_{n-2} - \alpha_{n-1} v_{n-1}$ with $\alpha_{n-1} \neq 0$ and $r_{n-1} \in \mathcal{K}_{n-1}(A, r_0) \setminus \mathcal{K}_{n-2}(A, r_0)$. Hence $Z_n = [Z_{n-1}, \widetilde{r}_{n-1}]$ forms a basis of $\mathcal{K}_n(A, r_0)$. $\square$

It is known that the residual basis can be linearly dependent if the minimum residual method does not make any progress at given step, in particular when 0 belongs to the field of values of the matrix A it may happen that $\alpha_n = 0$ resulting in $r_n = r_{n-1}$. Therefore we have excluded the case $\nu = 1$ from Theorem 2.2 which can lead to a breakdown of the RB-SGMRES or GCR algorithms.

We recall the results on the maximum attainable accuracy of algorithms based on (1.4) studied in [7], which apply also for adaptive Simpler GMRES. We assume that the QR factorization at Step 2b of Algorithm 2.1 is constructed such that the upper triangular matrix U_n is computed in a backward stable way; see, e.g., [7, Equations (2.1) and (2.2)]. It is true in particular for Householder QR factorization, modified and iterated Gram-Schmidt algorithms. Let $\hat{x}_n$ be an approximate solution computed at iteration n of Algorithm 2.1 in finite precision arithmetic with unit roundoff u. In addition let $cu\kappa(A)\kappa(Z_n) < 1$, where the constant c is a low-order polynomial in n and N, which guarantees that AZ_n and U_n are of full numerical rank. Then the gap between the true residual $b - A\hat{x}_n$ and the updated residual r_n can be estimated as

$$\|b - A\hat{x}_n - r_n\| \leq \frac{cu\kappa(A)}{1 - cu\kappa(A)\kappa(Z_n)} \sum_{k=1}^{n} \frac{\|r_{k-1}\|}{\sigma_k(Z_k)}, \tag{2.2}$$

while the accuracy in terms of the backward error can be bounded as

$$\frac{\|b - A\hat{x}_n - r_n\|}{\|A\|\|\hat{x}_n\|} \leq cu\kappa(Z_n)\left(1 + \frac{\|x_0\|}{\|\hat{x}_n\|}\right). \tag{2.3}$$

The conditioning of the basis Z_n plays therefore an important role in the numerical stability of algorithms based on (1.4). In the following we analyze the condition number of Z_n produced by adaptive Simpler GMRES. First we prove three auxiliary propositions.

LEMMA 2.3. *Let p and q be two integers such that $1 \leq p < q$ and let $\widetilde{B}_{p,q} \in \mathbb{R}^{(q-p+1)\times(q-p+1)}$ be a lower Hessenberg matrix defined by*

$$\widetilde{B}_{p,q} := \begin{bmatrix} a_{p,q-1}/\rho_{p-1} & I_{q-p} \\ \rho_{q-1}/\rho_{p-1} & 0 \end{bmatrix},$$

where $a_{p,q-1} := [\alpha_p, \ldots, \alpha_{q-1}]^T$, $\alpha_k^2 = \rho_{k-1}^2 - \rho_k^2$ for $k = p, \ldots, q-1$, and $0 < \rho_{q-1} \leq \rho_{q-2} \leq \ldots \leq \rho_{p-1}$. Then

$$\kappa(\widetilde{B}_{p,q}) = \delta_{p,q} := \frac{\rho_{p-1} + \sqrt{\rho_{p-1}^2 - \rho_{q-1}^2}}{\rho_{q-1}}.$$

PROOF. The proof uses the similar technique as in [8, Theorem 2.3]. By direct computation we obtain

$$\begin{aligned}\widetilde{B}_{p,q}^T\widetilde{B}_{p,q} &= \begin{bmatrix} (\rho_{q-1}^2 + \|a_{p,q-1}\|^2)/\rho_{p-1}^2 & a_{p,q-1}^T/\rho_{p-1} \\ a_{p,q-1}/\rho_{p-1} & I_{q-p} \end{bmatrix} \\ &= \begin{bmatrix} 1 & a_{p,q-1}^T/\rho_{p-1} \\ a_{p,q-1}/\rho_{p-1} & I_{q-p} \end{bmatrix}.\end{aligned}$$

There exists an orthonormal matrix $U \in \mathbb{R}^{(q-p)\times(q-p)}$ such that

$$Ua_{p,q-1} = \|a_{p,q-1}\|e_1 = (\rho_{p-1}^2 - \rho_{q-1}^2)^{\frac{1}{2}}e_1$$

and hence

$$\begin{bmatrix} 1 & 0 \\ 0 & U \end{bmatrix} \widetilde{B}_{p,q}^T \widetilde{B}_{p,q} \begin{bmatrix} 1 & 0 \\ 0 & U^T \end{bmatrix} = \begin{bmatrix} 1 & \beta e_1^T \\ \beta e_1 & I_{q-p} \end{bmatrix} =: G,$$

where $\beta := (1 - \rho_{q-1}^2/\rho_{p-1}^2)^{\frac{1}{2}}$. The eigenvalues of G are equal to the eigenvalues of its leading principal 2×2 submatrix together with 1 of multiplicity $q - p - 1$. Since G is (orthogonally) similar to $\widetilde{B}_{p,q}^T \widetilde{B}_{p,q}$, the square roots of its eigenvalues are at the same time equal to the singular values of $\widetilde{B}_{p,q}$. The extremal singular values of $\widetilde{B}_{p,q}$ can be evaluated as

$$\sigma_1^2(\widetilde{B}_{p,q}) = 1 + \beta, \qquad \sigma_{q-p+1}^2(\widetilde{B}_{p,q}) = 1 - \beta. \tag{2.4}$$

Note that $0 \le \beta < 1$ and 1 is neither minimal nor maximal eigenvalue of G unless $\beta = 0$. A simple algebraic manipulation gives

$$\kappa(\widetilde{B}_{p,q}) = \frac{\rho_{p-1} + \sqrt{\rho_{p-1}^2 - \rho_{q-1}^2}}{\rho_{q-1}}.$$

□

LEMMA 2.4. *Let q and m be two integers such that $1 \le q < m$ and $\widetilde{C}_{q,m} \in \mathbb{R}^{(m-q+1)\times(m-q+1)}$ be a lower triangular matrix*

$$\widetilde{C}_{q,m} := \operatorname{diag}([a_{q,m-1}^T, \rho_{m-1}]) L_{m-q+1}^{-1} \operatorname{diag}(r_{q-1,m-1})^{-1},$$

where $a_{q,m-1} := [\alpha_q, \ldots, \alpha_{m-1}]^T$, $r_{q-1,m-1} := [\rho_{q-1}, \ldots, \rho_{m-1}]^T$, $\alpha_n^2 = \rho_{n-1}^2 - \rho_n^2$ for $n = q, \ldots, m-1$, $0 < \rho_{m-1} < \rho_{m-2} < \ldots < \rho_{q-1}$. The matrix L_{m-q+1} of the order $m-q+1$ is lower bidiagonal with 1 on the main diagonal and -1 on the first subdiagonal. Then

$$1 \le \kappa(\widetilde{C}_{q,m}) \le \gamma_{q,m}, \qquad \gamma_{q,m} := (m-q+1)^{\frac{1}{2}} \left(1 + \sum_{n=q}^{m-1} \frac{\rho_{n-1}^2 + \rho_n^2}{\rho_{n-1}^2 - \rho_n^2}\right)^{\frac{1}{2}}.$$

PROOF. The inverse of L_{m-q+1} is a matrix with ones on the main diagonal and below and with zeros elsewhere. By direct computation we have $\sigma_1(\widetilde{C}_{q,m}) = \|\widetilde{C}_{q,m}\| \le \|\widetilde{C}_{q,m}\|_F = \sqrt{m-q+1}$. The inverse of $\widetilde{C}_{q,m}$ exists, since $\alpha_n \neq 0$ for $n = q, \ldots, m-1$ and $\rho_{m-1} \neq 0$, and it is a lower bidiagonal matrix

$$\widetilde{C}_{q,m}^{-1} = \operatorname{diag}(r_{q-1,m-1}) L_{m+q-1} \operatorname{diag}([a_{q,m-1}^T, \rho_{m-1}])^{-1}.$$

The minimal singular value of $\widetilde{C}_{q,m}$ can be estimated by $[\sigma_{m-q+1}(\widetilde{C}_{q,m})]^{-1} = \|\widetilde{C}_{q,m}^{-1}\| \le \|\widetilde{C}_{q,m}^{-1}\|_F$, where

$$\|\widetilde{C}_{q,m}^{-1}\|_F = \sqrt{1 + \sum_{n=q}^{m-1} \frac{\rho_{n-1}^2 + \rho_n^2}{\rho_{n-1}^2 - \rho_n^2}}.$$

□

The proof of the previous lemma was already given in [7, Theorem 3.4] for the context of RB-SGMRES (for $q = 1$), which was shown to be conditionally backward stable provided that the stagnation factor $\gamma_{1,m}$ is reasonably small. Another bound on the conditioning of the residual basis can be established using the Gershgorin theorem [5] (see also, e.g., [13, Theorem 1.11]).

LEMMA 2.5. *Let the assumptions of Lemma 2.4 be satisfied and let*

$$\underline{\lambda}_n := \begin{cases} \frac{\rho_n}{\rho_{n+1}+\rho_n} & \textit{for} \quad n = q-1, \\ \frac{\rho_n}{\rho_{n+1}+\rho_n} - \frac{\rho_n}{\rho_n+\rho_{n-1}} & \textit{for} \quad n = q, \dots, m-2, \\ \frac{\rho_{n-1}}{\rho_n+\rho_{n-1}} & \textit{for} \quad n = m-1, \end{cases}$$

$$\overline{\lambda}_n := \begin{cases} \frac{\rho_n}{\rho_n-\rho_{n+1}} & \textit{for} \quad n = q-1, \\ \frac{\rho_n}{\rho_{n-1}-\rho_n} + \frac{\rho_n}{\rho_n-\rho_{n+1}} & \textit{for} \quad n = q, \dots, m-2, \\ \frac{\rho_{n-1}}{\rho_{n-1}-\rho_n} & \textit{for} \quad n = m-1. \end{cases}$$

Then

$$1 \leq \kappa(\widetilde{C}_{q,m}) \leq \left(\frac{\max\limits_{n=q-1,\dots,m-1} \overline{\lambda}_n}{\min\limits_{n=q-1,\dots,m-1} \underline{\lambda}_n} \right)^{\frac{1}{2}}.$$

PROOF. The matrix $\widetilde{C}_{q,m}^{-1}\widetilde{C}_{q,m}^{-T}$ can be written in the form

$$\widetilde{C}_{q,m}^{-1}\widetilde{C}_{q,m}^{-T} = \operatorname{diag}(r_{q-1,m-1})\, T \operatorname{diag}(r_{q-1,m-1}),$$

where

$$T = \begin{bmatrix} \frac{1}{\alpha_q^2} & -\frac{1}{\alpha_q^2} & & & \\ -\frac{1}{\alpha_q^2} & \frac{1}{\alpha_q^2} + \frac{1}{\alpha_{q+1}^2} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & \frac{1}{\alpha_{m-2}^2} + \frac{1}{\alpha_{m-1}^2} & -\frac{1}{\alpha_{m-1}^2} \\ & & & -\frac{1}{\alpha_{m-1}^2} & \frac{1}{\alpha_{m-1}^2} + \frac{1}{\rho_{m-1}^2} \end{bmatrix}.$$

It is straightforward to show, that the matrix $\widetilde{C}_{q,m}^{-1}\widetilde{C}_{q,m}^{-T}$ is diagonally dominant. Let $\eta_{q-1}, \dots, \eta_{m-1}$ and $\delta_{q-1}, \dots, \delta_{m-1}$ denote the diagonal entries and the sum of absolute values of the off-diagonal entries in rows $1, \dots, m-q+1$. Note that the diagonal entries are positive, while the off-diagonal ones are negative. Since $\widetilde{C}_{q,m}^{-1}\widetilde{C}_{q,m}^{-T}$ is symmetric, its eigenvalues are real and belong to $\cup_{n=q-1}^{m-1}[\eta_n - \delta_n, \eta_n + \delta_n]$ due to the Gershgorin theorem [5]. We find that $\eta_n - \delta_n = \underline{\lambda}_n$ and $\eta_n + \delta_n = \overline{\lambda}_n$ and the proof of the statement is finished. □

The bound using the Gershgorin theorem will be employed below in order to establish the a priori estimate on the condition number of the basis provided we have a prescribed value of the threshold parameter ν. Whenever we want to explain the local contributions of intermediate residual norm decreases to the conditioning of the Krylov subspace basis, the estimate in Lemma 2.4 is however more usefull. We exploit it in the following theorem where we consider the case where at the steps $n = 2, \dots, q$ of Algorithm 2.1 the vector z_n is chosen as in Simpler GMRES, i.e., $z_n = v_{n-1}$, and $z_n = \widetilde{r}_{n-1}$ as in RB-SGMRES for $n = q+1, \dots, m$. It corresponds to adaptive Simpler GMRES applied to a problem with some initial stagnation of the minimum residual norm and a fast convergence afterwards.

Theorem 2.6. *Let $Z_m = [\widetilde{r}_0, v_1, \dots, v_{q-1}, \widetilde{r}_q, \dots, \widetilde{r}_{m-1}]$ for some integer q such that $1 < q < m$ and let $0 < \|r_{m-1}\| < \cdots < \|r_{q-1}\|$. Then*

$$Z_m = [V_{m-1}, \widetilde{r}_{m-1}]H_m,$$

with $H = C_m B_m$, $B_m := \operatorname{diag}(\widetilde{B}_{1,q}, I_{m-q})$, $C_m := \operatorname{diag}(I_{q-1}, \widetilde{C}_{q,m})$. The vectors $a_{1,q-1}$, $a_{q,m-1}$, and $r_{q-1,m-1}$ and the matrices $\widetilde{B}_{1,q}$ and $\widetilde{C}_{q,m}$ are defined as in Lemma 2.3 and 2.4 (with $p = 1$), where $\rho_n := \|r_n\|$. The condition number of Z_m can then be bounded as follows:

$$\delta_{1,q} \le \kappa(Z_m) \le \delta_{1,q}\gamma_{q,m}. \tag{2.5}$$

Proof. From (1.5) we have

$$\widetilde{r}_0 = [V_{q-1}, \widetilde{r}_{q-1}] \begin{bmatrix} a_{1,q-1}/\rho_0 \\ \rho_{q-1}/\rho_0 \end{bmatrix}.$$

Hence $[\widetilde{r}_0, V_{q-1}] = [V_{q-1}, \widetilde{r}_{q-1}]\widetilde{B}_{1,q}$ and

$$Z_m = [V_{q-1}, \widetilde{r}_{q-1}, \dots, \widetilde{r}_{m-1}]B_m. \tag{2.6}$$

Again using (1.5) we find that $[\widetilde{r}_{q-1}, \dots, \widetilde{r}_{m-1}] = [v_q, \dots, v_{m-1}, \widetilde{r}_{m-1}]\widetilde{C}_{q,m}$ and

$$[V_{q-1}, \widetilde{r}_{q-1}, \dots, \widetilde{r}_{m-1}] = [V_{m-1}, \widetilde{r}_{m-1}]C_m. \tag{2.7}$$

Combining (2.6) and (2.7), and applying Lemma 2.3 and 2.4 concludes the proof. □

Corollary 2.7. *Let the assumptions of Theorem 2.6 be satisfied. In addition, let $\|r_n\| \le \nu\|r_{n-1}\|$ for $n = q, \dots, m-1$ for some $\nu < 1$ and $\|r_n\| > \nu\|r_{n-1}\|$ for $n = 1, \dots, q-1$. Then*

$$1 \le \kappa(Z_m) \le \frac{2\sqrt{2}}{\nu^{q-1}} \frac{1+\nu}{1-\nu}. \tag{2.8}$$

Proof. From $\|r_n\| \le \nu\|r_{n-1}\|$ it follows:

$$\frac{1}{(1+\nu)\|r_{n-1}\|} \le \frac{1}{\|r_{n-1}\| + \|r_n\|} \le \frac{1}{2\|r_n\|}$$

and

$$\frac{1}{\|r_{n-1}\|} \le \frac{1}{\|r_{n-1}\| - \|r_n\|} \le \frac{1}{(1-\nu)\|r_{n-1}\|},$$

and therefore

$$\frac{1}{2}\frac{1-\nu}{1+\nu} \le \underline{\lambda}_n \le \overline{\lambda}_n \le \frac{1+\nu}{1-\nu}$$

for $n = q-1, \ldots, m-1$. Then the result follows from Theorem 2.6 and Lemma 2.5 (with $\rho_n = \|r_n\|$) and from the assumption $\|r_n\| > \nu\|r_{n-1}\|$ ($n = 1, \ldots, q-1$), which implies that $\|r_{q-1}\| > \nu^{q-1}\|r_0\|$ and $1 \leq \delta_{1,q} \leq 2/\nu^{q-1}$. ☐

Theorem 2.6 and Corollary 2.7 show that at the iteration steps where the residual norm (nearly) stagnates, the contribution of vectors from Simpler GMRES to the conditioning of Z_m is given approximately by the inverse of the relative residual norm decrease during the (near) stagnation. At steps where the residual norm is sufficiently reduced, the conditioning of Z_m in the adaptive Simpler GMRES is affected by the stagnation factor $\gamma_{q,m}$. Considering (2.3) and (2.8) we can estimate the backward error of adaptive Simpler GMRES as

$$\frac{\|b - A\hat{x}_m - r_m\|}{\|A\|\|\hat{x}_m\|} \leq cu\frac{1}{\nu^{q-1}}\frac{1+\nu}{1-\nu}\left(1 + \frac{\|x_0\|}{\|\hat{x}_m\|}\right).$$

Provided that the factor dependent on ν in the right-hand side of the inequality is not large, the adaptive variant of Simpler GMRES is backward stable. It means that whenever the updated residual r_m is small enough, the approximate solution $\hat{x}_m$ is an exact solution of $(A + \Delta A)x_m = b + \Delta b$ with slightly perturbed data $A + \Delta A$ and $b + \Delta b$, where $\|\Delta A\| = O(u)\|A\|$ and $\|\Delta b\| = O(u)\|b\|$.

In the inequality (2.8) of Corollary 2.7 we can find a quasi-optimal value of $\nu = \nu_{\text{opt}}$ minimizing the right-hand side of the bound (i.e., not the actual value of $\kappa(Z_m)$). It is clear that $q - 1 \leq m$, so

$$\kappa(Z_m) \leq \frac{2\sqrt{2}}{\nu^m}\frac{1+\nu}{1-\nu}. \tag{2.9}$$

The value of ν minimizing the right-hand side of (2.9) is given by

$$\nu_{\text{opt}}(m) = \frac{\sqrt{1+m^2}-1}{m}.$$

It can be shown that the first term $[\nu_{\text{opt}}(m)]^{-m}$ grows with m and approaches $e \approx 2.7183$ as $m \to \infty$. For the second term we have $\frac{1+\nu_{\text{opt}}(m)}{1-\nu_{\text{opt}}(m)} \sim 2m$ with $m \to \infty$. Hence the quasi-optimal bound in (2.9) behaves like

$$\kappa(Z_m) = O(m) \qquad \text{for} \qquad m \to \infty.$$

The threshold parameter $\nu_{\text{opt}}(m)$ is asymptotically reaching the value 1 for growing m, where m can be associated with the maximum number of iterations or the restart parameter. We observed in numerical experiments that $\nu_{\text{opt}}(m)$ minimizing the right-hand side of (2.9) does not always lead to optimal conditioning of the basis and the smaller value, say $\nu = 0.9$, can do better. On the other hand, we have shown that the quasi-optimal value $\nu_{\text{opt}}(m)$ leads to at worst linearly growing $\kappa(Z_m)$.

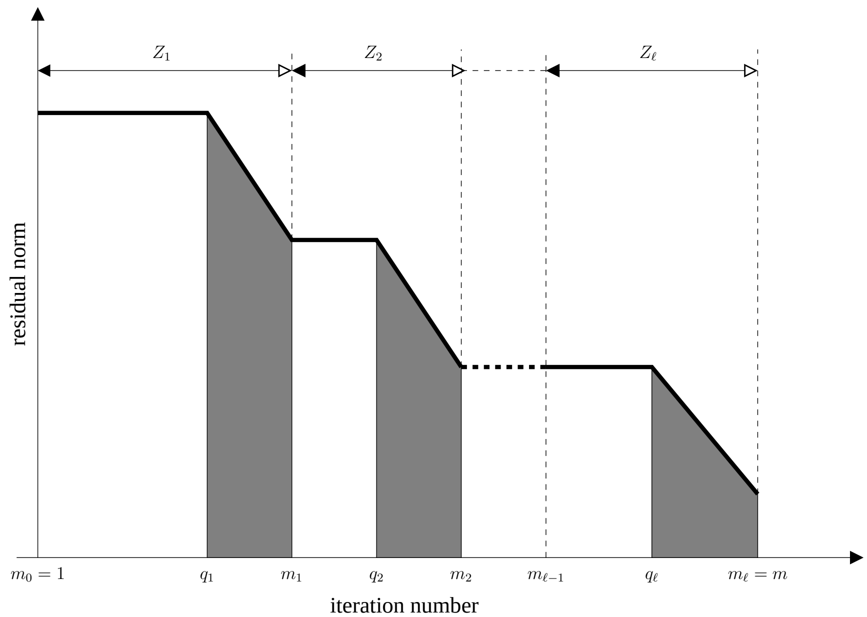

FIGURE 1. Multiple switching between the Simpler GMRES basis and the residual basis in the case of the occurrence of local stagnations in the residual norm. In the run of adaptive Simpler GMRES, the white areas correspond to the Simpler GMRES basis, while the gray areas correspond to the normalized residual basis of RB-SGMRES.

Theorem 2.6 can be generalized to the case with multiple switching between the bases from Simpler GMRES basis and RB-SGMRES. Such situation is more realistic since it can happen that there are some intermediate stagnations in the residual norm; see Figure 1 for the illustration and the explanation of the notation in the corollary below.

COROLLARY 2.8. *Let* m *be such that* $\dim \mathcal{K}_m(A, r_0) = m$ *and let* Z_m *has the block form* $Z_m = [\widetilde{Z}_1, \ldots, \widetilde{Z}_\ell, \widetilde{r}_{m-1}]$*, where*

$$\widetilde{Z}_j := [\widetilde{r}_{m_{j-1}-1}, v_{m_{j-1}}, \ldots, v_{q_j-1}, \widetilde{r}_{q_j}, \ldots, \widetilde{r}_{m_j-2}] \in \mathbb{R}^{N\times(m_j - m_{j-1})},$$

$m_0 = 1$*,* $m_\ell = m$*,* $m_{j-1} < q_j < m_j$ *and* $0 < \|r_{m_j-1}\| < \cdots < \|r_{q_j-1}\|$ *for* $j = 1, \ldots, \ell$*. Then*

$$\max_{j=1,\ldots,\ell} \delta_{m_{j-1},q_j} \leq \kappa(Z_m) \leq \gamma(\{q_j, m_j\}_{j=1}^{\ell}) \max_{j=1,\ldots,\ell} \delta_{m_{j-1},q_j}, \tag{2.10}$$

where

$$\gamma(\{q_j, m_j\}_{j=1}^{\ell}) := \left(1 + \sum_{j=1}^{\ell}(m_j - q_j)\right)^{\frac{1}{2}} \left(1 + \sum_{j=1}^{\ell}\sum_{i=q_j}^{m_j-1} \frac{\|r_{i-1}\|^2 + \|r_i\|^2}{\|r_{i-1}\|^2 - \|r_i\|^2}\right)^{\frac{1}{2}}.$$

PROOF. As in Theorem 2.6 we use (1.5) repeatedly in order to relate Z_m (which forms the basis of $\mathcal{K}_m(A, r_0)$ due to the assumptions of the corollary) to the orthonormal basis $[V_{m-1}, \widetilde{r}_{m-1}]$. In each $\widetilde{Z}_j$ we relate the first residual $\widetilde{r}_{m_{j-1}-1}$ to $\widetilde{r}_{q_j-1}$ using the vectors $v_{m_{j-1}}, \ldots, v_{q_j-1}$. Thus we obtain

$$
\begin{aligned}
\widetilde{Z}_j &= [\widetilde{r}_{m_{j-1}-1}, v_{m_{j-1}}, \ldots, v_{q_j-1} \,|\, \widetilde{r}_{q_j}, \ldots, \widetilde{r}_{m_j-2}] \\
&= [v_{m_{j-1}}, \ldots, v_{q_j-1}, \widetilde{r}_{q_j-1} \,|\, \widetilde{r}_{q_j}, \ldots, \widetilde{r}_{m_j-2}] \mathrm{diag}(\widetilde{B}_{m_{j-1},q_j}, I_{m_j-q_j-1}) \\
&= \widetilde{Y}_j B_{m_{j-1},q_j},
\end{aligned}
$$

where $\widetilde{Y}_j := [v_{m_{j-1}}, \ldots, v_{q_j-1}, \widetilde{r}_{q_j-1}, \widetilde{r}_{q_j}, \ldots, \widetilde{r}_{m_j-2}]$, $\widetilde{B}_{m_{j-1},q_j}$ is defined in Lemma 2.3, and $B_{m_{j-1},q_j} := \mathrm{diag}(\widetilde{B}_{m_{j-1},q_j}, I_{m_j-q_j-1})$. Hence it follows that

$$
Z_m = [\widetilde{Y}_1, \ldots, \widetilde{Y}_\ell, \widetilde{r}_{m-1}] B_m, \tag{2.11}
$$

with the matrix B_m defined by $B_m := \mathrm{diag}(B_{m_0,q_1}, \ldots, B_{m_{\ell-1},q_\ell}, 1)$. We now relate $[\widetilde{Y}_1, \ldots, \widetilde{Y}_\ell, \widetilde{r}_{m-1}]$ to $[V_{m-1}, \widetilde{r}_{m-1}]$, More precisely, we express the columns of $[V_{m-1}, \widetilde{r}_{m-1}] = [\widetilde{V}_1, \ldots, \widetilde{V}_\ell, \widetilde{r}_{m-1}]$ in terms of $[\widetilde{Y}_1, \ldots, \widetilde{Y}_\ell, \widetilde{r}_{m-1}]$, where $\widetilde{V}_j := [v_{m_{j-1}}, \ldots, v_{m_j-1}]$. From (1.5) we have

$$
[r_{q_j-1}, \ldots, r_{m_j-1}] L_{m_j-q_j+1, m_j-q_j} = [v_{q_j}, \ldots, v_{m_j-1}] \mathrm{diag}(a_{q_j,m_j-1}). \tag{2.12}
$$

Here $L_{m_j-q_j+1,m_j-q_j}$ is defined as $L_{m_j-q_j+1,m_j-q_1} := [L^T_{m_j-q_j}, -e_{m_j-q_j}]^T$, where $e_{m_j-q_j}$ stands for the last column of $I_{m_j-q_j}$. From (2.12) it follows that

$$
[v_{q_j}, \ldots, v_{m_j-1}] = [\widetilde{r}_{q_j-1}, \ldots, \widetilde{r}_{m_j-2}] \widetilde{G}_{q_j,m_j} - \frac{1}{\alpha_{m_j-1}} r_{m_j-1} e^T_{m_j-q_j}, \tag{2.13}
$$

with $\widetilde{G}_{q_j,m_j}$ defined by $\widetilde{G}_{q_j,m_j} := \mathrm{diag}(r_{q_j-1,m_j-2}) L_{m_j-q_j} [\mathrm{diag}(a_{q_j,m_j-1})]^{-1}$. Since r_{m_j-1} (or $\widetilde{r}_{m_j-1}$) is not in $[Y_1, \ldots, Y_\ell, \widetilde{r}_{m-1}]$ (for $j = 1, \ldots, \ell-1$), we express it in terms of the residual $r_{q_{j+1}-1}$ and the vectors $v_{m_j}, \ldots, v_{q_{j+1}-1}$ as

$$
r_{m_j-1} = r_{q_{j+1}-1} + [v_{m_j}, \ldots, v_{q_{j+1}-1}] a_{m_j,q_{j+1}-1} = \widetilde{Y}_{j+1} \begin{bmatrix} a_{m_j,q_{j+1}-1} \\ \rho_{q_{j+1}-1} \\ \mathbf{0}_{m_{j+1}-q_{j+1}-1} \end{bmatrix}
$$

for $j = 1, \ldots, \ell-1$. Here $\mathbf{0}_{m_{j+1}-q_{j+1}-1}$ denotes the column zero vector of the indicated dimension. From (2.13) we hence obtain

$$
\begin{aligned}
\widetilde{V}_j &= \widetilde{Y}_j \,\mathrm{diag}(I_{q_j-m_{j-1}}, \widetilde{G}_{q_j,m_j}) - \frac{1}{\alpha_{m_j-1}} r_{m_j-1} e^T_{m_j-m_{j-1}} \\
&= \widetilde{Y}_j \,\mathrm{diag}(I_{q_j-m_{j-1}}, \widetilde{G}_{q_j,m_j}) - \frac{1}{\alpha_{m_j-1}} \widetilde{Y}_{j+1} \begin{bmatrix} a_{m_j,q_{j+1}-1} \\ \rho_{q_{j+1}-1} \\ \mathbf{0}_{m_{j+1}-q_{j+1}-1} \end{bmatrix} e^T_{m_j-m_{j-1}} \\
&= \widetilde{Y}_j \widetilde{D}_{j,j} + \widetilde{Y}_{j+1} \widetilde{D}_{j+1,j}, \qquad j = 1, \ldots, \ell-1,
\end{aligned} \tag{2.14}
$$

and

$$\begin{aligned}\widetilde{V}_\ell &= \widetilde{Y}_\ell \operatorname{diag}(I_{q_\ell - m_{\ell-1}}, \widetilde{G}_{q_\ell, m_\ell}) - \frac{\rho_{m_\ell - 1}}{\alpha_{m_\ell - 1}} \widetilde{r}_{m_\ell - 1} e^T_{m_\ell - m_{\ell-1}} \\ &= \widetilde{Y}_\ell \widetilde{D}_{\ell,\ell} + \widetilde{r}_{m-1} \widetilde{D}_{\ell+1,\ell}.\end{aligned} \tag{2.15}$$

Combining (2.14) and (2.15), we get

$$[V_{m-1}, \widetilde{r}_{m-1}] = [\widetilde{Y}_1, \ldots, \widetilde{Y}_\ell, \widetilde{r}_{m-1}] D_m, \tag{2.16}$$

where D_m is a lower block bidiagonal matrix in the form

$$D_m := \begin{bmatrix} \widetilde{D}_{1,1} & & & & \\ \widetilde{D}_{2,1} & \widetilde{D}_{2,2} & & & \\ & \ddots & \ddots & & \\ & & & \widetilde{D}_{\ell,\ell} & \\ & & & \widetilde{D}_{\ell+1,\ell} & 1 \end{bmatrix}.$$

Using (2.11) and (2.16) we get the desired relation $Z_m = [V_{m-1}, \widetilde{r}_{m-1}] D_m^{-1} B_m$. Since $[V_{m-1}, \widetilde{r}_{m-1}]$ has orthonormal columns, it follows that

$$\kappa(B_m) \le \kappa(Z_m) \le \kappa(D_m)\kappa(B_m). \tag{2.17}$$

Due to (2.4) we have

$$\kappa(B_m) = \max_{j=1,\ldots,\ell} \kappa(\widetilde{B}_{m_{j-1}, q_j}) = \max_{j=1,\ldots,\ell} \delta_{m_{j-1}, q_j}. \tag{2.18}$$

To estimate the norm of D_m we find a permutation matrix Π such that

$$\Pi D_m \Pi^T = \begin{bmatrix} I & 0 \\ 0 & \widetilde{D}_m \end{bmatrix}, \tag{2.19}$$

where we moved the identities from the matrices $\widetilde{D}_{j,j}$ into the leading principal identity of $\Pi D_m \Pi^T$. It hence follows that $\|D_m\| = \max\{1, \|\widetilde{D}_m\|\} \le \max\{1, \|\widetilde{D}_m\|_F\}$. Since

$$\begin{aligned}\|\widetilde{D}_m\|_F^2 &= 1 + \sum_{j=1}^{\ell} (\|\widetilde{G}_{q_j, m_j}\|_F^2 + \|\widetilde{D}_{j+1,j}\|_F^2) \\ &= 1 + \sum_{j=1}^{\ell} \sum_{i=q_j}^{m_j - 1} \frac{\rho_{i-1}^2 + \rho_i^2}{\rho_{i-1}^2 - \rho_i^2},\end{aligned}$$

and $\|\widetilde{D}_m\|_F \ge 1$, we can bound the norm of the matrix D_m as

$$\|D_m\|^2 \le 1 + \sum_{j=1}^{\ell} \sum_{i=q_j}^{m_j - 1} \frac{\rho_{i-1}^2 + \rho_i^2}{\rho_{i-1}^2 - \rho_i^2}. \tag{2.20}$$

The inverse of D_m can be computed either directly from D_m or making the relation between $[\widetilde{Y}_1, \ldots, \widetilde{Y}_\ell, \widetilde{r}_{m-1}]$ and $[V_{m-1}, \widetilde{r}_{m-1}]$ in the opposite direction, which is more simple. Taking into account (1.5) we can express the residuals $\widetilde{r}_k$ in $\widetilde{Y}_j$ $(j = 1, \ldots, \ell)$ using $\widetilde{r}_{m-1}$ and the corresponding direction vectors $v_{k+1}, \dots, v_{m-1}$ from V_{m-1}. But since $[V_{m-1}, \widetilde{r}_{m-1}]$ has orthonormal columns and the residuals in $\widetilde{Y}_j$ are normalized, it follows that their coordinates in the basis $[V_{m-1}, \widetilde{r}_{m-1}]$ have unit norms. Considering the same permutation matrix Π as in (2.19) we can show that the columns of the lower triangular matrix $\widetilde{D}_m^{-1}$ contain the permuted coordinates of the residuals in $\widetilde{Y}_j$ $(j = 1, \dots, \ell)$ in the basis $[V_{m-1}, \widetilde{r}_{m-1}]$, and thus they have unit norms. Hence we obtain the bound

$$\|D_m^{-1}\|^2 \leq 1 + \sum_{i=1}^{\ell} (m_j - q_j). \tag{2.21}$$

Combining (2.17), (2.18), (2.20), and (2.21) concludes the proof. $\square$

3. Numerical experiments

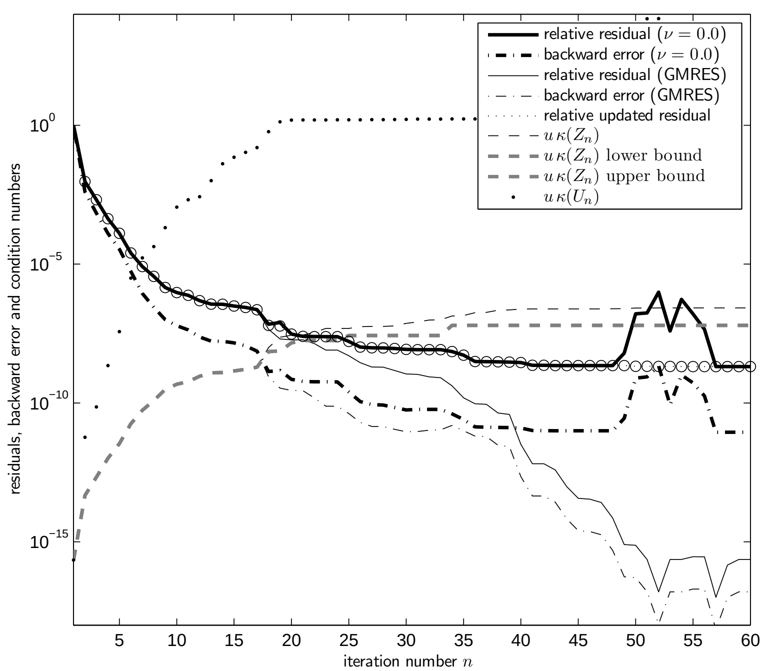

FIGURE 2. Test problem with `FS1836` and $b = A[1, \dots, 1]^T$ solved by Simpler GMRES ($\nu = 0$): relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

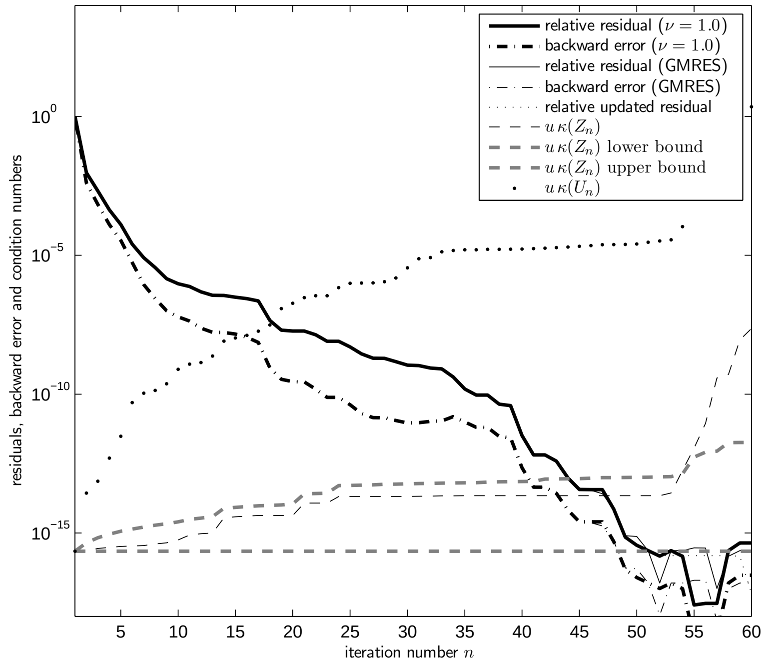

FIGURE 3. Test problem with `FS1836` and $b = A[1,\ldots,1]^T$ solved by RB-SGMRES ($\nu = 1$): relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

We illustrate our theoretical results on numerical examples selected from Matrix Market [**2**] and performed in MATLAB® using double precision arithmetic with $u \approx 10^{-16}$. Results for the adaptive Simpler GMRES and classical implementation of GMRES applied to the system with the matrix `FS1836` ($N = 183$, $\|A\| \approx 1.2 \cdot 10^9$, $\kappa(A) \approx 1.7 \cdot 10^{11}$) are illustrated on Figures 2–7. The right-hand side vector b is equal either to $A[1,\ldots,1]^T$ (Figures 2–4) or to the left singular vector corresponding to the smallest singular value of A (Figures 5–7). On each plot we show the relative true residual norms (bold solid lines) and normwise backward errors (bold dash-dotted lines) corresponding to the approximate solutions x_n computed by adaptive Simpler GMRES with three considered values of the threshold parameter: $\nu = 0$ (Figures 2 and 5) where adaptive Simpler GMRES is equivalent to Simpler GMRES of Walker and Zhou [**15**], $\nu = 1$ (Figures 3 and 6) leading to RB-SGMRES [**7**], and $\nu = 0.9$ (Figures 4 and 7). In each plot we also

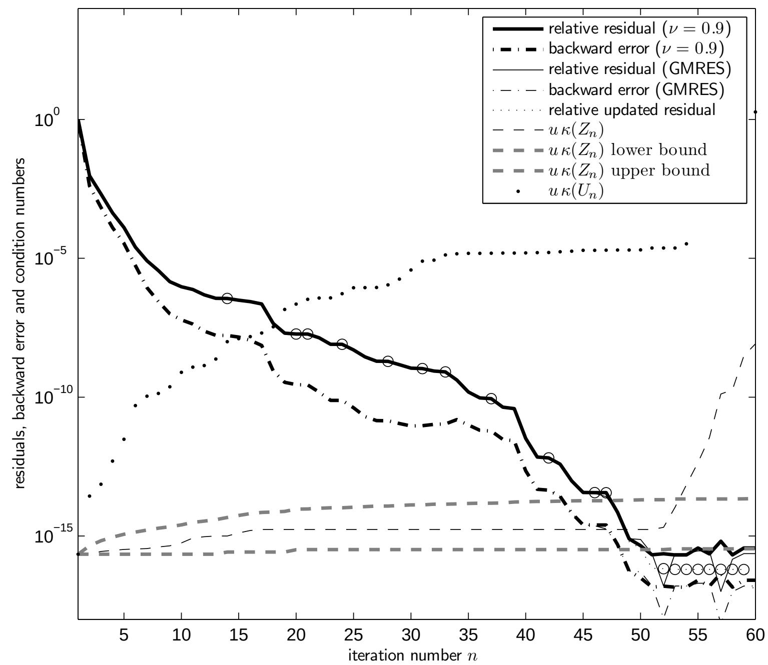

FIGURE 4. Test problem with FS1836 and $b = A[1, \ldots, 1]^T$ solved by adaptive SGMRES with $\nu = 0.9$: relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

include the relative residual norms and normwise backward errors for approximate solutions computed by classical GMRES of Saad and Schultz [12] (solid and dash-dotted lines). The relative norms of the updated residual r_n are plotted by dotted lines. The actual values of condition numbers of Z_n and U_n are plotted by dashed lines and dots, respectively. The estimates on $\kappa(Z_n)$ computed using (2.10) are plotted by gray dashed lines. Both the upper and lower bounds are quite tight until the maximum attainable accuracy is reached. The iteration steps, where the Simpler GMRES basis is used, are indicated by circles in the figures.

It is clear from our experiments that both Simpler GMRES and RB-SGMRES may lead to low accuracy of the computed approximate solution due to the ill-conditioning of Z_n in the case of a rapid initial convergence with $b = A[1, \ldots, 1]^T$ or long initial stagnation in the residual norm with b equal to the left singular vector corresponding to the smallest singular value, respectively; see Figures 2 and 6. However, as can be observed from

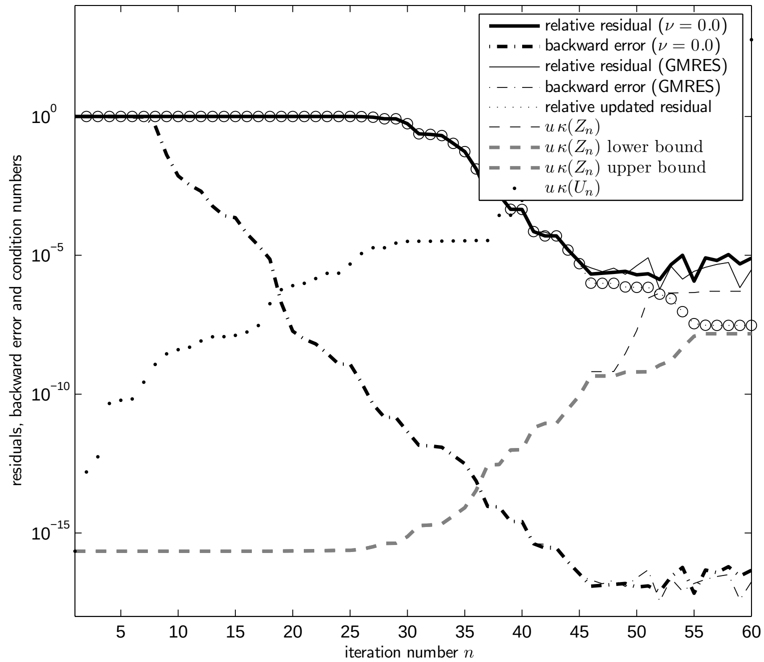

FIGURE 5. Test problem with FS1836 and b equal to the left singular vector corresponding to the smallest singular value of A solved by Simpler GMRES ($\nu = 0$): relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

Figures 4 and 7, the adaptive version of Simpler GMRES with the threshold value $\nu = 0.9$ leads to reasonably conditioned bases for both right-hand sides.

Figure 8 shows the dependence of $\kappa(Z_m)$ with respect to the threshold parameter ν for several real problems with various condition numbers and of dimensions from 225 up to 1080. For each problem we stop the method at the iteration step m, where the normwise backward error associated with the approximate solution x_m dropped below the level 10^{-14}. Note that for each problem and each value of ν varying between 0 and 1, adaptive version of Simpler GMRES was able to reach such high accuracy and thus the ill-conditioning of the basis does not necessarily lead to a low level of the maximum attainable accuracy. This phenomenon can be explained using (2.2), which shows that large $\kappa(Z_k)$ can be damped with the small residual norm $\|r_{k-1}\|$. We were not, however, able to prove this for the normwise

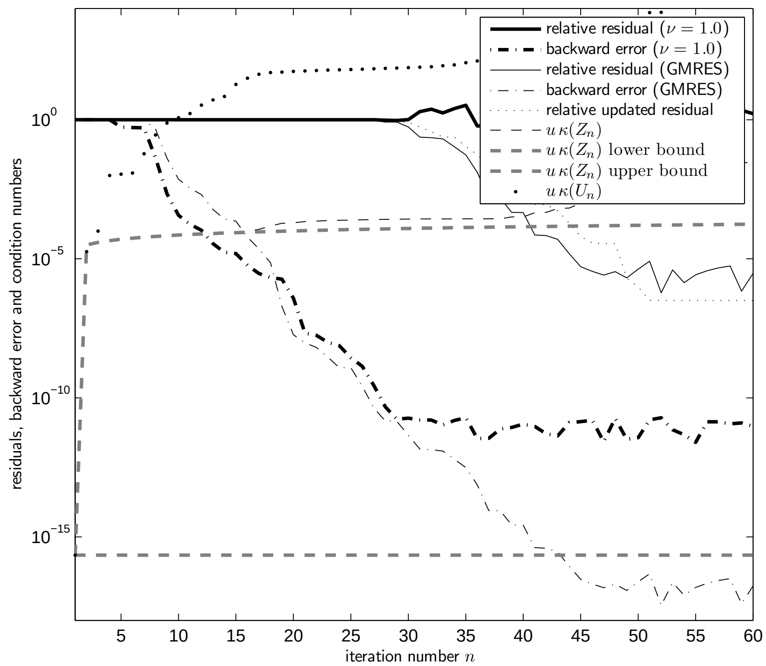

FIGURE 6. Test problem with `FS1836` and b equal to the left singular vector corresponding to the smallest singular value of A solved by RB-SGMRES ($\nu = 1$): relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

backward error in [7]. Nevertheless, as we have shown there are examples where ill-conditioning of Z_m leads to low maximum attainable accuracy of the computed approximate solution; cf. Figures 2 and 6. It is therefore reasonable to keep conditioning of the basis on a reasonably small level and consequently to keep the columns of Z_m linearly independent as well as the matrix U_m numerically nonsingular. It is clear from Figure 8 that, for our examples, the value of ν close (but not equal) to 1 leads to a nearly optimal conditioning of Z_m in adaptive Simpler GMRES and, therefore, the residual vectors should be preferred in Z_m even for a moderate intermediate residual norm decrease. The important issue however is here to preserve the linear independence of Z_m. Therefore, such adaptive switches seems to be useful whenever the Simpler GMRES method is used.

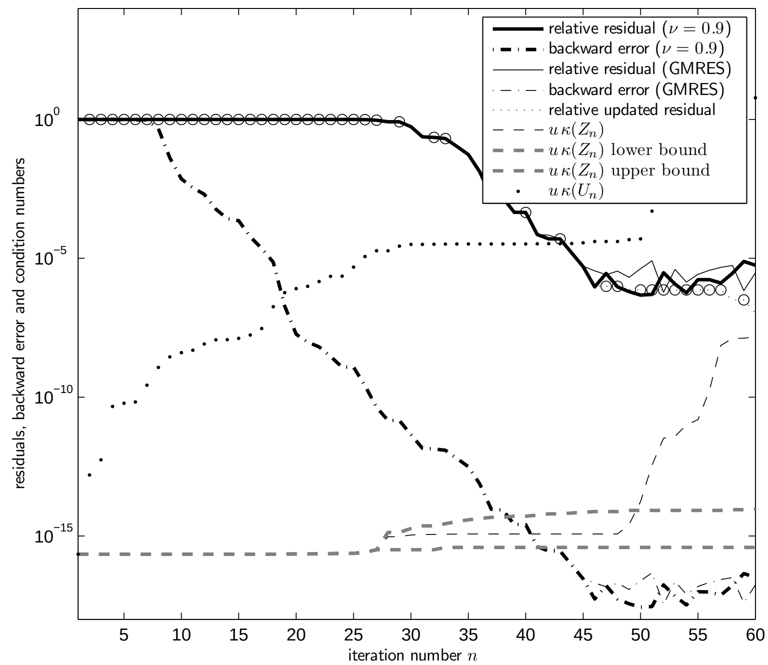

FIGURE 7. Test problem with `FS1836` and b equal to the left singular vector corresponding to the smallest singular value of A solved by adaptive SGMRES with $\nu = 0.9$: relative residual norms and normwise backward errors (bold solid and dash-dotted lines), relative residual norms and normwise backward errors of GMRES (solid and dash-dotted lines), relative updated residual norms (dotted lines), condition numbers $\kappa(Z_n)$ and $\kappa(U_n)$ multiplied by unit roundoff u (dashed lines and dots) including the bounds on $u\kappa(Z_n)$ (gray dashed lines).

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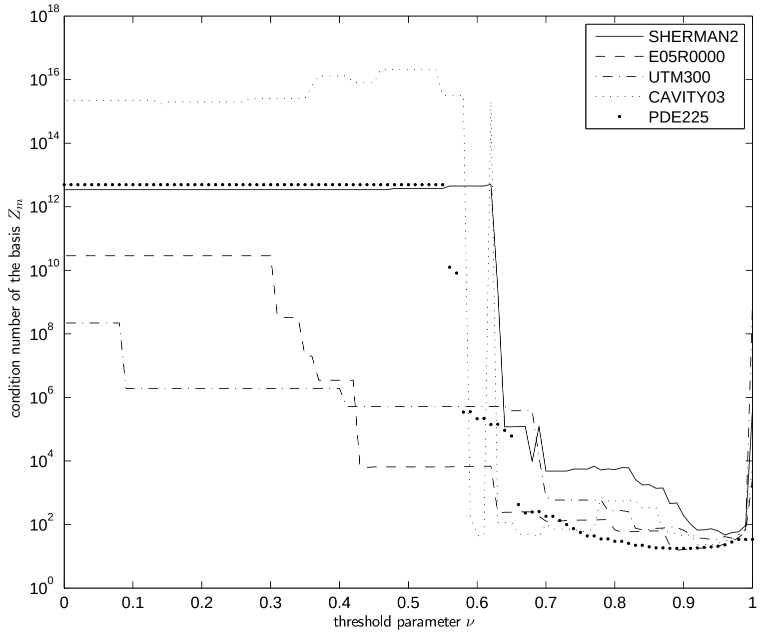

FIGURE 8. The dependence of the condition number of Z_m on the choice of the threshold parameter ν for various matrices and right-hand sides taken from Matrix Market.

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