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On the stable implementation of the generalized minimal error method

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Abstract

The paper reviews several implementations of the Generalized minimal error method (GMERR method) for solving nonsymmetric systems of linear equations that minimize the Euclidean norm of the error in the related generalized Krylov subspace. We show the relation to the methods in the symmetric indefinite case. A new variant of the GMERR method is proposed and the stable implementation based on the Householder transformations is discussed. Numerical stability of the most frequent implementations is analyzed and the theoretical results are illustrated by numerical examples. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let $Ax = b$ be a system of linear algebraic equations, where A is a real nonsingular matrix of order N and b, x are N-dimensional real vectors.

Among the broad variety of iterative Krylov space methods for the solution of this system (surveys can be found e.g. in [8, 12, 24, 5]) we consider the method that starts with an initial approximation x_0 and generates the nth approximate solution x_n in the form

$$x_n \in x_0 + A^{\mathrm{T}} K_n(A^{\mathrm{T}}, r_0), \tag{1}$$

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satisfying the error minimization property

$$\|x - x_n\| = \min_{u \in x_0 + A^T K_n(A^T, r_0)} \|x - u\|, \tag{2}$$

where $r_0 = b - Ax_0$ is the initial residual and $A^T K_n(A^T, r_0) \equiv K_n(A^T, A^T r_0)$ is the nth generalized Krylov subspace generated by the transpose of the matrix A and the vector $A^T r_0$

$$K_n(A^T, A^T r_0) = \text{span } \{A^T r_0, A^T(A^T r_0), \ldots, (A^T)^{n-1}(A^T r_0)\}. \tag{3}$$

It can be easily shown that the error minimization property (2) is equivalent to the condition that the nth error $x - x_n$ orthogonal to the space $A^T K_n(A^T, r_0)$, i.e.

$$x - x_n \perp A^T K_n(A^T, r_0) \equiv b - Ax_n \perp K_n(A^T, r_0). \tag{4}$$

The approximation given by conditions (1) and (2) always exists and is unique. The convergence of the error norms is assured to be monotonic. The GMERR method, however, does not have, in general, the finite termination property. In general nonsymmetric case one can construct examples for which the GMERR method terminates with the nonzero residual norm at the iteration $n < N$. Moreover it was shown in [34] that GMERR without restarts converges for every right-hand side if and only if the system matrix is normal.

For A symmetric, several algorithms generating the approximations determined by (2) were proposed and discussed in [10, 23, 17, 6]. Although these methods are mathematically equivalent, their behavior in the finite precision arithmetic may substantially differ. It was reported that some of them are numerically unstable and the most efficient and stable ones were proposed.

The first method for solving symmetric indefinite systems which is characterized by the minimal error property

$$\|x - x_n\| = \min_{u \in x_0 + K_n(A, Ar_0)} \|x - u\| \tag{5}$$

is the orthogonal direction (OD) method proposed by Fridman in [10]. However, this implementation is unstable (see e.g. [23, 24]). The first numerically stable algorithms for symmetric indefinite systems were proposed by Paige and Saunders in [17]. They considered the symmetric Lanczos method to generate an orthonormal basis of the Krylov subspace $K_n(A, r_0)$ and using this basis proposed a stable algorithm SYMMLQ which produces at every step an auxiliary approximation x_n^L satisfying the minimal error property (5).

Another approach was taken by Fletcher [6] who described the Bi-CG algorithm for nonsymmetric systems and then modified its symmetric variant to obtain the OD method by Fridman. This algorithm computes the orthogonal, but not normalized, basis of the subspace $K_n(A, Ar_0)$ and it faces some numerical difficulties. A stabilization of the OD method, named STOD, was proposed by Freund and Stoer [23]. Theoretical equivalence of the SYMMLQ method and OD method developed from the Bi-CG algorithm was already known by Fletcher [6]. Another stable implementation of the symmetric indefinite minimal error method (ME) was presented by Freund in [7].

In the nonsymmetric case, the concept of error minimization was introduced in [30], where the Generalized minimal error method (GMERR) has been proposed. In this paper, we describe the original implementation and propose other variants of the GMERR method, where the approximate solution in the form (1) is constructed via different set of orthonormal vectors that span the generalized Krylov space (3) and the Krylov space $K_n(A^T, r_0)$ generated by the transpose of the matrix

A and the initial residual r_0. We show their relation to the methods in the symmetric indefinite case and we investigate the numerical stability of the implementation based on the Householder transformations.

The paper is organized as follows. In Section 2, we review the original implementation of the GMERR method and show some theoretical results. Section 3 is devoted to other variants of GMERR based on the orthonormal bases of the generalized Krylov space $A^{\mathrm{T}}K_n(A^{\mathrm{T}}, r_0)$ and the Krylov space $K_n(A^{\mathrm{T}}, r_0)$. The connection to symmetric methods is discussed and some questions concerning their numerical stability are examined. In Section 4, a new stable implementation of GMERR based on Householder transformations is proposed and discussed. Finally, we present several numerical examples and give some conclusions.

2. Generalized minimal error method (GMERR)

The original implementation, presented in [30] is based on the generating two sequences of vectors $w_1, \ldots, w_n$ and $u_1, \ldots, u_n$ and is implemented as follows:

Algorithm 2.1. Generalized minimal error method (GMERR)

$$
\begin{aligned}
&x_0, r_0 = b - Ax_0, w_1 = r_0/\|A^{\mathrm{T}}r_0\|, u_1 = A^{\mathrm{T}}w_1,\\
&n = 1, 2, \ldots,\\
&x_n = x_{n-1} + [(b, w_n) - (x_{n-1}, u_n)]u_n,\\
&\alpha_{j,n} = -(A^{\mathrm{T}}u_n, u_j),\ j = 1, \ldots, n,\\
&\tilde{u}_{n+1} = A^{\mathrm{T}}u_n + \sum_{j=1}^{n} \alpha_{j,n}u_j,\\
&\tilde{w}_{n+1} = u_n + \sum_{j=1}^{n} \alpha_{j,n}w_j,\\
&w_{n+1} = \tilde{w}_{n+1}/\|\tilde{u}_{n+1}\|,\\
&u_{n+1} = \tilde{u}_{n+1}/\|\tilde{u}_{n+1}\|.
\end{aligned}
$$

From the algorithm 2.1 it is clear that the vectors $u_1, \ldots, u_n$ build up the orthonormal basis of the subspace $A^{\mathrm{T}}K_n(A^{\mathrm{T}}, r_0)$, the vectors $w_1, \ldots, w_n$ build up the AA^{T}-orthonormal basis of the subspace $K_n(A^{\mathrm{T}}, r_0)$ and both bases are generated by the scheme equivalent to the classical Gram–Schmidt orthogonalization. It is well known, that this orthogonalization technique is numerically unreliable and may be replaced by more stable modified Gram–Schmidt scheme or even iterated classical or modified Gram–Schmidt orthogonalization. For details of different orthogonalizations which can be used we refer to [2, 20, 11, 15].

If we denote the AA^{T}-orthonormal basis $W_n = [w_1, \ldots, w_n]$ of the Krylov space $K_n(A^{\mathrm{T}}, r_0)$, then the recurrences from the algorithm 2.1 can be written as a recursive column-by-column QR decomposition of the matrix $[r_0, A^{\mathrm{T}}W_{n-1}]$ assuming the innerproduct $(u, v)_{AA^{\mathrm{T}}} = u^{\mathrm{T}}AA^{\mathrm{T}}v$

$$
[r_0, A^{\mathrm{T}}W_{n-1}] = W_nG_n,\ W_n^{\mathrm{T}}AA^{\mathrm{T}}W_n = I_n \tag{6}
$$

with an upper triangular matrix G_n. The nth approximate solution x_n can be written in the form

$$x_n = x_0 + A^{\mathrm{T}} W_n f_n \tag{7}$$

and condition (4) which is equivalent to the error minimization condition (2) implies

$$f_n = (A^{\mathrm{T}} W_n)^{\mathrm{T}}(x - x_0) = W_n^{\mathrm{T}} r_0. \tag{8}$$

Then the approximation solution x_n and the nth residual can be updated step by step

$$x_n = x_{n-1} + (r_0, w_n) A^{\mathrm{T}} w_n, \tag{9}$$

$$r_n = r_{n-1} - (r_0, w_n) A A^{\mathrm{T}} w_n. \tag{10}$$

From condition (4) the inner product (r_0, w_n) in (9) and (10) can be replaced by (r_{n-1}, w_n) or, when the residual vector not computed, by $(b, w_n) - (x_{n-1}, A^{\mathrm{T}} w_n)$.

By (9) GMERR can be formulated so that only one matrix–vector multiplication is needed per iteration step if the residuals are not calculated. For realistic problems the matrix–vector multiplication dominates the work of the other operations like dot products and triadic expressions. As matrix–vector multiplications and triadic operations can be efficiently implemented on vector and parallel machines [31], GMERR is well suited for today's supercomputers.

A problem for GMERR is the controlling of the convergence because the errors decrease but they cannot be calculated. If we observe the norm of the residuals, it may increase or may oscillate even the errors decrease. Moreover, an additional matrix–vector multiplication is needed for the calculation of the residuals. Therefore, we propose to calculate the residuals only every mth step (e.g. $m = 20$) and to apply residual-minimizing smoothing [14, 22, 28, 33]. The norm of the smoothed residuals can be used for control.

The exact variant presented here cannot be calculated with a short recurrence unless certain favorable conditions are valid. For example for A symmetric, the calculation of the u_n and w_n is possible with a short recurrence. For practical applications with large and sparse systems a restarted version has to be applied. Minimization properties corresponding to (2) are valid in the restart interval.

We remark that the original GMERR definition [30] is a little more general than stated in (1) and (2). The approximation is chosen such that

$$x_n \in x_0 + A^{\mathrm{T}} K_n(A^{\mathrm{T}}, w_1), \tag{11}$$

where w_1 is arbitrary, and

$$\|x - x_n\| = \min_{u \in x_0 + A^{\mathrm{T}} K_n(A^{\mathrm{T}}, w_1)} \|x - u\|. \tag{12}$$

The optimal choice of w_1 would be $w_1 = A^{-T}(x - x_0) = A^{-T} A^{-1} r_0$ because then the solution is obtained in the first step following from (12). But the calculation of this optimal w_1 would be as difficult as the solution of the original system. A natural choice for w_1 is the here considered $w_1 = r_0 / \|A^{\mathrm{T}} r_0\|$.

We recognize for GMERR a similar structure as for GMRES [20]. Both methods distinguish in the Krylov space chosen for the approximations and in the minimization principle. GMRES minimizes the residuals instead of the errors and converges to the exact solution in a finite number of iteration steps. For symmetric matrices the spanned Krylov spaces are close and numerical tests confirm that the methods behave in a similar way. We also remark that if we apply GMERR to the

normal equations $A^{\mathrm{T}}Ax = A^{\mathrm{T}}b$, then we obtain a method mathematically equivalent to Craig's method CGNE [3].

The analysis of the convergence of GMERR is not yet settled. At least we can state the following result for normal matrices:

Theorem 2.1. *Let $\sigma(A)$ be the spectrum of A, Π_{n-1} the set of all polynomials of degree $n-1$ with the constant coefficient equal to unity, i.e. $p(0)=1$ for $p \in \Pi_{n-1}$. If A is normal, then for the errors of GMERR*

$$\|x - x_n\| \leqslant \min_{p \in \Pi_{n-1}} \max_{\lambda \in \sigma(A)} |(1 - p'(0)\lambda)p(\lambda)| \|x - x_0\| \tag{13}$$

is satisfied, where p' denotes the derivative of the polynomial p.

Proof. As A is normal, there exists an orthonormal matrix C and a diagonal matrix D such that $A = C^{-1}DC$. From Eq. (2) follows:

$$\begin{aligned}
\|x - x_n\| &= \min_{\beta_1,\dots,\beta_{n-1}} \left\| x - x_0 + \sum_{i=1}^{n-1} \beta_i (A^{\mathrm{T}})^i r_0 \right\| \\
&= \min_{\beta_1,\dots,\beta_{n-1}} \left\| x - x_0 + \sum_{i=1}^{n-1} \beta_i (A^{\mathrm{T}})^i A(x - x_0) \right\| \\
&= \min_{\beta_1,\dots,\beta_{n-1}} \left\| x - x_0 + \sum_{i=1}^{n-1} \beta_i (C^{\mathrm{T}} D^{\mathrm{T}} C^{-T})^i C^{-1} DC(x - x_0) \right\| \\
&\leqslant \min_{\beta_1,\dots,\beta_{n-1}} \left\| \sum_{i=1}^{n-1} \beta_i C^{\mathrm{T}} (D^{\mathrm{T}})^i C^{-\mathrm{T}} C^{-1} DC + I \right\| \|x - x_0\| \\
&\leqslant \min_{\beta_1,\dots,\beta_{n-1}} \|C^{-1}\| \left\| \sum_{i=1}^{n-1} \beta_i CC^{\mathrm{T}} (D^{\mathrm{T}})^i C^{-T} C^{-1} D + I \right\| \|C\| \|x - x_0\| \\
&= \min_{\beta_1,\dots,\beta_{n-1}} \left\| \sum_{i=1}^{n-1} \beta_i (D^{\mathrm{T}})^i D + I \right\| \|x - x_0\| \\
&\quad \text{as } C \text{ is orthonormal} \\
&\leqslant \min_{\beta_1,\dots,\beta_{n-1}} \max_{\lambda \in \sigma(A)} \left| \sum_{i=1}^{n-1} \beta_i \lambda^{i+1} + 1 \right| \|x - x_0\|,
\end{aligned}$$

as D is a diagonal matrix consisting of the eigenvalues. The polynomial in the last inequality is of degree n, the constant coefficient equal to unity and the first power of λ is missing. Thus, it can be written as $(1 - p'(0)\lambda)p(\lambda)$, where $p \in \Pi_{n-1}$. □

A direct consequence of Theorem 2.1 is that GMERR converges fast for normal matrices if the eigenvalues are clustered. By substituting the polynomial p in (13) by a normalized Chebyshev polynomial further results similar to those of residual-minimizing methods involving the condition number of A can be derived. Note that the polynomial $(1 - p'(0)\lambda)p(\lambda)$ in (13) is a polynomial

of degree n, where the first power of λ is missing and the constant coefficient is equal to unity. If $p'(0)=0$, then the polynomial in (13) simplifies. The result for the errors of GMERR is similar to the well known result for the residuals of GMRES [20] applied to normal matrices:

$$\|r_n\| \leqslant \min_{p\in\Pi_n} \max_{\lambda\in\sigma(A)} |p(\lambda)|\|r_0\|. \tag{14}$$

However, if A is similar to a diagonal matrix, we do not obtain for GMERR an analogue to the estimate for GMRES where the right-hand side of (14) is multiplied by the condition number of the eigenvector matrix.

The investigations in [7] show that GMERR is competitive with GMRES if the matrix is symmetric. The residual reduction is slightly better for GMRES while the error reduction is slightly better for GMERR. This could be expected from Theorem 2.1. Theorem 2.1 further suggests that GMERR behaves similar as GMRES also for normal matrices because the estimate is similar to the GMRES estimate (14). For nonnormal matrices there are no theoretical results up to now. Practical tests give a rather confusing impression. There are examples where GMRES works fine while GMERR converges very slowly. There are also few examples where GMERR is very fast but GMRES is very bad. The later presented tests show this behavior.

The valuation becomes more difficult for the restarted variant. For restarted GMRES the iterate is in the same space as for the exact method and, therefore, the restarted version is always worse than the exact. For restarted GMERR the iterate is in a different space than for the exact method. Numerical tests show that restarted GMERR can be sometimes substantially better than the exact method for distinct problems. As regards a valuation of GMERR for non-normal matrices further research is necessary.

3. Other variants of the GMERR method

In this section, we formulate two other variants of the GMERR method based on the generation of the set of orthonormal vectors that span either the generalized Krylov space $K_n(A^T, A^T r_0)$ or the Krylov subspace $K_n(A^T, r_0)$, respectively.

First we consider the formulation of GMERR, which is analogical to the variant of the GMRES method [20] presented by Walker and Lu Zhou (for details see [29]) and which computes an orthonormal basis $Q_n=[q_1,\ldots,q_n]$ of the generalized Krylov space $K_n(A^T, A^T r_0)\equiv A^T K_n(A^T, r_0)$. Analogously to GMRES, this can be done via recursive column by column QR factorization of the matrix $[A^T r_0, A^T Q_{n-1}]$

$$A^T[r_0, Q_{n-1}] = Q_n S_n, \quad Q_n^T Q_n = I_n, \tag{15}$$

where S_n is an upper triangular matrix. Then, the approximation (1) has the form

$$x_n = x_0 + Q_n t_n \tag{16}$$

and from the optimality condition (4) written as $Q_n^T(x_n - x)=0$ we obtain

$$t_n = Q_n^T(x - x_0). \tag{17}$$

From (16) and denoting $t_n = [\zeta_1, \ldots, \zeta_n]^T$ it is clear that the approximate solution x_n and the residual vector r_n can be updated step by step

$$x_n = x_{n-1} + \zeta_n q_n, \tag{18}$$

$$r_n = r_{n-1} - \zeta_n A q_n. \tag{19}$$

Since t_n cannot be computed directly from (17), consider the optimality condition (4) in the form

$$[A^T r_0, A^T Q_{n-1}]^T (x - x_n) = 0. \tag{20}$$

Using (20) with (16) and factorization (15) we receive the lower triangular system for the unknown vector t_n

$$S_n^T t_n = [r_0, Q_{n-1}]^T r_0, \tag{21}$$

which can be solved easily and ζ_n can be obtained as

$$\zeta_n = \frac{(q_{n-1}, r_0) - \sum_{i=1}^{n-1} s_{i,n}\zeta_i}{s_{n,n}}, \tag{22}$$

where $[s_{1,n}, \ldots, s_{n,n}]^T$ is the nth column of the upper triangular matrix S_n. Alternatively, when the residual is computed, from the optimality condition (4), rewritten as $[r_0, Q_{n-1}]^T r_n = 0$ we get the formula for the coefficient ζ_n in the form

$$\zeta_n = \frac{(r_{n-1}, q_n)}{s_{n,n}}. \tag{23}$$

It can be easily seen that in the symmetric case, this variant of GMERR reduces to the OD method proposed by Fridman in [10] and known as numerically unstable. From this point we can expect poor numerical behavior of the particular implementations of this variant. We think that this behavior can be explained by arguments very similar to ones presented by Walker and Lu Zhou for the GMRES method in [29, Section 3]. Consider the matrix

$$B_n = [r_0, q_1, \ldots, q_{n-1}], \tag{24}$$

where $q_1, \ldots, q_{n-1}$ are computed via the shifted Arnoldi recurrence (15). Similarly to Walker and Lu Zhou we can conclude that the matrix B_n may become ill-conditioned for some initial residual r_0. Then from (15) we would have

$$s_{1,1}/s_{n,n} \leqslant \kappa(S_n) \leqslant \kappa(A^T)\kappa(B_n) \tag{25}$$

and $s_{n,n}$ used in (22) or in (23) may become very small. Then we can expect this variant to be numerically unstable.

We note here that the original formulation of GMERR from [30] reduces in the symmetric case to the STOD, introduced by Stoer and Freund [23]. The STOD method was designed as a stabilization of the unstable OD method for the symmetric indefinite systems. From this we can deduce that the numerical behavior of original variant can be more stable than that of the variant analogical to the Walker and Lu Zhou variant of GMRES. This can be the case, especially when more reliable orthogonalization than classical Gram–Schmidt used in the original algorithm (see the comments at the end of previous section).

In the following we describe a formulation of GMERR which we consider to be superior to other formulation when considering the numerical stability and when considering the stable orthogonalization such as one based on the Householder transformations. This formulation of GMERR is, in some sense, analogical to the classical formulation of GMRES (see e.g. the classical paper [20]) and it is based on the orthonormal basis $V_n = [v_1, \ldots, v_n]$ of the Krylov space $K_n(A^T, r_0)$, computed via the Arnoldi recurrence

$$v_1 = r_0/\|r_0\|, \quad A^T V_n = V_{n+1} H_{n+1,n}, \quad V_{n+1}^T V_{n+1} = I_{n+1}, \tag{26}$$

where $H_{n+1,n}$ is upper Hessenberg matrix of order $(n+1) \times n$. Then the nth approximate solution (1) can be written in the form

$$x_n = x_0 + A^T V_n y_n. \tag{27}$$

The unknown vector y_n can be obtained from condition (4) and rewritten as

$$(A^T V_n)^T (A^T V_n) y_n = (A^T V_n)^T (x - x_0) = V_n^T r_0. \tag{28}$$

Using the Arnoldi recurrence (26) with the matrix A^T we obtain

$$H_{n+1,n}^T H_{n+1,n} y_n = \|r_0\| e_1. \tag{29}$$

Consider, analogously to classical variant of GMRES, the upper Hessenberg matrix $H_{n+1,n}$ reduced to the upper triangular matrix via Givens rotations

$$J_n(J_{n-1} \ldots J_2 J_1) H_{n+1,n} = \begin{pmatrix} R_n \\ 0 \end{pmatrix}. \tag{30}$$

Then, the system (29) can be solved easily by backsubstitution solving two triangular systems

$$R_n^T R_n y_n = \|r_0\| e_1. \tag{31}$$

Slightly different approach of computing the unknown vector y_n can be found in [5].

From (27) it also for the residual of the approximate solution r_n follows that

$$r_n = r_0 - A A^T V_n y_n \tag{32}$$

and from the equality (28) we have

$$r_n = -(I - V_n V_n^T) A A^T V_n y_n. \tag{33}$$

We note here that in the symmetric case, this formulation of the GMERR method reduces to the stable implementation presented by Freund in [7] and is also closely related to the SYMMLQ algorithm presented by Paige and Saunders in [17], which is also numerically stable.

4. Implementation of GMERR method based on the Householder transformations

In the previous section, we discussed the variant of GMERR based on the generating the orthonormal basis $V_n = [v_1, \ldots, v_n]$ of the Krylov subspace $K_n(A^T, r_0)$. Particular implementations can be

obtained from the general formulation by specifying the orthogonalization technique. Here we shall concentrate on the Householder orthogonalization which is numerically more reliable, but requires somewhat more arithmetic and storage than usual Gram–Schmidt factorization. For details we refer to [26, 27]. We consider the following algorithm:

Algorithm 4.1. Householder implementation of GMERR method

$$
\begin{aligned}
&x_0, r_0 = b - Ax_0,\\
&P_1 = I - 2s_1 s_1^{\mathrm{T}}, \quad \|s_1\| = 1, \quad P_1 r_0 = \|r_0\| e_1, \quad v_1 = P_1 e_1,\\
&n = 1, 2, \ldots,\\
&P_{n+1} = I - 2s_{n+1} s_{n+1}^{\mathrm{T}}, \quad \|s_{n+1}\| = 1,\\
&P_{n+1}(P_n P_{n-1} \ldots P_1 A v_n) = (h_{1,n}, \ldots, h_{n+1,n}, 0, \ldots, 0)^{\mathrm{T}},\\
&v_{n+1} = P_1 P_2 \ldots P_{n+1} e_{n+1},\\
&J_n(J_{n-1} \ldots J_2 J_1) H_{n+1,n} = \begin{pmatrix} R_n \\ 0 \end{pmatrix},\\
&R_n^{\mathrm{T}} z_n = \|r_0\| e_1,\\
&R_n y_n = z_n,\\
&x_n = x_0 + A^{\mathrm{T}} V_n y_n.
\end{aligned}
$$

In the following we will present three different examples that illustrate the efficiency of GMERR in comparison to other iterative solvers, the efficiency of the here proposed stable implementation and the influence of the restart parameter on the convergence. We also study different implementations for the restarted version of the method.

Artificial examples showing the efficiency of GMERR in comparison to other iterative solvers were presented in [30]. Here we give an example obtained by courtesy of the manufacturer Pfisterer in Stuttgart, Germany. The electrostatic field of a 145 kV plug as used in interfaces between power cables and gas-insulated circuits is modelled by solving Poisson's differential equation

$$\Delta\phi = -\frac{\rho}{\varepsilon} \tag{34}$$

with Dirichlet and Neumann boundary conditions. The quantity ϕ is the electric scalar potential, ρ is the space charge density and ε is the permitivity constant; for details see [32]. Eq. (34) was solved by the boundary element method using concentrated charges with a "region-oriented" charge simulation method [1]. The dimension of the linear system is 1346. The eigenvalues of the system matrix are scattered over the complex plane and there is a cluster at zero. We compare the original implementation of GMERR (denoted by GS) and the implementation using Householder reflections (denoted by HT) with the Gram–Schmidt implementation of GMRES; see Fig. 1. Both GMERR implementations perform similarly except in the last step, where the Householder implementation achieves better final accuracy close to the multiple of machine precision. If we consider the reduction of the relative residuals GMRES initially seems to converge better than GMERR. But the errors show a quite different behavior (the "exact" solution was calculated by Gaussian elimination). While GMERR reduces the relative errors by one order of magnitude very fast the GMRES errors oscillate

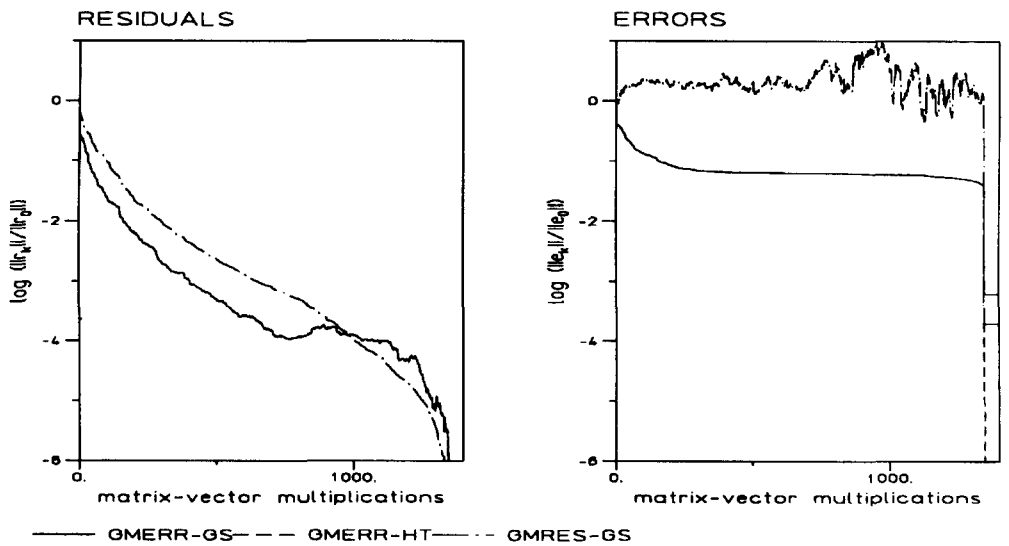

Fig. 1. GMERR and GMRES for the electric plug example.

heavily and stay above the initial error until iteration step N (note that the number of matrix–vector multiplications corresponds to the number of iterations). The reduction of the GMRES residuals gives a completely wrong information; GMERR proceeds at least to the solution. We also remark that we applied to this example other iterative methods. CGNE did not come closer to the solution until iteration step N. Other Krylov subspace methods like BiCGSTAB [25] and QMR [9] did not perform better – as could be expected because they do not fulfil a minimization property in the Euclidean norm. Even preconditioning by approximate inverses did not improve the convergence.

The next example considers the numerical stability of different implementations. We compared the performance of the variant of GMERR analogical to the classical variant of GMRES with the original implementation. We considered the implementations with Householder orthogonalization as well as classical and modified Gram–Schmidt orthogonalization on the problem $Ax = b$, where the matrix A and the solution x were chosen as

$$\mathrm{TP1}(n,\alpha) \quad A = \begin{bmatrix} 1 & 0 & \dots & \alpha \\ 0 & 2 & \dots & 0 \\ \cdot & \cdot & \dots & \cdot \\ 0 & 0 & \dots & n \end{bmatrix} \quad x = \begin{bmatrix} 1 \\ 1 \\ \cdot \\ 1 \end{bmatrix}.$$

This example was taken from [27, 16]; computing was done in a double precision using the Matlab on SGI Crimson workstation with processor R4000.

In Fig. 2 we plotted the logarithm of the error norm on the problem TP1 versus iteration number for the implementation using the Householder reflections (solid line), implementations based on the modified and classical Gram–Schmidt (dashed and dash–dotted lines) and the original implementation of GMERR (dotted line). Here the parameter α and the dimension of the system N were set to $\alpha = 20000$ and $N = 100$. From Fig. 2 it can be seen, that the algorithm using the Householder reflections performed markedly better than other implementations based on the Gram–Schmidt for both variants. The Gram–Schmidt implementations for both original variant and variant analogous to

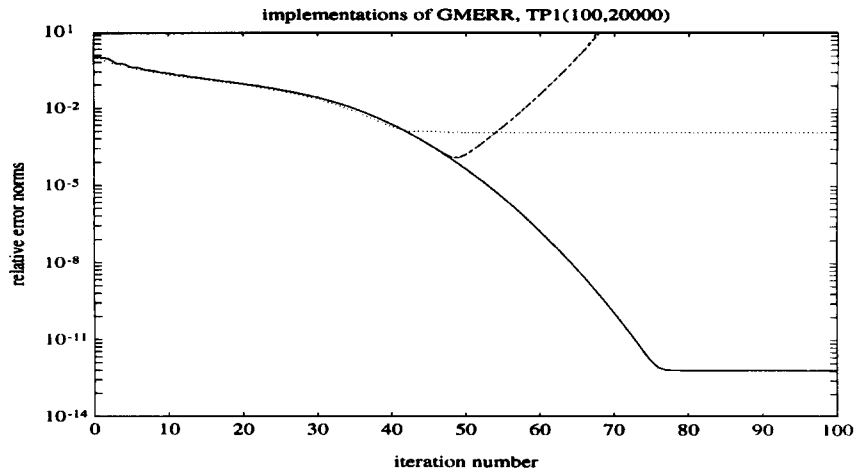

Fig. 2. Comparison of different implementations of GMERR.

the classical variant of GMRES behaved quite badly (note that the original implementation is based on the classical Gram–Schmidt) and did not achieve the final error reduction of the Householder implementation. While for the original implementation of GMERR, the error norm tends to stagnate after a number of iterations, both classical and modified Gram–Schmidt implementations of the variant analogous to the Saad and Schultz variant of GMRES initially converge to the slightly lower error norm than the original implementation, but then suddenly start to diverge. Following the previous considerations we did not include to our comparison the implementations of the variant analogous to the Walker and Lu Zhou variant of GMRES, which seem similarly to the OD method, numerically less stable.

We note that while for the GMRES method it was observed and theoretically justified that the linear independence of the computed vectors is important (see [13, 19]), preserving the orthogonality to some sufficient level (say, to the square root of the machine precision) seems to have a crucial role in the stability analysis of the variant of GMERR analogical to the Saad, Schultz variant of GMRES.

In order to analyze the restarted GMERR versions let us consider now a rough model of the three-dimensional Navier–Stokes equations. We will solve the following partial differential equation for the velocity $v = (v_1, v_2, v_3)^T$,

$$\Delta v + v + \rho(v^T \nabla)v = h \tag{35}$$

with Dirichlet boundary conditions on the unit cube. The parameter ρ simulates a Reynolds number and in our tests we set $\rho = 1$. The right-hand side $h = (h_1, h_2, h_3)^T$ is determined so that equation (35) has trigonometric functions as solution. The linear system is generated by the FIDISOL program package [21]. It arises from finite difference discretizations with consistency orders 2 and 4 and from the linearization in the first Newton step. The calculations have been performed on a $20 \times 20 \times 20$ grid. The matrix is normalized, i.e. every row is divided by the sum of the absolute entries in that row and all diagonal entries have a positive sign. The dimension of the system is $N = 24000$.

In Fig. 3 the influence of the restart parameter on GMERR and GMRES is shown for a fourth order discretization. The convergence of GMRES becomes better if the restart interval becomes larger. This

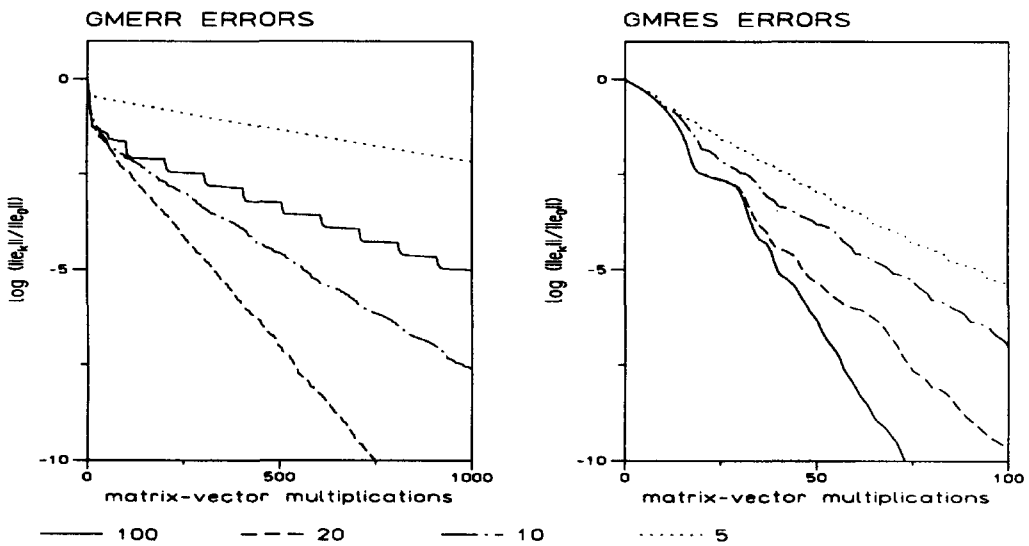

Fig. 3. Dependence on the restart parameter.

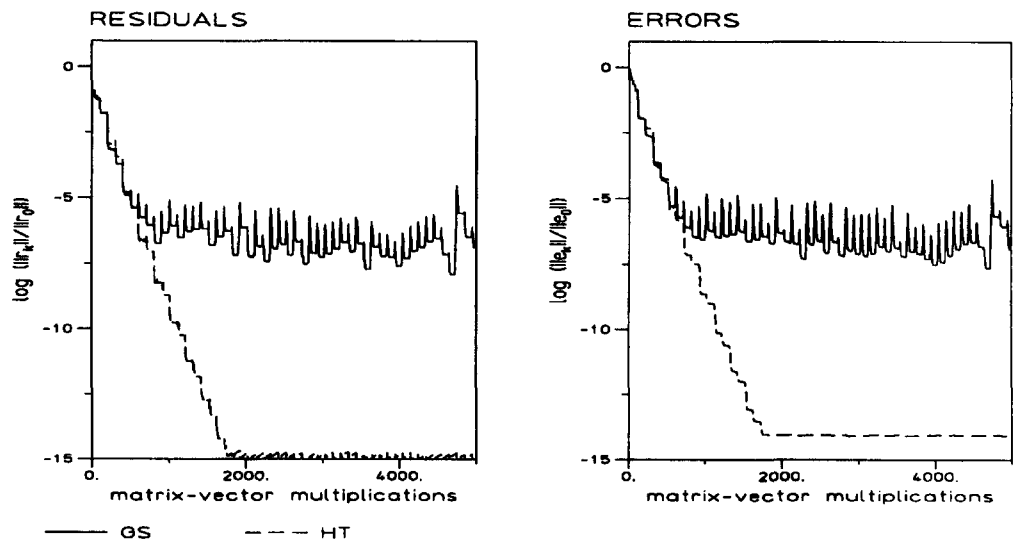

Fig. 4. Different implementations of restarted GMERR.

could be expected because all approximations are in the same Krylov space. For GMERR the space spanned is different for different restart parameters. Consequently, there is no monotonous dependence of the convergence on the restart parameter. We obtain for this example the best convergence for restart parameter 20, followed by the values 10, 100 and 5.

For a second-order discretization of (35) the original implementation (denoted by GS in Fig. 4) and the implementation using Householder reflections (denoted by HT in Fig. 4) is analyzed for the restarted version of GMERR with the restart parameter 100. If the restart parameter is smaller the

differences become less visible. However, rounding errors are cummulated in the restart intervals as well. Only the stable implementation achieves an accuracy of the magnitude of the machine precision; see Fig. 4. For original implementation the error-minimizing property is lost after a residual reduction of 5 orders of magnitude.

5. Conclusions

In this paper we reviewed several implementations of the GMERR method for solving nonsymmetric systems of linear equations and showed their relation to the methods used in the symmetric indefinite case. We proposed a new implementation of the GMERR method based on the Householder reflections and showed that this implementation is numerically superior on some examples. Although the full version of the GMERS method seems to be not competitive with the residual minimizing GMRES method our numerical experiments also illustrate that restarting of the GMERR method may be an attractive alternative. The choice of the restart parameter and deep understanding of the convergence of all and also restarted method still remain as open questions.

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