VARIATIONAL ANALYSIS OF SOME CONJUGATE GRADIENT METHODS

DANIEL B. SZYLD* AND OLOF B. WIDLUND†

Abstract.

A number of conjugate gradient methods are considered for a class of linear systems of real algebraic equations. This class includes all symmetric and certain special nonsymmetric problems, which give rise to three-term recursions. All the algorithms are characterized variationally. This makes it possible to derive error estimates systematically in terms of certain polynomial approximation problems. Bounds are obtained, which are functions of the extreme eigenvalues of the basic iteration operator.

Key Words. linear systems, conjugate gradients, variational formulation, sparse matrices, error bounds

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1. Introduction. It is the purpose of this survey article to present some standard and not-so-standard conjugate gradient methods in a common framework. We consider iterative methods for solving $n \times n$ linear systems of real algebraic equations

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

We will focus our attention on general symmetric, not necessarily definite, and special nonsymmetric problems where

$$A = I - K, \quad K^T = -K. \tag{2}$$

Throughout the paper I denotes the identity matrix and K^T the transpose of K. We concentrate on the variational formulation of these methods, i.e. the fact that the iterates satisfy certain minimization criteria over a given subspace, even if the algorithms were not originally designed from this point of view. We use these properties to derive error bounds. This framework also has a computational aspect, since it indicates how to choose the basis for the subspaces so that the iterates can be obtained from the previous by adding only one or two vectors.

Many of the results presented here have been known to the authors and specialists in the field since the late seventies and most have already appeared in the literature. However, we know of no previous survey covering all these topics systematically.

* Department of Mathematics, Temple University TU 038-16, Philadelphia, Pennsylvania 19122-2585 (szyld@euclid.math.temple.edu). This work was supported by the National Science Foundation grant DMS-8807338.

† Department of Computer Science, Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012 (widlund@cs.nyu.edu). This work was supported in part by the National Science Foundation under Grant NSF-CCR-8903003 and, in part, by the U.S. Department of Energy under contract DE-FG02-88ER250553 at the Courant Mathematics and Computing Laboratory.

In their pioneering work, Hestenes and Stiefel [26] developed a theory for the positive definite, symmetric case. They also noted that any linear system with a nonsingular matrix can be transformed into a positive definite system by using the normal equations. Thus, in the terminology of Faddeev and Faddeeva [12], the first (left) Gauss transform can be used to obtain

$$A^T A x = A^T b. \tag{3}$$

The matrix-vector multiplication required in each iteration of a conjugate gradient method can be carried out by multiplying the vector with A and the resulting vector by A^T. The fact that such a factored form can be used was noticed already by Hestenes and Stiefel. The conjugate gradient method applied to the normal equations (3) is sometimes referred to as Craig's method, see e.g. Faddeev and Faddeeva [12], or as CGNE; see e.g. Elman [10]. The second (right) Gauss transform

$$\begin{aligned} A A^T y &= b, \\ x &= A^T y. \end{aligned} \tag{4}$$

can also be used to transform (1) into a different positive, definite symmetric problem. For the symmetric and special nonsymmetric cases considered in this paper, the coefficient matrices in (3) and (4) become A^2 and $I - K^2$, respectively. Since frequently the main computational cost of a conjugate gradient step is the matrix-vector multiplication, the use a Gauss transform increases the cost per step considerably. If the positive definite product matrix is not formed, the cost per step can be expected to approximately double; if it is formed, the product of A and A^T is usually less sparse than A.

The spectrum of the iteration operator affects the rate of convergence of the iterative methods; generally the convergence slows with an increase in the condition number. It is therefore desirable to avoid systems obtained by using the Gauss transforms since the condition number of $A^T A$ can be much worse than that of A. We therefore consider conjugate gradient type methods which produce a new approximation after only one matrix-vector multiply involving the original matrix, and with convergence rates that depend on the spectrum of A rather than $A^T A$. As we will see, there will be some disappointments.

In the absence of roundoff, the conjugate gradient method terminates in n steps or less. Because of this finite termination property, this method was originally viewed as a direct method; cf. Hestenes and Stiefel [26]. Reid [36] is credited with the revival of the algorithm as an iterative method. If the system is well conditioned, much fewer than n iterations can produce a very good approximation to the solution. For a detailed historical review of the conjugate gradient method for the period 1948-1976, see Golub and O'Leary [18].

In this paper, we will not attempt to discuss the effect of roundoff on the error bounds. We only note that this issue was first treated by Paige [32] and Reid [36] and

that recent results by Greenbaum [21] shed new light on the issue of the reliability of the error bounds, which are obtained while ignoring roundoff.

The preconditioning idea, which goes back at least to Hestenes [25], consists of replacing "the system given by another system with the same solution but with a different coefficient matrix A of smaller condition number"; see Rutishauser [37, p.38]. Thus, the preconditioned system is expected to have better convergence properties. We can use positive definite, symmetric preconditioners for all the methods considered for symmetric problems with virtually no change in the theory; see further Sections 2 and 4.

Many methods of conjugate gradient type can be derived variationally. This can be done systematically by selecting an expanding set of subspaces, known as the Krylov subspaces, and by defining a sequence of approximate solutions in these subspaces by using a Galerkin condition, or by minimizing the norm of the residual. For a special choice of the subspace, an approximate solution, which minimizes the Euclidean norm of the error, can also be computed. By exploiting the special form of A, we show in Section 2 that the Krylov subspaces can be defined in terms of Lanczos vectors, which satisfy a three-term recurrence relationship. As a consequence, the iterates obtained using these subspaces satisfy similar simple recursions; cf. Section 3. Faber and Manteuffel [11] have shown that the matrices for which it is possible to obtain such simply structured algorithms essentially are of the form $A = e^{i\theta}(T + i\sigma I)$, where $i := \sqrt{-1}$, θ and σ are real, and T is Hermitian. This paper covers these cases when the matrix A is real. An analysis of the complex case can be found in a recent paper by Freund [15].

For completeness, we include a derivation of the algorithms for the positive definite case. We use an approach quite similar to that of Paige and Saunders [33]. This sets the stage for a description of their algorithms SYMMLQ and MINRES, which were introduced in the same paper to solve indefinite symmetric problems. The main result of Subsection 3.3 shows that the auxiliary vectors, introduced by Paige and Saunders in the SYMMLQ algorithm in order to make the computation stable, are minimum error solutions; cf. also Fletcher [13]. An underlying variational formulation therefore makes it possible to derive error bounds for one of the sequences of solutions provided by the SYMMLQ algorithm using techniques very similar to the standard case; cf. Section 4.

The special nonsymmetric problems considered here naturally arise from linear systems with coefficient matrices with a positive definite symmetric part. In some applications, it is preferable to repeatedly solve a linear system with the symmetric part as coefficient matrix rather than solving the original system directly. There are also interesting applications with a series of problems with different coefficient matrices but with the same symmetric part; cf. Rapoport [35]. The symmetric part of the coefficient matrix serves as a preconditioner and the problem is reduced to the

special nonsymmetric form. We use the splitting

$$A = M - N, \tag{5}$$

where

$$M := (A + A^T)/2 \tag{6}$$

is the symmetric, positive definite and

$$-N := (A - A^T)/2$$

is the skew-symmetric part of A; see Concus and Golub [4] and Widlund [49]. The operator

$$K := M^{-1}N \tag{7}$$

plays a central role in the algorithm and in our analysis. It is easy to see that K is skew-symmetric with respect to the M-inner product defined by

$$(u, v)_M := (u, Mv) := u^T M v. \tag{8}$$

The results of the analysis of the algorithm obtained by using a Galerkin condition, known as the CGW algorithm, and of the alternative minimal residual algorithm given in the thesis of Rapoport [35], are disappointing. As first shown by Young [50], cf. Hageman, Luk and Young [22], the CGW algorithm is directly related to a doubling algorithm; we show in Subsection 3.5 that the CGW algorithm can be obtained using a Gauss transform.

In the final section, we collect the error bounds known to us. The analysis is based on best polynomial approximation problems on the spectrum of the operator which defines the Krylov subspaces. Such a result is well known for the positive definite case; cf. Daniel [5] and Luenberger [30]. The other cases are now also well understood primarily because of the efforts of Freund [14,15] and Freund and Ruscheweyh [16].

We also note that there are other conjugate gradient-type methods for general nonsymmetric problems that can be characterized variationally, but for which no three-term recurrence is possible. We refer to Dennis and Turner [6], Eisenstat, Elman and Schultz [9], Elman [10], Hageman and Young [23], Saad and Schultz [39], Young and Jea [51] and the references given therein, for descriptions of such methods. In particular, in Eisenstat, Elman and Schultz [9]and Elman [10] connections are established between minimum residual methods for the special matrices (2) and methods for general nonsymmetric matrices such as Orthomin, GCR and GMRES.

2. Krylov Spaces, Lanczos Vectors and the Restriction of the Operators to the Subspaces.

2.1. The symmetric case. The approximate solutions x_k of (1) are constructed using expanding affine spaces of the form $x_0 + S^k$, which are of dimension $k = 1, 2, \ldots$ The Krylov subspace, $S^k = S^k(A, v_1)$, is spanned by the first k vectors of the Krylov sequence

$$v_1, Av_1, \ldots, A^{k-1}v_1, \ldots \tag{9}$$

We note that for any constant α, $S^k(A + \alpha I, v_1) = S^k(A, v_1)$. We also ignore the normalization of the element v_1 and regard $S^k(A, \beta v_1)$, $\beta \neq 0$, as the same as $S^k(A, v_1)$. The operator A and the initial element v_1 completely determine these spaces. The Krylov sequence (9) was apparently introduced over half a century ago by Krylov [27], see also Faddeev and Faddeeva [12], but we do not know who first attributed Krylov's name to it.

In this subsection, we assume that A is symmetric. The system (1) can be preconditioned, from the left, by a positive definite matrix M. Preferably M should be close to A in the sense that the generalized eigenvalues of the pencil defined by A and M are close to each other; see Section 4. The transformed equation,

$$M^{-1}Ax = M^{-1}b,$$

is then solved using the Krylov subspaces $S^k(M^{-1}A, v_1)$. The operator $M^{-1}A$ is symmetric with respect to the the M-inner product (8). This inner product has to be used in the formulas which provide the parameters for the Lanczos vectors and the iterative methods, instead of the Euclidean inner product. Just as there are left and right Gauss transforms, there are left and right preconditioners. We can thus also transform equation (1) into

$$AM^{-1}y = b, \qquad x = M^{-1}y. \tag{10}$$

In this case, the use of the inner product $u^T M^{-1} v$ is appropriate.

The initial element v_1 of the Krylov sequences, which is relevant in this work, is the initial residual $r_0 := b - Ax_0$, where x_0 is the initial guess, or in the case of a left Gauss transform, Ar_0. For the left preconditioner, the initial element can be chosen as $v_1 = M^{-1}r_0$ or as $M^{-1}AM^{-1}r_0$. To simplify the notations, we will, except in the special nonsymmetric case, only discuss the case when no preconditioner is used.

The Lanczos vectors v_j, $j = 1, 2, \ldots$, provide an orthonormal basis for the subspaces S^k; cf. Lanczos [28]. They are defined recursively, are unique up to sign and are obtained by a Gram–Schmidt orthogonalization process:

$$\begin{aligned} &\text{Normalize } v_1, \\ &\beta_{k+1} v_{k+1} \;:=\; Av_k - \sum_{i=1}^{k} \delta_{ik} v_i, \qquad k = 1, 2, \ldots, \end{aligned} \tag{11}$$

where β_{k+1} is chosen so that v_{k+1} has unit norm. Since the vectors are orthonormal,

$$\delta_{ik} = (Av_k, v_i), \qquad i \leq k. \tag{12}$$

The Lanczos vectors depend on the operator A and the direction of the initial vector. They are uniquely defined by the Krylov sequence and the inner product used in (12).

We show that in the cases considered in this paper, equation (11) reduces to a three-term recurrence similar to those of the classical theory of orthogonal polynomials. This means that $\delta_{ik} = 0$, $i < k-1$. It is convenient to change our notations and let $\alpha_k := \delta_{kk}$, and $\gamma_k := \delta_{k-1,k}$.

LEMMA 2.1. *Let A be symmetric, let $v_0 := 0$, let v_1 be a given unit vector, and let*

$$\beta_{k+1} v_{k+1} \;:=\; A v_k - \alpha_k v_k - \gamma_k v_{k-1}. \tag{13}$$

If $\alpha_k := (Av_k, v_k)$, $\beta_{k+1} := (Av_k, v_{k+1})$ and $\gamma_k := (Av_k, v_{k-1})$, then $(v_{k+1}, v_j) = 0$, $j \le k$, i.e. $v_{k+1} \perp S^k$, for $k = 1, 2, \ldots$ The vectors have unit length, and $\beta_k = \gamma_k$, for $k = 2, 3, \ldots$

Proof. The fact that $\beta_k = \gamma_k$ follows directly from the symmetry of A.

For the orthogonality, we proceed by induction. The case of $k = 1$ is trivial. Assume that the conditions are valid for $j \le k$. We find that $\beta_{k+1}(v_{k+1}, v_k) = (Av_k, v_k) - \alpha_k = 0$. Using the symmetry of A and the induction hypothesis, we find that

$$\beta_{k+1}(v_{k+1}, v_{k-1}) = (v_k, Av_{k-1}) - \alpha_k(v_k, v_{k-1}) - \gamma_k = \beta_k - \gamma_k = 0.$$

Finally, for $j \le k-2$,

$$\beta_{k+1}(v_{k+1}, v_j) = (v_k, Av_j) - \alpha_k(v_k, v_j) - \gamma_k(v_{k-1}, v_j).$$

Since $v_j \in S^{k-2}$, $Av_j \in S^{k-1}$ and all three terms vanish by the induction hypothesis.

Finally, since $\beta_{k+1}(v_{k+1}, v_{k+1}) = (Av_k, v_{k+1}) = \gamma_{k+1}$, it follows that v_{k+1} has unit length. □

We can therefore write the three-term recurrence (13) as

$$\beta_{k+1} v_{k+1} \;=\; A v_k \;-\; \alpha_k v_k \;-\; \beta_k v_{k-1}. \tag{14}$$

Let

$$V_k \;:=\; [v_1, v_2, \ldots, v_k] \tag{15}$$

be the $n \times k$ matrix with the first k Lanczos vectors as columns. Then equation (14) gives

$$AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_{(k)}^T. \tag{16}$$

Here $e_{(k)}^T := (0, \ldots, 0, 1)$ and T_k is the $k \times k$ symmetric tridiagonal matrix

$$T_k := \begin{bmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & & \ddots & & & \\ & & \beta_i & \alpha_i & \beta_{i+1} & \\ & & & & \ddots & \\ & & & & \beta_k & \alpha_k \end{bmatrix}.$$

By the orthogonality of the Lanczos vectors,

$$V_k^T A V_k = T_k, \tag{17}$$

i.e. T_k is a matrix representation of the restriction of the operator A to the subspace $S^k = S^k(A, v_1)$ using the convenient basis provided by the Lanczos vectors.

2.2. The skew-symmetric case. We will now consider the special nonsymmetric case (5)-(6) with M positive definite. If the operator A is skew-symmetric, the Lanczos vectors can be constructed quite similarly to the symmetric case just considered.

LEMMA 2.2. *Let A be skew-symmetric, let $v_0 := 0$, let v_1 be a given nonzero vector, and let*

$$\beta_{k+1} v_{k+1} := A v_k - \gamma_k v_{k-1}.$$

If $\gamma_k := (Av_k, v_{k-1})/(v_{k-1}, v_{k-1})$, $k \geq 2$, then $(v_{k+1}, v_j) = 0$, $j \leq k$, i.e. $v_{k+1} \perp S^k$, $k = 1, 2, \ldots$

Note that β_{k+1} is not yet defined, i.e. the norm of the vector v_{k+1} has not been chosen. In the derivation of the CGW algorithm, cf. Subsection 3.4, it is convenient to use a special normalization of the vectors and we adopt this normalization from the start:

$$\beta_2 = 1, \quad \beta_{k+1} + \gamma_k = 1, \quad k \geq 2. \tag{18}$$

Proof of Lemma 2. We again use an induction proof. The case of $k = 1$ is easy, since the operator is skew symmetric, i.e. $(v, Av) = 0$ for all v. The orthogonality of v_{k+1} and v_k also follows from this formula and the induction hypothesis, and that of v_{k+1} and v_{k-1} from the formula for γ_k. The orthogonality of v_{k+1} and v_j, $j \leq k-2$, is established almost exactly as in the proof of Lemma 1. □

Lemma 2 applies directly to the operator K defined in (7) if the M-inner product (8) is used throughout. Thus,

$$\gamma_k := (Kv_k, v_{k-1})_M/(v_{k-1}, v_{k-1})_M = (Nv_k, v_{k-1})/(v_{k-1}, Mv_{k-1}), \tag{19}$$

and the vectors defined by

$$\beta_{k+1} v_{k+1} \;:=\; K v_k - \gamma_k v_{k-1}, \tag{20}$$

are M-orthogonal. Since the system (1) can be written as

$$(I - K)x = M^{-1} b, \tag{21}$$

the initial residual is $M^{-1}b - (I-K)x_0 = M^{-1} r_0$ and the relevant Krylov subspaces are $S^k = S^k(I-K, v_1) = S^k(K, v_1)$, with $v_1 = M^{-1} r_0$.

The following results will be used in Subsection 3.5.

LEMMA 2.3. *Let ϕ_o and ϕ_e be odd and even polynomials, respectively. Then $(\phi_e(K)v, \phi_o(K)v)_M = 0$, for all v.*

Proof. The operator $\phi_e(K)$ is symmetric with respect to the M-inner product. Therefore,

$$(\phi_e(K)v, \phi_o(K)v)_M = (v, \phi_e(K)\phi_o(K)v)_M.$$

Since $\phi_e(K)\phi_o(K)$ is an odd polynomial in K, it is skew-symmetric and the expression vanishes. □

Lemma 3 directly implies the following

COROLLARY 2.4. *$S^{2k}(K, v_1) = S^k(K^2, v_1) \oplus_M S^k(K^2, Kv_1)$, where $\oplus_M$ denotes a direct sum of M-orthogonal subspaces.*

Let

$$\rho_k \;:=\; (v_k, v_k)_M. \tag{22}$$

¿From (20), it follows

$$\beta_{k+1}\rho_{k+1} = (v_{k+1}, Kv_k)_M = (v_{k+1}, Nv_k).$$

Similarly from (19),

$$\gamma_k \rho_{k-1} = (Nv_k, v_{k-1}) = -(v_k, Nv_{k-1}).$$

Therefore,

$$\gamma_k = -\beta_k \rho_k / \rho_{k-1}. \tag{23}$$

If the coefficients β_k are chosen as in (18), they satisfy the recurrence relation

$$\beta_2 = 1, \quad \beta_{k+1} = 1 + \beta_k(\rho_k/\rho_{k-1}). \tag{24}$$

Let V_k be defined as in (15). Then from (20), it follows that

$$KV_k = V_k J_k + \beta_{k+1} v_{k+1} e_{(k)}^T, \tag{25}$$

where J_k is the tridiagonal matrix

$$J_k := \begin{bmatrix} 0 & \gamma_2 & & & & \\ \beta_2 & 0 & \gamma_3 & & & \\ & & \ddots & & & \\ & & \beta_i & 0 & \gamma_{i+1} & \\ & & & & \ddots & \\ & & & & \beta_k & 0 \end{bmatrix}.$$

Therefore,

$$V_k^T A V_k = V_k^T (M - N) V_k = V_k^T M (I - K) V_k = R_k (I - J_k), \tag{26}$$

where R_k is the diagonal matrix with entries $\rho_1, \rho_2, \ldots, \rho_k$; see (22). By using (23) and (24), we see that the parameters $\beta_i > 0$ and $\gamma_i < 0$ and that the matrix J_k is similar to a skew-symmetric tridiagonal matrix, via the diagonal similarity transformation $R_k^{1/2}$.

3. The Basic Algorithms.

3.1. The Standard Positive Definite Case. In this subsection, we derive the standard conjugate gradient, the minimum residual and the minimal error methods for the solution of (1), where A is symmetric, positive definite. The resulting approximate solutions belong to the k-dimensional affine subspaces $x_0 + S^k(A, r_0)$ or $x_0 + S^k(A, Ar_0)$. We choose to present the algorithms from the variational point of view, i.e. developing the formulae directly from the optimality conditions. We prefer this to the usual presentation of the conjugate gradient algorithm, in which the formulae are given first and the variational properties deduced later; see e.g. Golub and Van Loan [19] or Stoer and Bulirsch [42].

The conjugate gradient iterates x_k^c minimize the A-norm of the error. Thus,

$$\|x_k^c - x^\star\|_A^2 = \min \|x - x^\star\|_A^2, \quad x \in x_0 + S^k(A, r_0)\ . \tag{27}$$

Here $r_0 = b - Ax_0$, $x^\star$ is the solution of (1) and $\|y\|_A^2 = (y, Ay)$. The expression (27) can also be written as the square of the A^{-1}-norm of the residual.

The minimal residual solution is determined by minimizing the Euclidean norm of the residual over the same affine subspace while the minimal error solution is determined by minimizing the Euclidean norm of the error over a different affine subspace, namely $x_0 + S^k(A, Ar_0)$. We first discuss the standard conjugate gradient method in some detail.

Since

$$\|x - x^\star\|_A^2 = (x, Ax) - 2(x, b) + (x^\star, b), \tag{28}$$

the minimization problem (27) is, after dropping a constant term, equivalent to

$$\min\,[(x,Ax)-2(x,b)],\quad x\in x_0+S^k(A,r_0)$$

and to

$$\min\,[(x-x_0,A(x-x_0))-2(x-x_0,r_0)],\quad x\in x_0+S^k(A,r_0)\ .$$

By setting the gradient to zero, it follows that the same solution is obtained from the Galerkin equation

$$(b-Ax,v)=0,\ \text{for all } v\in S^k(A,r_0), \tag{29}$$

which can also be written as

$$(A(x-x_0),v)=(r_0,v),\ \text{for all } v\in S^k(A,r_0), \tag{30}$$

In the last two equations, we solve for $x\in x_0+S^k(A,r_0)$.

We now represent x_k^c in terms of the Lanczos vectors, i.e. we use the Lanczos vectors as the basis in which we represent $S^k(A,r_0)$. Thus,

$$x_k^c-x_0=V_k y_k^c, \tag{31}$$

where V_k is defined in (15) and $y_k^c:=(\eta_1^{(k)},\eta_2^{(k)},\ldots,\eta_k^{(k)})^T$.

Substituting this expression into the Galerkin equation (30), we obtain

$$V_k^TAV_k y_k^c=V_k^Tr_0. \tag{32}$$

By (17) and $\beta_1 v_1=r_0$, this is equivalent to the tridiagonal system

$$T_k y_k^c=\beta_1 e_{(1)}, \tag{33}$$

where $e_{(1)}:=(1,0,\ldots,0)^T$.

The residual

$$r_k\ :=\ b-Ax_k^c$$

is a multiple of the Lanczos vector v_{k+1} and the residuals are therefore orthogonal. To see this, we use (16) and obtain

$$AV_k y_k^c=V_kT_k y_k^c+\beta_{k+1}v_{k+1}e_{(k)}^T y_k^c.$$

By using that $\beta_1 v_1=r_0$, (31) and (33), we find that

$$r_k=-\eta_k^{(k)}\beta_{k+1}v_{k+1}. \tag{34}$$

Thus, by Lemma 1,

$$r_k \perp S^k(A, r_0) \ . \tag{35}$$

Orthogonality also follows immediately from the Galerkin condition (29). If $\beta_{k+1} = 0$, then $Ax_k^c = b$.

Following Paige and Saunders [33], we now provide further algorithmic details. Cholesky's method can be used to solve (33). The coefficient matrix is factored

$$T_k \ = \ E_k D_k E_k^T, \tag{36}$$

where D_k is a diagonal matrix with elements $\delta_1, \delta_2, \ldots, \delta_k$, and E_k is a unit lower bidiagonal matrix with off-diagonal elements $\lambda_2, \lambda_3, \ldots, \lambda_k$. These elements are obtained by using the recursions

$$\delta_1 = \alpha_1, \quad \lambda_j = \beta_j/\delta_{j-1}, \quad \delta_j = \alpha_j - \beta_j\lambda_j, \quad j = 2, \ldots, k. \tag{37}$$

Here the α_k and β_k are the coefficients of the three-term recurrence (14). The matrices E_{k-1}, D_{k-1} are the $(k-1) \times (k-1)$ principal minors of the matrices E_k, D_k, respectively. In step k of the algorithm, the new elements λ_k, δ_k are computed using only the values α_k, β_k and δ_{k-1}.

Similarly, $s_k = (\xi_1, \ldots, \xi_k)^T$, the solution of the lower triangular system

$$E_k D_k s_k = \beta_1 e_{(1)}, \tag{38}$$

has the same $k-1$ first components as s_{k-1}; cf. (33). The component ξ_k is obtained by the formula

$$\xi_k = -\delta_{k-1}\lambda_k\xi_{k-1}/\delta_k, \tag{39}$$

with $\xi_1 = \beta_1/\alpha_1$. On the other hand, the vector

$$y_k^c = E_k^{-T} s_k, \tag{40}$$

changes completely from one step to the next. It is therefore more convenient to work with an additional, A-orthogonal, basis for S^k. As in (31) let

$$x_k^c - x_0 = P_k s_k, \tag{41}$$

where

$$P_k = [p_1, p_2, \ldots, p_k] \ := \ V_k E_k^{-T}, \tag{42}$$

i.e.

$$x_k^c = x_0 + \sum_{i=1}^{k} \xi_i p_i = x_{k-1}^c + \xi_k p_k. \tag{43}$$

It follows from equation (42) that the vectors p_j can be computed directly from the v_j by the recursion

$$p_1 = v_1, \quad p_j = v_j - \lambda_j p_{j-1}, \quad j \geq 2. \tag{44}$$

By using (35), we find that

$$(r_k, p_j) = 0, \quad j \leq k. \tag{45}$$

Equations (43) and (44) show that the approximate solution x_k^c can be computed directly from the previous iterate x_{k-1}^c, and that the Lanczos vectors need not be saved.

In summary, a step of the conjugate gradient method proceeds by computing new values of α and β using the formulas in Lemma 1, a new Lanczos vector using (14), new values of δ and λ using (37), a new component ξ of s using (39), a new vector p using (44) and finally a new approximation to the solution using (43). In this implementation only five vectors of storage are necessary. The matrix A is only needed in terms of a subroutine which produces the matrix-vector product and, as previously pointed out, this makes the algorithm quite independent of the choice of data structures, etc.

The following computation shows that the vectors p_i are conjugate, i.e. A-orthogonal,

$$P_k^T A P_k = E_k^{-1} V_k^T A V_k E_k^{-T} = E_k^{-1} T_k E_k^{-T} = D_k.$$

The vectors p_i are often called search directions, since by (43), we move in the direction of p_k when we go from x_{k-1}^c to x_k^c. By using the conjugacy of the search directions, it is easy to show that x_k^c can be obtained by solving

$$\|x_k^c - x^\star\|_A^2 = \min_\mu \|(x_{k-1}^c + \mu p_k) - x^\star\|_A^2.$$

By setting the derivative with respect to μ equal to zero, we obtain an alternative formula for ξ_k

$$\xi_k = (p_k, r_{k-1})/(p_k, Ap_k). \tag{46}$$

¿From (43) it also follows that

$$x_k^c - x_{k-1}^c = \xi_k p_k.$$

By using formulas (34) and (44), we obtain

$$\xi_{k+1}^{-1}(x_{k+1}^c - x_k^c) = -(\eta_k^{(k)}\beta_{k+1})^{-1} r_k - \xi_k^{-1}\lambda_{k+1}(x_k^c - x_{k-1}^c),$$

and thus

$$x_{k+1}^c = x_k^c - \xi_{k+1}(\eta_k^{(k)}\beta_{k+1})^{-1}(r_k + \xi_k^{-1}\lambda_{k+1}\eta_k^{(k)}\beta_{k+1}(x_k^c - x_{k-1}^c)).$$

It follows from (40) that $\eta_k^{(k)} = \xi_k$. From (39) and (37) we then obtain the form of the algorithm, which is associated with Rutishauser [37],

$$x_{k+1}^c = x_k^c + (1/\delta_{k+1})(r_k + \lambda_{k+1}\beta_{k+1}(x_k^c - x_{k-1}^c)). \tag{47}$$

We now turn to the minimal residual algorithm. As we have previously noted, this solution is defined by minimizing the Euclidean norm of the residual over the same affine subspace that is used for the standard conjugate gradient method. By quite similar arguments, we obtain a five diagonal linear system of equations,

$$V_k^T A^2 V_k y_k^r = V_k^T A r_0. \tag{48}$$

By further straightforward computations using (16), we can rewrite this equation as

$$(T_k^2 + \beta_{k+1}^2 e_{(k)} e_{(k)}^T) y_k^r = \alpha_1\beta_1 e_{(1)} + \beta_1\beta_2 e_{(2)}. \tag{49}$$

We will return to a more detailed discussion of equation (49) in the next subsection.

In a similar way, we can derive a pentadiagonal linear system for the minimal error solution. This solution has the form

$$x_k^e = x_0 + A V_k y_k^e. \tag{50}$$

The resulting linear system has the same coefficient matrix as (49), but a different right hand side. The system has the form

$$V_k^T A^2 V_k y_k^e = V_k^T r_0,$$

or

$$(T_k^2 + \beta_{k+1}^2 e_{(k)} e_{(k)}^T) y_k^e = \beta_1 e_{(1)}. \tag{51}$$

These pentadiagonal linear systems of equations, which are nonsingular if A is nonsingular, can also be solved by Cholesky's method. A typical row of the resulting triangular matrices has two nonzero off-diagonal elements and the search directions can be computed recursively from the two previous search direction vectors and one Lanczos vector. We will return to a study of the minimal residual and minimal error solutions since they can be computed in a stable manner for any problem with an arbitrary nonsingular, symmetric but not necessarily positive definite, coefficient matrix.

3.2. The Indefinite Symmetric Case. In this and the next subsection, we consider the case where A is symmetric, nonsingular but indefinite. The Lanczos vectors and the Krylov spaces are defined exactly as in the positive definite case. The quadratic form (28) no longer has a minimum, but we can use the Galerkin condition (29) to try to find a unique saddle point. As in the previous subsection,

we then obtain the tridiagonal system of equations (33). The coefficient matrix is the restriction of an indefinite operator to a subspace and the tridiagonal matrix can therefore be singular. If it is almost singular, the solution of equation (33) can have a very large norm and catastrophic cancellation then makes the procedure, as developed for the positive definite case, numerically unstable. On the other hand, an elementary argument shows that if the tridiagonal matrix T_k is singular, then T_{k+1} is not, unless the off-diagonal element $\beta_{k+1} = 0$. By Lemma 1 and (34), this happens only if the residual $r_k = 0$. Because of these difficulties, it is natural to consider an alternative algorithm of solving equation (33).

We follow Paige and Saunders [33] and use an LQ factorization. Other possibilities have been explored in the literature. Thus Chandra [3] developed an alternative algorithm, SYMMBK, in which the tridiagonal matrix T_k is factored using both 1×1 and 2×2 pivots, as in the algorithm by Bunch and Kaufman [2]. Simon [40], on the other hand, proposed that the tridiagonal matrix and the norm of the residuals be computed first, without generating the iterates, and that when the norm of the residual is sufficiently small, the linear system (33) be solved by a stable method. Finally, the solution is assembled by retrieving the Lanczos vectors from secondary storage or by regenerating them; cf. Parlett [34]. Both, in the SYMMBK algorithm and in Simon's method, only the standard conjugate gradient approximation x_k^c is produced, while the SYMMLQ algorithm of Paige and Saunders also provides an additional sequence of approximate solutions which we further characterize.

Early on, Fridman [17] proposed that the minimum error approximations to the solution of (1) in the subspace $S^k(A, Ar_0)$ be used. As we will see, the choice of this initial element of the Krylov space is crucial. Let $v_i, i = 1, 2 \ldots$, be the Lanczos vectors spanning $S^k(A, Ar_0)$. Fridman's main observation was that the minimum error approximation can be written as

$$x_k^e = x_0 + \sum_{j=1}^{k} \varphi_j v_j \ , \quad \text{where } \varphi_j := (x^\star - x_0, v_j).$$

By the orthogonality of the Lanczos vectors, it is also true that $\varphi_k = (x^\star - x_{k-1}^e, v_k)$. By using (14), we find that

$$\varphi_k = (x^\star - x_{k-1}^e, Av_{k-1} - \alpha_{k-1}v_{k-1} - \beta_{k-1}v_{k-2})/\beta_k \ .$$

Since $x^\star - x_{k-1}^e$ is orthogonal to $S^{k-1}(A, Ar_0)$, we find that for $k > 1$

$$\varphi_k = (A(x^\star - x_{k-1}^e), v_{k-1})/\beta_k = (r_{k-1}, v_{k-1})/\beta_k \ .$$

Similarly, since the initial element of the Krylov sequence is Ar_0,

$$\varphi_1 = (x^\star - x_0, v_1) = (A(x^\star - x_0), r_0)/\|Ar_0\| = (r_0, r_0)/\|Ar_0\|.$$

Fridman's method is numerically unstable; see Paige and Saunders [33] or Stoer and Freund [43]. In the next subsection, we show that the additional sequence of

approximate solutions of the SYMMLQ algorithm provides a stable computation of the minimum error solution. This appears not to have been known to Paige and Saunders.

Adopting the notations of Paige and Saunders [33], we factor T_k

$$T_k = \bar{L}_k Q_k, \tag{52}$$

where Q_k is orthogonal and $\bar{L}_k$ is lower triangular. To fully understand the derivation of the SYMMLQ algorithm, we need to examine $\bar{L}_k$ and Q_k in some detail. The LQ factorization is computed recursively. The orthogonal matrix Q_k is the product of $k-1$ elementary orthogonal matrices $Q_{k-1,k} \cdots Q_{1,2}$. In the first step an elementary symmetric, orthogonal matrix $Q_{1,2}$ is used to eliminate the $(1,2)$ element of the tridiagonal matrix T_k. This orthogonal matrix is block diagonal with all diagonal elements equal to one, except for a leading 2×2 diagonal block of the form

$$\begin{bmatrix} c & s \\ s & -c \end{bmatrix}, \tag{53}$$

with $c^2 + s^2 = 1$. It is easy to see that if T_k is multiplied from the right by $Q_{1,2}$ changes occur only in the two first columns and that a nonzero element is introduced in the $(3,1)$ position. In the second step (and in the steps that follow), the elements of the first row and first column are not changed, while the elements in the three first rows and two first columns of what remains of the matrix are changed by multiplying by an elementary orthogonal matrix $Q_{2,3}$, constructed similarly to $Q_{1,2}$. Note that this $(k-1) \times (k-1)$ matrix involved in the second step is initially tridiagonal. A similarly situated element below the diagonal becomes nonzero but there is no further loss of sparsity. In the second step, which only affects the second and third column, the $(2,2)$ element is changed a second and final time. By the same arguments, the matrix $\bar{L}_k$ differs from the $k \times k$ leading minor of $\bar{L}_{k+1}$ only in the (k,k) element. After $k-1$ steps, the lower triangular matrix $\bar{L}_k$ is obtained. It has nonzero elements in positions at a distance up to two from the diagonal. This matrix is singular if and only the matrix T_k is singular. By simple matrix algebra, using the orthogonality of Q_k, it is also easy to see that $\bar{L}_k$ is a, possibly singular, Cholesky factor of T_k^2.

As in the positive definite case, we can in principle obtain the conjugate gradient solution, for those k for which it exists, by setting

$$x_k^c - x_0 = \bar{W}_k \bar{z}_k. \tag{54}$$

Here $\bar{z}_k$ is the solution of

$$\bar{L}_k \bar{z}_k = \beta_1 e_{(1)}, \tag{55}$$

and

$$\bar{W}_k = [w_1, w_2, \ldots, \bar{w}_k] \;:=\; V_k Q_k^T; \tag{56}$$

cf. (38), (41) and (42). By using the product form of Q_k given above, we see that only the k^{th} column of $\bar{W}_k$ changes when we update it to produce $\bar{W}_{k+1}$. Since the x_k^c iterates do not always exist or can be quite susceptible to roundoff, Paige and Saunders work with a different sequence x_k^L from which x_k^c can be computed upon demand. The sequence x_k^L is obtained by replacing $\bar{L}_k$ by L_k, the $k \times k$ leading minor of $\bar{L}_{k+1}$, and $\bar{W}_k$ by W_k, the first k columns of $\bar{W}_{k+1}$. Thus

$$x_k^L - x_0 = W_k z_k, \tag{57}$$

where z_k is the solution of

$$L_k z_k = \beta_1 e_{(1)}. \tag{58}$$

The first $k-1$ components of z_k coincide with z_{k-1} since all but the first component of the right hand side is zero. In the update step the k^{th} row of L_k is calculated to obtain ζ_k, the new element of z_k. A new approximation x_k^L is given by the formula

$$x_k^L = x_{k-1}^L + \zeta_k w_k; \tag{59}$$

cf. (43). By using the fact that only the last rows of $\bar{L}_k$ and L_k differ and (54)-(59), it is easy to see that the conjugate gradient approximation satisfies

$$x_{k+1}^c = x_k^L + \bar{\zeta}_{k+1} \bar{w}_{k+1}, \tag{60}$$

where $\bar{\zeta}_{k+1}$ is the last component of $\bar{z}_{k+1}$.

The SYMMLQ algorithm returns either x_k^L or x_k^c, depending on which one has the smallest residual norm, once a prescribed tolerance has been met. The residual norms are computed at a cost of a few scalar operations from quantities already available; see Paige and Saunders [33].

In the same paper, Paige and Saunders also discuss MINRES, the minimum residual algorithm. The Cholesky factorization of the matrix in equation (49) is

$$T_k^2 + \beta_{k+1}^2 e_{(k)} e_{(k)}^T = \bar{L}_k \bar{L}_k^T + \beta_{k+1}^2 e_{(k)} e_{(k)}^T = L_k L_k^T. \tag{61}$$

This Cholesky factor is the same matrix as in (58). This follows from the fact that L_k is the $k \times k$ leading minor of $\bar{L}_{k+1}$.

The vector y_k^r, defined by equation (49), changes completely from one step to the next. Therefore, in a way similar to the conjugate gradient solution, cf. (41)-(43), let

$$x_k^r - x_0 = M_k t_k, \tag{62}$$

where

$$M_k = [m_1, m_2, \ldots, m_k] \ := \ V_k L_k^{-T} \tag{63}$$

and $t_k = (\tau_1, \ldots, \tau_k)^T$ is the solution of

$$L_k t_k = \alpha_1 \beta_1 e_{(1)} + \beta_1 \beta_2 e_{(2)}.$$

The first $k-1$ components of t_k coincide with t_{k-1} since all but the first two components of the right hand side are zero. We obtain,

$$x_k^r = x_{k-1}^r + \tau_k m_k.$$

Since the last row of L_k has nonzeros only in the last three positions, the search direction m_k can be computed recursively from the Lanczos vector v_k, m_{k-1} and m_{k-2}.

We also show how to obtain the conjugate gradient solution from the minimal residual solution. From (61), it follows that L_k and $\bar{L}_k$ differ only in the (k,k) position. Let C_k be the diagonal matrix with entries $1,\ldots,1,c_k$ such that $\bar{L}_k = L_k C_k$. The quantity c_k appears on the diagonal of the 2×2 matrix (53) of $Q_{k-1,k}$.

Premultiplying (32) by $T_k = V_k^T A V_k$, we see that y_k^c satisfies

$$T_k^2 y_k^c = L_k C_k^2 L_k^T y_k^c = V_k^T A r_0,$$

while y_k^r satisfies

$$L_k L_k^T y_k^r = V_k^T A r_0,$$

and $t_k = L_k^T y_k^r$. Thus,

$$C_k^2 L_k^T y_k^c = t_k.$$

We rewrite (31) using (63) as

$$x_k^c - x_0 = V_k L_k^{-T} L_k^T y_k^c = M_k C_k^{-2} t_k.$$

¿From (62) and the form of C_k, we finally obtain

$$x_k^c = x_k^r + M_k(C_k^{-2} - I)t_k = x_k^r + \tau_k(c_k^{-2} - 1)m_k.$$

3.3. Variational Formulation of the SYMMLQ Algorithm. Paige and Saunders introduced the second sequence of iterates x_k^L primarily to obtain a stable algorithm. They also noted that x_k^L is a better approximation than x_k^c of $x^\star$ in the l_2-norm. This follows from (60) since from (56), $W_k^T \bar{w}_{k+1} = 0$. Fletcher [13] rediscovered Fridman's method independently, while considering a class of biconjugate gradient methods, and showed that the resulting iterates are the same as x_k^L. Here we present a different proof of this fact. It follows then, that since one of the iterative sequences can be characterized variationally, it is possible to derive an error bound for the SYMMLQ Algorithm; see Subsection 4.2.

THEOREM 3.1. *The sequence x_k^L of the SYMMLQ algorithm is the minimum error approximation in the subspace $S^k(A, Ar_0)$.*

Proof. By using equations (51), (50), (61), (57) and (58), we see that the theorem follows by showing that

$$W_k = A V_k L_k^{-T}. \tag{64}$$

The matrix W_k consists of the first k columns of $\bar{W}_{k+1} = V_{k+1}Q_{k+1}^T$. Postmultiplying the $m \times (k+1)$ matrix $\bar{W}_{k+1}$ by $\bar{L}_{k+1}^T$, we obtain, cf. (52),

$$V_{k+1}T_{k+1} = AV_{k+1}.$$

The first k columns of AV_{k+1} coincide with AV_k. The matrix L_k^{-T} is upper triangular and is the $k \times k$ principal minor of $\bar{L}_{k+1}^{-T}$. Being upper triangular, the last row of $\bar{L}_{k+1}^{-T}$ has a nonzero only in the $(k+1, k+1)$ position. Therefore, $AV_kL_k^{-T}$ consists of the first k columns of $AV_{k+1}\bar{L}_{k+1}^{-T}$ and (64) is established. □

3.4. The Special Nonsymmetric Case. If the matrix A in (1) is skew-symmetric, the Lanczos vectors, which span the Krylov subspaces are constructed as in Lemma 2. Similarly, as we have seen in Sections 1 and 2.2, if the matrix A is nonsymmetric but can be split as in (5)-(6) with M positive definite, then the matrix $K = M^{-1}N$ is skew-symmetric with respect to the M-inner product and the relevant Krylov space is $S^k(K, v_1)$, where

$$v_1 = M^{-1}r_0 = M^{-1}b - (I - K)x_0. \tag{65}$$

In this case, the Galerkin procedure works and gives invertible linear systems of equations and approximations for which error bounds can be derived. We first describe the method developed by Concus, Golub [4] and Widlund [49], which is commonly known as the CGW method. The Galerkin condition has the form (30) and, as in the symmetric, positive definite case, it is satisfied by $x_k^g - x_0 = V_k y_k^g$, where y_k^g is the solution of

$$V_k^T A V_k y_k^g = V_k^T r_0. \tag{66}$$

¿From (22), (26) and (65), it follows that (66) is equivalent to

$$R_k(I - J_k)y_k^g = \rho_1 e_{(1)}. \tag{67}$$

We note that $\rho_1 = (v_1, Mv_1)$ is the first element of the diagonal matrix R_k and that we therefore can simplify equation (67) to

$$(I - J_k)y_k^g = e_{(1)}. \tag{68}$$

With the normalization given by (18), the LU factorization of $(I - J_k) = L_kU_k$ becomes exceptionally easy, requiring no arithmetic; this is the reason for chosing β_k in this way. The factors are

$$L_k = \begin{bmatrix} 1 & & & & & & \\ -1 & 1 & & & & & \\ & -1 & 1 & & & & \\ & & \ddots & \ddots & & & \\ & & & -1 & 1 & & \\ & & & & -1 & 1 \end{bmatrix}, \qquad U_k = \begin{bmatrix} \beta_2 & -\gamma_2 & & & & & \\ & \beta_3 & -\gamma_3 & & & & \\ & & \ddots & & & & \\ & & & & \beta_i & -\gamma_i & \\ & & & & & \ddots & \\ & & & & & & \beta_{k+1} \end{bmatrix}.$$

It is also easy to see that

$$L_k \bar{e}_{(k)} = e_{(1)},$$

where $\bar{e}_{(k)}^T := (1, 1, \ldots, 1)^T$. The triangular system

$$U_k y_k^g = \bar{e}_{(k)}$$

remains to be solved. We wish to obtain $y_k^g = U_k^{-1} \bar{e}_{(k)}$ directly from y_{k-1}^g. Using block Gaussian elimination, we find that since

$$U_k = \left[\begin{array}{c|c} & 0 \\ U_{k-1} & \vdots \\ & 0 \\ & -\gamma_k \\ \hline 0 & \beta_{k+1} \end{array}\right],$$

its inverse is

$$U_k^{-1} = \left[\begin{array}{c|c} U_{k-1}^{-1} & (\gamma_k/\beta_{k+1}) u_{k-1} \\ \hline 0 & 1/\beta_{k+1} \end{array}\right],$$

where $u_{k-1} := U_{k-1}^{-1} e_{(k-1)}$, $e_{(k-1)} := (0, \ldots, 0, 1)^T$. Thus,

$$y_k^g = U_k^{-1} \bar{e}_{(k)} = U_k^{-1} \begin{bmatrix} \bar{e}_{(k-1)} \\ 1 \end{bmatrix} = \begin{bmatrix} U_{k-1}^{-1} \bar{e}_{(k-1)} + (\gamma_k/\beta_{k+1}) u_{k-1} \\ 1/\beta_{k+1} \end{bmatrix} = \begin{bmatrix} y_{k-1}^g \\ 0 \end{bmatrix} + u_k,$$

where $u_k = \begin{bmatrix} (\gamma_k/\beta_{k+1}) u_{k-1} \\ 1/\beta_{k+1} \end{bmatrix} = U_k^{-1} e_{(k)}$. We can therefore obtain y_k^g and u_k directly from y_{k-1}^g and u_{k-1}. The Galerkin solution is then

$$x_k^g - x_0 = V_k y_k^g = V_k U_k^{-1} \bar{e}_{(k)} = V_{k-1} y_{k-1}^g + V_k u_k. \tag{69}$$

The first term on the right in (69) is $x_{k-1}^g - x_0 = V_{k-1} y_{k-1}^g$ while the second is $\Delta x_k^g := x_k^g - x_{k-1}^g = V_k u_k$. We can therefore write (69) as

$$\Delta x_k^g = \frac{\gamma_k}{\beta_{k+1}} V_{k-1} u_{k-1} + \frac{1}{\beta_{k+1}} v_k = \frac{\gamma_k}{\beta_{k+1}} \Delta x_{k-1}^g + \frac{1}{\beta_{k+1}} v_k. \tag{70}$$

Since by (18), $\gamma_k = 1 - \beta_{k+1}$,

$$\frac{\gamma_k}{\beta_{k+1}} = \frac{1}{\beta_{k+1}} - 1.$$

Only the parameter

$$\omega_k := 1/\beta_{k+1}, \tag{71}$$

is needed and we rewrite (70) as

$$\Delta x_k^g = (\omega_k - 1)\Delta x_{k-1}^g + \omega_k v_k,$$

or equivalently

$$x_k^g = x_{k-2}^g + \omega_k(v_k + x_{k-1}^g - x_{k-2}^g). \tag{72}$$

LEMMA 3.2. *Let v_k be the Lanczos vectors constructed as in Lemma 2 with the initial vector given by (65), and the normalization (18). Let the residuals of the CGW method be $r_k := b - Ax_k^g$. Then $v_{k+1} = M^{-1}r_k$, $k = 0, \ldots$*

Proof. We use induction. From (65) the assertion holds for $k = 0$. Let $x_{-1} = 0$. From (72),

$$r_k = b - Ax_k^g = r_{k-2} - \omega_k(Av_k - r_{k-1} + r_{k-2}).$$

Premultiplying by M^{-1}, we obtain

$$M^{-1}r_k = M^{-1}r_{k-2} - \omega_k((I - K)v_k - M^{-1}r_{k-1} + M^{-1}r_{k-2}),$$

which by the induction hypothesis is

$$\begin{aligned} M^{-1}r_k &= v_{k-1} - \omega_k((I - K)v_k - v_k + v_{k-1}) = \\ &= \omega_k K v_k + (1 - \omega_k)v_{k-1}. \end{aligned} \tag{73}$$

The lemma follows from (71) and (18), and by comparing (73) with (20). □

A consequence of Lemma 6 is that $\rho_k = (v_k, r_{k-1})$; cf. (22). Also note that from (24), $1/\omega_k = 1 + (\rho_k/\rho_{k-1})/\omega_{k-1}$, $k > 1$ and this is how ω_k is actually computed.

We conclude the subsection with a brief description of the algorithm developed by Rapoport [35] in his 1978 dissertation, which is the minimal residual analog to the CGW algorithm. The algorithm is derived, straightforwardly, by minimizing the M^{-1}-norm of the residual of the equation (1) over the same affine subspace. Just as in the symmetric case, cf. (48)-(49), a pentadiagonal linear system results. As noted by Rapoport, all elements next to the diagonal vanish. However, it does not seem to be possible to realize any direct savings by using this structure. We cannot see any convincing reason to prefer this method over the CGW algorithm.

3.5. Variational Formulation of the CGW Algorithm. We conclude this section by showing that the approximations produced by the CGW algorithm with even and odd indices, $\{x_{2k}^w\}$ and $\{x_{2k+1}^w\}$, also can be generated by applying the standard conjugate gradient method to the system obtained after using the second Gauss transform and the initial guesses x_0 and x_1^w, respectively. This result is closely related to Corollary 4 and greatly simplifies the error analysis, given in the next section, since the theory for the standard symmetric, positive definite case applies.

It is disappointing that the CGW algorithm offers so little new and that the error bound depends on the spectrum of $I - K^2$. However, as in the SYMMLQ algorithm, the CGW algorithm provides two subsequences, the odd and even. There are cases when one of them converges appreciably faster than the other and in such cases the CGW algorithm can be faster than if only one of the subsequences were used.

The result can be derived from a result by David Young [50], who appears to have been the first to observe a relationship between the CGW algorithm and a standard algorithm using the operator $I - K^2$. His result is presented in a context different than ours in Hageman, Luk and Young [22]. Further results are given in two papers by Eisenstat [7] [8]. Connections with the symmetric system obtained by using the second Gauss transform were established in these papers; see also Elman [10] and Freund [14].

The use of the second Gauss transform amounts to a change of variables

$$x = (I + K)z. \tag{74}$$

The system (21) becomes

$$(I - K^2)z = M^{-1}b\ . \tag{75}$$

When the standard conjugate gradient method, with the M-inner product, is applied to (75) the relevant Krylov subspace is $S^k(I - K^2, v_1) = S^k(K^2, v_1)$, where v_1 is the initial residual given by

$$v_1 = M^{-1}b - (I - K^2)z_0 = M^{-1}b - (I - K)x_0 = M^{-1}r_0. \tag{76}$$

We also note that by a direct calculation using (72), with $\omega_1 := 1$ and $x_{-1} := 0$, the approximation after the first step of the CGW algorithm is given by

$$x_1^w = x_0 + v_1. \tag{77}$$

By Lemma 6, the residual after the first step and the second Lanczos vector are given by

$$r_1 = MKr_0 \quad \text{and} \quad v_2 = Kv_1. \tag{78}$$

The main result is formulated as follows.

THEOREM 3.3. *Let $\{x_k^w\}$, $k = 0, 1, \ldots$, be the CGW approximations to $x^\star$ for the special nonsymmetric problem (5)-(6). Let z_0 and z_1 be defined by $x_0 = (I+K)z_0$ and $x_1^w = (I + K)z_1$ and consider the system obtained after the second Gauss transform*

$$(I - K^2)z = M^{-1}b\ . \tag{79}$$

Let z_k be the conjugate gradient solution of (79) using the initial guess z_0. Then the approximations with even indices, x_{2k}^w, $k = 0, 1, \ldots$, coincide with $(I + K)z_k$. The odd

subsequence can similarly be obtained by the conjugate gradient solution of the same system using the initial guess z_1.

Proof. By the Galerkin condition (30), the solution x_{2k}^w is the unique element in $x_0+S^{2k}(K,v_1)$ with a residual $M^{-1}b-(I-K)x_{2k}^w$, which is M-orthogonal to $S^{2k}(K,v_1)$. Similarly, z_k is the unique element in $z_0+S^k(K^2,v_1)$ such that the residual

$$\overline{r}_k := v_1-(I-K^2)(z_k-z_0)$$

is M-orthogonal to $S^k(K^2,v_1)$. Since $(I+K)(z_k-z_0)\in(I+K)S^k(K^2,v_1)$ and $(I+K)S^k(K^2,v_1)\subset S^{2k}(K,v_1)$, we can by Corollary 4 complete the proof of the theorem for the even case by proving that $\overline{r}_k$ is M-orthogonal to all of $S^{2k}(K,v_1)$. Since $\overline{r}_k\in S^{k+1}(K^2,v_1)$, this follows directly from Lemma 3. The result for the odd subsequence is obtained in almost exactly the same way, by using the formulas given in (77)-(78). □

4. Error Bounds. It is easy to see that any element of the Krylov space $S^k(A,v_1)$ can be represented as $\phi_{k-1}(A)v_1$, where $\phi_{k-1}\in\mathcal{P}_{k-1}$, the space of polynomials of degree $k-1$. The errors of the conjugate gradient methods considered in this paper can be estimated from above in terms of the solution of certain best polynomial approximation problems. This is well known for the standard conjugate gradient method; cf. Daniel [5] and Luenberger [30]. As we will see, the same estimate can also be used for several other cases, but for others, more complicated polynomial approximation problems arise. These problems are also quite well understood, primarily because of the efforts of Freund [15] and Freund and Ruscheweyh [16].

Throughout, $x^\star$ denotes the solution of (1). Two affine polynomial spaces of dimension k will be used. They are

$$\mathcal{P}_{k-1}^0 := 1+t\mathcal{P}_{k-1},$$

in other words the polynomials of degree k that are equal to 1 at the origin, and

$$\bar{\mathcal{P}}_{k-1}^0 := 1+t^2\mathcal{P}_{k-1}\ ,$$

or the polynomials of degree $k+1$ that are equal to 1 at the origin and have zero first derivative at the same point. It is easy to see that the natural bases of $t\mathcal{P}_{k-1}$ and $t^2\mathcal{P}_{k-1}$ form so-called Haar systems; cf. Meinardus [31]. The existence and uniqueness of the solution of the approximation problems that we are going to formulate follows immediately.

4.1. The Standard Estimate. We begin by reviewing the standard case. The conjugate gradient solution x_k^c of (1) is the minimizing element for (27). Thus, the error $e_k := x_k^c-x^\star$ satisfies

$$e_k^TAe_k = \min_{\phi_{k-1}\in\mathcal{P}_{k-1}}(\phi_{k-1}(A)r_0+e_0)^TA(\phi_{k-1}(A)r_0+e_0). \tag{80}$$

Since $r_0 = -Ae_0$, (80) can be rewritten as

$$e_k^T A e_k = \min_{\psi_{k-1} \in \mathcal{P}_{k-1}^0} (\psi_{k-1}(A)e_0)^T A (\psi_{k-1}(A)e_0).$$

By expanding the initial error e_0 in eigenvectors of A, it is easy to show, that

$$\frac{e_k^T A e_k}{e_0^T A e_0} \leq \min_{\psi_{k-1} \in \mathcal{P}_{k-1}^0} \max_{\sigma_i \in \sigma(A)} \psi_{k-1}^2(\sigma_i), \tag{81}$$

where $\sigma(A)$ is the spectrum of A.

We can now obtain an upper bound of (81) for the symmetric positive definite case; see Daniel [5] and Luenberger [30].

THEOREM 4.1. *Let $\{x_k^c\}$, $k = 0, 1, \ldots$, be the conjugate gradient approximations to $x^\star$, and let $A = A^T$ be positive definite. Let $0 < \alpha := \min \sigma(A)$, $\beta := \max \sigma(A)$, $\kappa := \kappa(A) =$ the condition number of $A = \beta/\alpha$, and $\rho = (\sqrt{\kappa} + 1)/(\sqrt{\kappa} - 1)$. Then, the error $e_k := x_k^c - x^\star$ satisfies*

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \frac{2}{\rho^k + \rho^{-k}} \quad . \tag{82}$$

Proof. From (81), it follows that

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq \min_{\psi_{k-1} \in \mathcal{P}_{k-1}^0} \max_{\sigma \in [\alpha, \beta]} |\psi_{k-1}(\sigma)| \ .$$

This approximation problem has a known unique solution, namely, the normalized Chebyshev polynomial given by

$$\psi_{k-1}(\zeta) = \frac{T_k(\frac{-2\zeta + \beta + \alpha}{\beta - \alpha})}{T_k(\frac{\beta + \alpha}{\beta - \alpha})}, \tag{83}$$

where $T_k(\eta) = \cos(k \ arc \cos \eta)$ is the k^{th} Chebyshev polynomial. By using a standard formula, see e.g. Luenberger [30], we obtain the bound (82). □

By dropping a term in the denominator, we obtain a standard form of the bound

$$\frac{\|e_k\|_A}{\|e_0\|_A} \leq 2(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1})^k.$$

These upper bounds depend only on the condition number κ. If more information on the distribution of the eigenvalues of A is available, better bounds can be obtained; see Axelsson [1], Greenbaum [20], Hayes [24], Lebedev [29], Saad [38], van der Vorst [47] and Widlund [49]. See the discussion below of the symmetric indefinite case for a sample argument of this kind.

The analysis of the algorithms based on the straightforward use of the first and second Gauss transforms is very similar to the standard case. A direct calculation

shows that the resulting bounds, which compare the l_2- norm of the residual and the error, respectively, after k steps with the corresponding initial error measure, reduces to the standard case. The same bounds based on Chebyshev polynomials result, except that the relevant spectrum is that of A^TA.

By Theorem 7, the CGW algorithm provides two subsequences of iterates, each of which can be derived via the second Gauss transform. If Λ is the spectral radius of K, i.e. $\sigma(K) \subseteq [-i\Lambda, i\Lambda]$, the condition number of the matrix in (79) is bounded by $1+\Lambda^2$. In practical applications, either $0 \in \sigma(K)$, or there is an eigenvalue very close to zero. Thus, we can assume that the condition number of $I-K^2$ is equal to $1+\Lambda^2$.

THEOREM 4.2. *Let $\{x_k^g\}$, $k = 0, 1, \ldots$, be the CGW approximations to $x^\star$ for the special nonsymmetric problem (5)-(6). Let Λ be the spectral radius of K, i.e. $\sigma(K) \subseteq [-i\Lambda, i\Lambda]$. Denote the error by $e_k^g := x_k^g - x^\star$. Then, the even subsequence satisfies*

$$\frac{\|e_{2k}\|_M}{\|e_0\|_M} \leq \frac{2}{\rho^k + \rho^{-k}}, \tag{84}$$

where $\rho = (\sqrt{1+\Lambda^2}+1)/(\sqrt{1+\Lambda^2}-1)$. The bound (84) also holds for $\|e_{2k+1}\|_M/\|e_1\|_M$.

Proof. By Theorem 7, $e_{2k} = (I+K)(z_k - z^\star)$, where $(I+K)z^\star = x^\star$ and z_k is the conjugate gradient solution of (79) using the initial guess z_0 defined by $(I+K)z_0 = x_0$. Since K is skew-symmetric with respect to the M-inner product,

$$(e_{2k}, e_{2k})_M \;=\; (z_k - z^\star, (I-K)(I+K)(z_k - z^\star))_M \;\; .$$

Thus, by Theorem 8, the bound (84) holds for the even case. The odd case is completely analogous. □

4.2. The Other Estimates. We first consider the minimal residual method for the special nonsymmetric case (2), first considered in Rapoport [35]. It is easy to obtain an upper bound for the error in terms of a comparison polynomial by using the same techniques as for the standard case. The spectrum is confined to an interval $1 + i[-\Lambda, \Lambda]$. This polynomial approximation problem has been solved completely by Freund and Ruscheweyh [16]. The following bound is best possible if we have no information except that the spectrum is confined to this interval.

THEOREM 4.3. *Let $\{x_k^r\}$, $k = 0, 1, \ldots$, be the minimum residual approximations to $x^\star$ for the special nonsymmetric problem (5)-(6). Let Λ be the spectral radius of K, i.e. $\sigma(K) \subset [-i\Lambda, i\Lambda]$. Then, the residual $r_k := b - Ax_k^r$ satisfies*

$$\frac{\|r_k\|_{M^{-1}}}{\|r_0\|_{M^{-1}}} \leq \frac{2}{\tilde{\rho}^k + \tilde{\rho}^{k-2}},$$

where $\tilde{\rho} = (\sqrt{1+\Lambda^2}+1)/\Lambda$.

For large values of Λ this bound is asymptotically similar and as disappointing as the bound in Theorem 9. For a proof of Theorem 10, we refer to Freund and Ruscheweyh [16]. For the more general case of $A = e^{i\theta}(T + i\sigma I)$, θ and σ real, T Hermitian, Freund [15] gives useful upper and lower bounds for the decay of the norm of the residuals. We also note that Widlund [49] contains a result on superlinear convergence for cases with clustered eigenvalues.

We now turn to the symmetric, indefinite case. We have shown in Theorem 5 that one of the sequences produced by the SYMMLQ algorithm, x_k^L, is the minimum error solution of the equation (1) and $x_k^L - x_0 \in S^k(A, Ar_0)$. Therefore, the error $\bar{e}_k := x_k^L - x^\star$ satisfies

$$\begin{aligned} \bar{e}_k^T \bar{e}_k &= \min_{\phi_{k-1} \in \bar{\mathcal{P}}_{k-1}} (\phi_{k-1}(A)Ar_0 + \bar{e}_0)^T (\phi_{k-1}(A)Ar_0 + \bar{e}_0) = \\ &= \min_{\chi_{k-1} \in \bar{\mathcal{P}}^0_{k-1}} (\chi_{k-1}(A)\bar{e}_0)^T (\chi_{k-1}(A)\bar{e}_0), \end{aligned} \tag{85}$$

Expanding $\bar{e}_0$ in the eigenvectors of A, we find that

$$\frac{\bar{e}_k^T \bar{e}_k}{\bar{e}_0^T \bar{e}_0} \leq \min_{\chi_{k-1} \in \bar{\mathcal{P}}^0_{k-1}} \max_{\sigma_i \epsilon \sigma(A)} \chi_{k-1}^2(\sigma_i).$$

Fletcher [13] appears to have been the first to understand the relation between the minimum error solution and SYMMLQ, but he did not use that result to produce error bounds. The analysis above of the convergence of SYMMLQ was given by Widlund [48]; see also Stoer and Freund [43], Szyld [44] and Szyld and Widlund [46].

If A is indefinite, its spectrum has both positive and negative eigenvalues. If we only know that $\sigma(A) \subseteq [-\beta, -\alpha] \cup [\alpha, \beta]$, $\beta \geq \alpha > 0$, we obtain the bound

$$\begin{aligned} \frac{\|\bar{e}_k\|}{\|\bar{e}_0\|} &\leq \min_{\chi_{k-1} \in \bar{\mathcal{P}}^0_{k-1}} \max_{\alpha \leq |\sigma| \leq \beta} |\chi_{k-1}(\sigma)| \\ &= \min_{\psi_{\bar{k}-1} \in \mathcal{P}^0_{\bar{k}-1}} \max_{\alpha^2 \leq \tau \leq \beta^2} |\psi_{\bar{k}-1}(\tau)|, \end{aligned}$$

where $\bar{k} := [(k+1)/2]$ is the integer part of $(k+1)/2$. The last equality follows from the fact that the minimizing polynomial must be even, and from a change of variables $\tau = \sigma^2$. Using Chebyshev polynomials as in Theorem 8, it follows that

$$\frac{\|\bar{e}_k\|}{\|\bar{e}_0\|} \leq 2 \left(\frac{\kappa - 1}{\kappa + 1} \right)^{\bar{k}}, \tag{86}$$

where $\kappa = \beta/\alpha$; see Freund [14] and Stoer [41].

The bound (86) can be very pessimistic. A better bound is obtained if we assume that $\sigma(A) \subseteq \{\lambda_1, \lambda_2, \cdots, \lambda_m\} \cup [\alpha, \beta]$, where λ_i, $i = 1, \cdots, m$ are negative eigenvalues and $\beta \geq \alpha > 0$. This is typical in many applications, e.g. for the linear systems of inverse iteration; see Szyld [44,45]. The bound obtained below is asymptotically

similar to that of the standard conjugate gradient method; cf. (82). This explains the excellent convergence properties observed in practice for SYMMLQ. The relevant quantity $\tilde{\kappa} := \beta/\alpha$ is sometimes called the reduced condition number of A.

THEOREM 4.4. *Let $\{x_k^L\}$, $k = 0, 1, \ldots$, be the auxiliary sequence of SYMMLQ approximations to $x^\star$, obtained for a symmetric indefinite problem. Let $\sigma(A) \subseteq \{\lambda_1, \lambda_2, \cdots, \lambda_m\} \cup [\alpha, \beta]$, where λ_i, $i = 1, \cdots, m$ are negative eigenvalues and $\beta \geq \alpha > 0$. Then, for $k > m$, the error $\bar{e}_k := x_k^L - x^\star$ satisfies,*

$$\frac{\|\bar{e}_k\|}{\|\bar{e}_0\|} \leq \Omega_k \ \frac{2}{\rho^{k-m} + \rho^{m-k}} \quad . \tag{87}$$

Here $\rho = (\sqrt{\tilde{\kappa}} + 1)/(\sqrt{\tilde{\kappa}} - 1)$, $\tilde{\kappa} = \beta/\alpha$, and Ω_k is a linear function of k, which is given in the proof.

Proof. We use a construction due to Freund [14] to obtain a comparison polynomial in $\bar{\mathcal{P}}_{k-1}^0$

$$p_m(\sigma) q(\sigma) \psi_{k-m}(\sigma).$$

Here $\psi_{k-m}(\sigma)$ is the normalized Chebyshev polynomial (83) of degree $k-m$ associated with the interval $[\alpha, \beta]$, chosen so that $\psi_{k-m}(0) = 1$. The polynomial $p_m(\sigma)$ of degree m vanishes at $\lambda_i = 0$, $i = 1, \cdots, m$ and $p_m(0) = 1$, i.e.

$$p_m(\sigma) = \prod_{j=1}^{m} (1 - \frac{\sigma}{\lambda_j}).$$

The parameter μ in the linear function $q(\sigma) = 1 + \mu\sigma$ is chosen so that $\chi'_{k+1}(0) = 0$, which leads to the formula

$$\mu = \sum_{j=1}^{m} \frac{1}{\lambda_j} + \frac{2}{(\beta - \alpha)} \ \frac{T'_{k-m}(\gamma)}{T_{k-m}(\gamma)} \ ,$$

where $\gamma = (\beta+\alpha)/(\beta-\alpha)$. It can be shown that $T'_{k-m}(\gamma)/T_{k-m}(\gamma) \leq (k-m)/\sqrt{\gamma^2 - 1}$. Therefore,

$$\begin{aligned} \frac{\|\bar{e}_k\|}{\|\bar{e}_0\|} &\leq \max_{\sigma \epsilon \sigma(A)} |p_m(\sigma) q(\sigma) \psi_{k-m}(\sigma)| = \max_{\sigma \epsilon [\alpha,\beta]} |p_m(\sigma) q(\sigma) \psi_{k-m}(\sigma)| \\ &\leq \max_{\sigma \epsilon [\alpha,\beta]} |p_n(\sigma) q(\sigma)| \max_{\sigma \epsilon [\alpha,\beta]} |\psi_{m-k}(\sigma)| \leq \Omega_k \ \frac{2}{\rho^{k-m} + \rho^{m-k}} \quad , \end{aligned}$$

where

$$\Omega_k = \left(\prod_{j=1}^{m} (1 - \frac{\beta}{\lambda_j}) \right) \left(1 - \beta \sum_{j=1}^{m} \frac{1}{\lambda_j} + (k-m)\sqrt{\tilde{\kappa}} \right) \quad . \qquad \square$$

We remark that in the case when there are small isolated positive eigenvalues the bound (87) can be improved using a similar comparison polynomial.

The MINRES algorithm, also considered by Paige and Saunders [33] only generates one sequence of approximate solutions. Under the assumptions on the spectrum given in Theorem 11, the decrease of the norm of the residuals satisfies the bound given in that theorem, where

$$\Omega_k = \prod_{j=1}^{m} (1 - \frac{\beta}{\lambda_j})$$

is independent of k. This follows from a straightforward argument, since the comparison polynomial need not satisfy the additional constraint of a zero derivative at the origin.

We end this section by mentioning an interesting polynomial approximation problem related to the study of the minimum error solution for symmetric problems, in the positive definite case. In a recent paper Freund identifies the optimal polynomial in terms of certain Zolotarev polynomials. The optimal polynomial is given in terms of a parameter which can be determined by solving a certain nonlinear equation; see Freund [15]. These formulas are relatively complicated to use but Freund also provides the following bounds for the decrease of the norm of the error in the positive definite case:

$$\frac{\|x_k^e - x^\star\|}{\|x_0 - x^\star\|} \leq 2 \, \frac{(k-1)b_{k-1}(\rho) + k b_k(\rho)}{b_{2k-1}(\rho) + (2k-1)b_1(\rho)},$$

where $\rho = (\sqrt{\kappa} + 1)/(\sqrt{\kappa} - 1)$ and $b_l(\rho) = (1/2)(\rho^l - \rho^{-l})$. By considering the worst case, it can also be shown that the best upper bound must exceed

$$\frac{2}{\rho^k + \rho^{-k}} \; .$$

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