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s-STEP ITERATIVE METHODS FOR (NON)SYMMETRIC (IN)DEFINITE LINEAR SYSTEMS*

A. T. CHRONOPOULOS†

Abstract. In this paper a class of s-step methods for nonsymmetric linear systems of equations is introduced. These methods are obtained from nonsymmetric generalizations of the conjugate residual method, which apply to nonsymmetric definite systems [S. C. Eisenstat, H. C. Elmans and M. H. Schultz, *SIAM J. Numer. Anal.*, 20 (1983), pp. 345–357]. The s-step methods are derived then in a way similar to obtaining the s-step conjugate gradient [G. E. Forsythe, *Numer. Math.*, 11 (1968), pp. 57–76], [A. T. Chronopoulos and C. W. Gear, *J. Comput. Math.*, 25 (1989), pp. 153–168], [A. T. Chronopoulos, *Ph.D. thesis*, Dept. of Computer Science, University of Illinois, Urbana, IL, 1986). It is proven that the s-step methods (with $s \geqq 2$) converge for all symmetric indefinite matrices, for nonsymmetric matrices with positive definite symmetric part and for a class of nonsymmetric indefinite problems. The s-step methods require less computational work but $s-1$ more vectors of main memory storage than the standard ones. These methods are also more suitable for parallel computations.

Key words. iterative methods, conjugate gradient based, s-step, nonsymmetric indefinite

AMS(MOS) subject classifications. 65F10, 65J10

1. Introduction.

Consider the linear system of equations

$$Ax = f \tag{1.1}$$

where A is a nonsingular matrix of order n. If the matrix A is symmetric and positive definite then the conjugate gradient (CG) method [11] can be applied to approximate the solution of (1.1). At each iteration it computes an approximate solution x_i which minimizes the error functional $E(x_i) = (x - x_i)^T A(x - x_i)$. The conjugate residual (CR) method is a variant of the conjugate gradient method that minimizes the residual error $E(x_i) = \|f - Ax_i\|_2^2$ at each iteration.

It is assumed (unless otherwise stated) throughout this paper that the matrix in (1.1) is nonsingular and nonsymmetric with symmetric part $M = (A + A^T)/2$ being either positive definite or indefinite. If the matrix M is (positive or negative) definite then the matrix A is called (positive or negative) definite. Luenberger [13] and Paige and Saunders [16] have obtained conjugate residual and Lanczos based methods for indefinite symmetric systems. A survey of conjugate gradient methods for symmetric indefinite linear systems can be found in [1]. Generalizations of the conjugate gradient method were derived by Concus and Golub [4] and Widlund [18] for a nonsymmetric system with positive real coefficient matrix. However, on each iteration an auxiliary symmetric system of equations must be solved. Axelsson [2], Eisenstat, Elman, and Schultz [9], and Young and Jea [19] devised generalizations of the conjugate residual method, which apply when the matrix of the system is positive real. Saad and Schultz [17] obtained an algorithm called GMRES(m), which is based on the Arnoldi iteration but with residual error minimization property.

In this article, some generalizations of CR are reviewed which can be used to solve the linear system (1.1). Then s-step iterative methods are derived in a way similar

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† Department of Computer Science, University of Minnesota, Minneapolis, Minnesota 55455.

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to the methods for the symmetric positive definite problems [5], [7]. These methods are shown to converge. In § 2, the generalized conjugate residual (GCR) and Orthomin(k) methods are presented. In § 3, the s-step minimal residual method (MR) is introduced. It is shown that the s-step MR method possesses the residual error minimizing property and subsequent convergence for indefinite symmetric and skew-symmetric, for positive real nonsymmetric, and for a class of indefinite nonsymmetric systems. In § 4, s-step generalizations for GCR and Orthomin (k) are derived. In § 5, convergence theorems for the s-step methods are proved. It is also shown that the s-step methods are equivalent to the standard methods for positive real matrices. In § 6, the work and storage requirements for the new s-step methods is discussed. There is a modest increase in the main memory storage ($s-1$ vectors), but less work is required than with one-step methods.

2. Generalizations of the conjugate residual method. The CR method applied to the symmetric positive definite (SPD) problem minimizes $\|r_{i+1}\|_2^2$ along the direction p_i in order to determine the steplength a_i in

$$x_{i+1}=x_i+a_ip_i.$$

Also, p_i is made $A^T A$-orthogonal to p_{i-1}. Symmetry is used to obtain

$$(Ap_i, Ap_j)=0 \quad \text{for } i\neq j.$$

Positive definiteness is necessary to guarantee that $a_i=(r_i, Ap_i)/(Ap_i, Ap_i)=(r_i, Ar_i)/(Ap_i, Ap_i)$ is positive, and so there is progress towards the solution in every step. The orthogonality and the norm reducing properties of CR guarantee its convergence in at most n iterations.

If A is nonsymmetric but definite then the norm reducing property of CR is still valid but the orthogonality only holds locally. That is, p_i is guaranteed to be $A^T A$-orthogonal only to p_{i-1}. This shortcoming is improved in some of the generalizations of CR.

ALGORITHM 2.1. (Nonsymmetric generalizations of CR).
x_0, $p_0=r_0=f-Ax_0$
For $i=0$ **Until** Convergence **Do**

$$a_i=\frac{(r_i, Ap_i)}{(Ap_i, Ap_i)}$$

$$x_{i+1}=x_i+a_ip_i$$

$$r_{i+1}=r_i-a_iAp_i$$

Compute p_{i+1}, Ap_{i+1}

EndFor.

Since $(r_i, Ar_i)>0$ the norms of the residuals form a decreasing sequence. The direction vectors must be constructed to reduce the norm significantly at each step. Next, in (i) and (ii) below, two ways are presented to compute p_{i+1}, Ap_{i+1}.

(i) Generalized conjugate residual method (GCR):

$$p_{i+1}=r_{i+1}+\sum_{j=0}^{i} b_j^ip_j,\quad b_j^i=-\frac{(Ar_{i+1}, Ap_j)}{(Ap_j, Ap_j)},\qquad j\leqq i.$$

Here $\|r_{i+1}\|_2$ is minimized over $x_0+\{r_0, Ar_0, \cdots, A^ir_o\}$. GCR gives the exact solution in at most n iterations [9]. However, if more than a few iterations are needed then the

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storage requirements become prohibitive. To circumvent this, GCR can be restarted periodically every $(k+1)$ iterations. This method is called GCR (k) [9]. An alternative is to $A^T A$-orthogonalize p_{i+1} to the k preceding directions. This defines Orthomin (k).

(ii) Orthomin (k):

$$p_{i+1} = r_{i+1} + \sum_{j=i-k+1}^{i} b_j^i p_j$$

where the $\{b_j^i\}$ are defined as in (i). Both methods coincide for $k \geqq 1$ with CR in the symmetric case. Note that CR applied to the nonsymmetric problem is Orthomin (1). Orthomin (0) is a one-dimensional steepest descent method called the minimal residual method (MR).

In both (i) and (ii) Ap_{i+1} must be computed. This can be done either directly or via the recursion

$$Ap_{i+1} - Ar_{i+1} + \sum_{j=j_i}^{i} b_j^i Ap_j \tag{2.1}$$

where $j_i = 0$ for GCR and $j_i = \max(0, i-k+1)$ for Orthomin (k). Note that the work for Orthomin (k) is (a) that of GCR for $j < k-1$ and (b) that of the $(k-1)$th iteration of GCR for $k-1 \leqq j$.

Assuming (2.1) is used for computing Ap, the work and storage for these methods is shown in Table 2.1. The work is given in terms of number of inner products (Dotprods), vector updates (Vupdates), and matrix vector multiplications (Matvecs). These operations are called vector operations and they involve vectors of size n. Operations on vectors of dimension s have been ignored in the operations count. The vector operations and storage requirements in each method for completing the i first iterations are tabulated. Storage includes the matrix A and the vectors x, r, Ar, $\{p_j\}_{j=j_i}^{j=i+1}$, $\{Ap_j\}_{j=j_i}^{j=i+1}$, for GCR the vector Ar is stored in Ap_{i+1}.

TABLE 2.1.

Vector operations for completing the interations $j = 0, \cdots, i$ *in* GCR(Orthomin (k), MR *and in* GCR (k) *(with* $k \neq 0$ *and* (i/k) *integer.*

Vector Operation	GCR	Orthomin (k)	GCR (k)	MR
Dotprods	$(i+1)(i+6)/2$	$i(k+2)+2+k(3-k)/2$	$(i/k)(k+1)(k+6)/2$	$2(i+1)$
Vupdates	$(i+1)(i+4)$	$2i(k+1)+k(3-k)+2$	$(i/k)(k+1)(k+4)$	$2(i+1)$
MatVecs	$(i+1)$	$(i+1)$	$(i+1)$	$(i+1)$
Storage	$2i+6$	$(2k+3)$	$(2k+3)$	3

In the next section a nonsymmetric s-step minimal residual method is introduced and it is shown that it converges for $s \geqq 2$ for all symmetric or skew-symmetric indefinite and for some nonsymmetric indefinite systems.

3. The s-step minimal residual method. In solving a linear system of equations using the MR method the choice of steplength a_i minimizes the quadratic function $E(x_{i+1}) = \|f - Ax_{i+1}\|_2^2$. This method guarantees reduction of the residual error at every iteration only if the matrix A is positive definite. Otherwise, the steplength a_i may be zero. Here, the MR method is extended to an s-step method (s-step MR). It is then proved that the s-step MR converges for a class of indefinite matrices, in addition to the definite matrices. Steepest descent methods similar to s-step MR have been studied in [10] and [12].

DEFINITION 3.1. The minimal polynomial of a nonzero vector v with respect to matrix A is defined to be the least degree monic polynomial $q_k(\lambda)$ so that $q_k(A)v=0$.

Notation 3.1. Let L_i denote the affine subspace

$$\left\{x_i+\sum_{j=0}^{s-1} a_j A^j r_i : a_j \textit{ scalars} \text{ and } r_i=f-Ax_i\right\}$$

If it is assumed that the degree of the minimal polynomial of r_i is not less than s then the dimension of L_i equals s. Next, the s-step MR method is introduced, which is an s-dimensional steepest descent method provided that the dimension of L_i equals s for all i.

ALGORITHM 3.1 (The s-step minimal residual method (s-MR)).
x_0, $r_0=f-Ax_0$
For $i=0$ **Until** Convergence **Do**
  $x_{i+1}=x_i+a_i^1r_i+\cdots+a_i^sA^{s-1}r_i$,
  where x_{i+1} minimizes $E(x)$ over L_i
  $r_{i+1}=r_i-a_i^1Ar_i-\cdots-a_i^sA^sr_i$, or $r_{i+1}=f-Ax_{i+1}$
EndFor

Since x_{i+1} minimizes $E(x)$ over the affine subspace L_i the residual r_{i+1} must be orthogonal to A times the span of $\{r_i, Ar_i, \cdots, A^{s-1}r_i\}$. Thus $a_i^1, \cdots, a_i^s$ can be determined by the s conditions

$$\begin{aligned}-(r_i, Ar_i)+a_i^1(Ar_i, Ar_i)+\cdots+a_i^s(Ar_i, A^sr_i)&=0,\\ &\cdots\\ -(r_i, A^sr_i)+a_i^1(A^sr_i, Ar_i)+\cdots+a_i^s(A^sr_i, A^sr_i)&=0.\end{aligned} \tag{3.1}$$

DEFINITION 3.2. For $k=0, \pm1, \pm2, \cdots$, and $z_k=A^kr$ let the moments μ_{kj} of the vector $r\neq 0$ be defined by $\mu_{kj}=z_k^Tz_j$.

Remark 3.1. Let $W_i=(AR_i)^T(AR_i)$ and $m_i=r_i^TAR_i$ where $R_i=[r_i, \cdots, A^{s-1}r_i]$. The system (3.1) above can be written as $W_i\underline{a}=m_i$ where $\underline{a}=[a_i^1, \cdots, a_i^s]^T$.

The matrix W_i is nonnegative semidefinite [3]. It is positive definite if the subspace R_i has dimension s.

Remark 3.2. The error functional $E(x)$ has a nontrivial minimum $x_{i+1}\neq x_i$ on the affine subspace L_i if the zeroth moment of A^j, $j=1, \cdots, s$ with respect to the vector r_i is nonzero for at least one index j.

Proof. Consider the approximate solution $\bar{x}_{i+1}=x_i+(\mu_{0,j}/\mu_{j,j})A^{j-1}r_i$. Since $\mu_{0,j}\neq 0$ the inequality $E(x_{i+1})\leqq E(\bar{x}_{i+1})<E(x_i)$ holds. □

The condition $m_i\neq 0$ guarantees that a (unique) solution $\underline{a}\neq 0$ exists for W_i nonsingular. If W_i is singular then it has rank greater than or equal to 1, because $r_i\neq 0$ implies that the entry $\mu_{1,1}\neq 0$. In this case $\underline{a}$ can be computed by using the generalized inverse of W_i.

Remark 3.3. If A is definite $E(x)$ has a nontrivial minimum, because $\mu_{0,1}=(r_i, Mr_i)>0$ where M is the symmetric part of A.

Remark 3.4. The s-step MR method in exact arithmetic generates the same iterates x_i as the GMRES (s) method. However, GMRES (s) is stable, for large s, because it forms an orthonormal basis for the Krylov basis which generates the affine subspace L_i. The s-step MR may suffer from instability for large s.

The rest of this section contains results on convergence of the s-step minimal residual and GMRES (s) methods. All that is needed is to find conditions under which

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the error functional $E(x)$ has a nontrivial minimum in L_i. Let the eigenvalues of a symmetric matrix B of dimension n be denoted by

$$\lambda_n(B) \leqq \cdots \leqq \lambda_1(B).$$

LEMMA 3.1. *For the nonsingular matrix A let $M = (A + A^T)/2$ and $N = (A - A^T)/2$ be its symmetric and skew-symmetric parts. Then the symmetric and skew-symmetric parts of A^2 are $M^2 + N^2$ and $MN + NM$, respectively. The matrices M^2 and N^2 are symmetric with eigenvalues $0 \leqq \lambda_n(M^2) \leqq \cdots \leqq \lambda_1(M^2)$ and $\lambda_n(N^2) \leqq \cdots \leqq \lambda_1(N^2) \leqq 0$, respectively.*

Proof. Computing the symmetric and skew-symmetric part of A^2 yields $M^2 + N^2$ and $MN + NM$, respectively. Since M is symmetric, M^2 is symmetric with positive eigenvalues. Since N is skew symmetric, N^2 is symmetric with negative eigenvalues. $\square$

The following theorem provides sufficient conditions under which s-MR and GMRES (s) (with $s \geqq 2$) converge.

THEOREM 3.1. *Assume that the degree of the minimal polynomial r_0 is greater than $s \geqq 2$. If* (a) *$d = \lambda_n(M^2) + \lambda_n(N^2) > 0$ or* (b) *$d = -[\lambda_1(N^2) + \lambda_1(M^2)] > 0$, then the matrix A^2 is definite and s-*MR *or* GMRES (s) *converge to the solution. The residuals satisfy*

$$(r_{i+1}, r_{i+1}) = \leqq [1 - d^2/\lambda_1(A^{2T}A^2)]^i (r_0, r_0).$$

Proof. It is easy to show that in a direction p_i the residual norm is minimized for $\alpha_i = (r_i, Ap_i)/(Ap_i, Ap_i)$ and the minimum is $\|\bar{r}_{i+1}\|^2 = \|r_i\|^2 - (r_i, Ap_i)^2/Ap_i, Ap_i)$. Now, to prove the inequality note that if the one-dimensional steepest descent in the direction $p_i = Ar_i$ is followed, instead of the steepest descent defined by the s directions R_i, the following inequality is obtained

$$\|r_{i+1}\|_2^2 \leqq \|\bar{r}_{i+1}\|_2^2 = \|r_i\|_2^2 - \frac{(r_i, A^2 r_i)^2}{(A^2 r_i, A^2 r_i)}. \tag{3.2}$$

The following inequality also holds:

$$(r_i, r_i)/(r_i, A^{2T}A^2 r_i) \geqq 1/\lambda_1(A^{2T}A^2). \tag{3.3}$$

Since M^2 and N^2 are symmetric matrices the following inequalities hold

$$\lambda_n(M^2) + \lambda_n(N^2) \leqq \lambda_n(M^2 + N^2), \tag{3.4}$$

$$-[\lambda_1(M^2) + \lambda_1(N^2)] \leqq -\lambda_1(M^2 + N^2) \leqq -\lambda_n(M^2 + N^2). \tag{3.5}$$

Inequality (3.4) or (3.5) combined with assumptions (a) or (b), respectively, yields $|\lambda_n(M^2 + N^2)| \geqq d > 0$. Thus, under (a) or (b) the symmetric part of A^2 is either positive or negative definite and

$$|(r_i, A^2 r_i)/(r_i, r_i)| = |(r_i, [M^2 + N^2] r_i)/(r_i, r_i)| \geqq \min_{k=1,\cdots,n} |\lambda_k(M^2 + N^2)| \geqq d.$$

The last inequality combined with inequalities (3.2) and (3.3) proves the inequality in the theorem statement. $\square$

This result is of interest only for indefinite matrices. Note that in Theorem 3.1 condition (a) means that the matrix A has a *small* skew-symmetric part, while condition (b) means that it has a *large* skew-symmetric part.

COROLLARY 3.1. *For A nonsingular, symmetric, or skew-symmetric indefinite, the s-step* MR *and* GMRES (s) *methods (with $s \geqq 2$) yield residuals satisfying*

$$\|r_{i+1}\|_2^2 \leqq [1-(\lambda_n(A^2))^2/\lambda_1(A^{2T}A^2)]^i(r_0, r_0),$$

and the methods converge.

The following example gives an application of Theorem 3.1.

Example. Let A be of even dimension and with skew-symmetric part consisting of the repeated diagonal block $[\begin{smallmatrix} 0 & -b \\ b & 0 \end{smallmatrix}]$, with $b>0$. If either $d=[-b^2+\lambda_n(M^2)]>0$ or $d=[b^2-\lambda_1(M^2)]>0$ then s-MR and GMRES (s) (with $s \geqq 2$) converge.

In the next section s-step generalizations for the nonsymmetric extensions of conjugate residual in [9] are introduced.

4. The s-step GCR and s-step Orthomin (k) methods. The s-step MR is used to obtain s-step generalizations for GCR and Orthomin (k). The s directions $\{r_i, \cdots, A^{s-1}r_i\}$ are formed and are $A^T A$-orthogonalized simultaneously to all (in GCR) or k (in Orthomin (k)) of the preceding directions $\{p_j^1, \cdots, p_j^s\}_{j=j_i}^{j=i}$, where $j_i=0$ or $i-k+1$ for GCR or Orthomin (k), respectively. The norm of the residual $\|r_{i+1}\|$ is minimized simultaneously in all s new directions in order to obtain x_{i+1}. This method is summarized in the following algorithm.

ALGORITHM 4.1 (The s-step generalized conjugate residual method (s-GCR)).

x_0, $p_0^1=r_0=f-Ax_0, \cdots, p_0^s=A^{s-1}r_0$

For $i=0$ **Until** Convergence **Do**

Select a_i^j to minimize $E(x_{i+1})=\|f-Ax_{i+1}\|$ in

$x_{i+1}=x_i+a_i^1p_i^1+\cdots+a_i^sp_i^s$

over $L_i=\left\{x_i+\sum_{j=1}^{s} a_i^jp_i^j\right\}$

Compute $r_{i+1}=f-Ax_{i+1}$, and $Ar_{i+1}, \cdots, A^{s-1}r_{i+1}$

Select $\{b_j^{(l,m)}\}$ to A^TA-orthogonalize $\{p_{i+1}^1, \cdots, p_{i+1}^s\}$ against $\{p_j^1, \cdots, p_j^s\}_{j=j_i}^{j=i}$, where

$$p_{i+1}^1=r_{i+1}+\sum_{j=j_i}^{i}\{b_j^{(1,1)}p_i^1+\cdots+b_j^{(1,s)}p_j^s\}$$

$$p_{i+1}^2=Ar_{i+1}+\sum_{j=j_i}^{i}\{b_j^{(2,1)}p_j^1+\cdots+b_j^{(2,s)}p_j^s\}$$

$\cdots$

$$p_{i+1}^s=A^{s-1}r_{i+1}+\sum_{j=j_i}^{i}\{b_j^{(s,1)}p_j^1+\cdots+b_j^{(s,s)}p_j^s\}.$$

EndFor

The parameters $\{b_j^{(l,m)}\}$ and a_i^l are determined by solving linear systems of equations of order s. For simplicity in the notation the i index is dropped from the parameters b. Next some notation is introduced in order to specify the algorithm more precisely.

Remark 4.1. (1) Let $W_i=[(Ap_i^j, Ap_i^l)]$, where $1 \leqq j, l \leqq s$.

(2) Let $a_i=[a_i^1, \cdots, a_i^s]^T$ be the steplengths in updating x_i and $\underline{m}_i=[(r_i, Ap_i^1), \cdots, (r_i, Ap_i^s)]^T$.

(3) $\underline{c}_j^l=[(A^lr_{i+1}, Ap_j^1), \cdots, (A^lr_{i+1}, Ap_j^s)]^T$ and $\underline{b}_j^l=\{b_j^{(l,m)}\}_{m=1}^s$ for $j=j_i, \cdots, i$ and $l=1, \cdots, s$.

(4) $P_i=[p_i^1, \cdots, p_i^s]$.

(5) $R_i=[r_i, Ar_i, \cdots, A^{s-1}r_i]$

The notation P_i and R_i will also be used to denote the subspaces generated by $\{p_i^1, \cdots, p_i^s$ and $\{r_i, Ar_i, \cdots, A^{s-1}r_i\}$, respectively.

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The following linear systems of order s must be solved in executing one step of s-step GCR (Orthomin (k)):

$$W_i\underline{a}_i - \underline{m}_i = 0,$$
$$W_j\underline{b}_j^l + \underline{c}_j^l = 0 \quad \text{for } j = j_i, \cdots, i \text{ and } l = 1, \cdots, s,$$

The matrix W_i is invertible if and only if $p_i^1, \cdots, p_i^s$ are linearly independent. This follows from the fact that the bilinear form $(A^T A\cdot, \cdot)$ is an inner product.

Next, both the s-step GCR and the s-step Orthomin (k) are presented in one algorithm.

ALGORITHM 4.2 (The s-step GCR, Orthomin (k) algorithm).

x_0, $P_0 = [r_0 = f - Ax_0, Ar_0, \cdots, A^{s-1}r_0]$

For $i = 0$ **Until** Convergence **Do**

Compute $\underline{m}_i$, W_i

Call Scalar1

$x_{i+1} = x_i + P_i\underline{a}_i$

$r_{i+1} = r_i - AP_i\underline{a}_i$

Compute $\underline{c}_j^i$, $j = j_i, \cdots, i$

Call Scalar2

Compute R_i

$P_{i+1} = R_{i+1} + \sum_{j=j_i}^{i} P_j[\underline{b}_j^l]_{l=1}^m$

Compute AP_{i+1} or,

$AP_{i+1} = AR_{i+1} + \sum_{j=j_i}^{i} AP_j[\underline{b}_j^l]_{l=1}^m$

EndFor

*Scalar*1: Decomposes W_i and solves $W_i\underline{a}_i = \underline{m}_i$.

*Scalar*2: Solves $W_j\underline{b}_j^l = -\underline{c}_j^l$ for $j = j_i, \cdots, i$ and $l = 1, \cdots, s$, where $j_i = 0$, $i - k + 1$ for s-step GCR and s-step Orthomin (k), respectively.

Obviously, for $s = 1$ the algorithm coincides with the standard GCR and Orthomin (k) algorithms. Note that in s-step Orthomin (0), s directions are used to improve the solution. The s-step Orthomin (0) is the s-step MR method. The s-step Orthomin (1) method coincides with s-step conjugate residual if A is SPD [5], [7]. This will be shown in § 5. In general, s will be chosen to be less than k, because s must be small for stability as in the SPD case [5].

The solution of the linear systems may cause a quick loss of orthogonality of the s-dimensional direction subspaces P_i because the matrix W_i may have a very large condition number. Numerical tests [5], [6], [8] have shown that the condition number of W_i is small for $s \leqq 5$. For $s > 5$ iterative refinement could be used, without increasing the amount of vector computation (for s small). Also, the direction vectors within each subspace P_i could $A^T A$-orthogonalized. Then no linear systems need be solved at each iteration. However, this would slightly increase the computational work.

5. Convergence of s-step GCR and s-step Orthomin (k). In this section convergence proofs for the s-step methods are given and their relation to their one-step counterparts is discussed. Unlike the standard GCR and Orthomin (k) (i.e., $s = 1$) it will be shown that the s-step GCR and Orthomin (k) converge even for some indefinite matrices.

Next relations among the direction and the residual vectors of s-GCR (see [9] for analogous relations for GCR) are established. This will prove the convergence of s-GCR in at most $\lceil n/s \rceil$ iterations.

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THEOREM 5.1. *Let A be either definite or indefinite with A^s definite. The solution vectors x_i and the subspaces R_i, P_i generated by s-GCR at the ith iteration satisfy the following relations provided that the degree of the minimal polynomial of r_0 does not exceed $s(i+1)$ and $s(i+1) \leqq n$.*

(i) *P_i is $A^T A$-orthogonal to P_j for $i \neq j$,*
(ii) *r_i is orthogonal to AP_j for $i > j$,*
(iii) *$(r_i, Ap_i^l) = (r_i, A^l r_i)$ for $l = 1, \cdots, s$,*
(iv) *r_i is orthogonal to AR_j for $i > j$,*
(v) *AP_i is orthogonal to AR_j for $i > j$,*
(vi) *$(Ap_i^l, Ap_i^j) = (Ap_i^l, A^j r_i)$ for $1 \leqq l, j \leqq s$,*
(vii) *$(r_j, Ap_i^l) = (r_0, Ap_i^l)$ for $j \leqq i$ and $1 \leqq l \leqq s$.*
(viii) *$\{R_0, R_1, \cdots, R_i\} = \{P_0, P_1, \cdots, P_i\} = \{r_0, Ar_0, \cdots, A^{(i+1)s-1} r_0\}$.*
(ix) *If $r_i \neq 0$, then $a_{i-1}^s \neq 0$.*
(x) *x_{i+1} minimizes $\|r_{i+1}\|_2^2$ over the translated subspace $x_0 + \{P_0, \cdots, P_i\}$.*

Proof. The definition of the direction vectors P_i implies (i). From $r_i = r_{i-1} - AP_{i-1}\underline{a}_{i-1}$ and (i), (ii) follows by induction. The defining relations for $\{p_i^1, \cdots, p_i^s\}$ and (ii) give (iii).

To prove (iv) the defining identity for AP_j is rewritten

$$AR_j = AP_j - l\{AP_{j-1}, \cdots, AP_0\}$$

where $l\{\ \}$ is a linear combination of the vectors involved. Then (iv) is obtained by use of (ii). The same equation and (i) gives (v). Condition (vi) is shown from the definition of p_i^j, $j = 1, \cdots, s$ and (i). The identity $r_j = r_{j-1} - AP_{j-1}\underline{a}_{j-1}$ and induction give (vii).

To prove (viii) note that the Krylov subspace basis contains the other two sets of vectors defined in (viii). Also, it is easy to check that $\{P_0, \cdots, P_i\}$ is contained in $\{R_0, \cdots, R_i\}$ because every direction can be written in terms of $A^l r_i$, $l = 1, \cdots, s$. By (i) the dimension of $\{P_0, \cdots, P_i\}$ equals $(i+1)s$, which is the dimension of the Krylov basis given as the last set in (viii). Therefore all the subspaces are equal.

Condition (ix) states that the new (nonzero) residual lifts the iteration out of the current Krylov subspace. Then the assumption on the degree of the minimal polynomial of r_0 proves that the directions $\{p_i^1, \cdots, p_i^s\}$ are independent.

First, let A be definite. If Gramm-Schmidt $A^T A$-orthogonalization of P_i starting with the vector p_i^1 is used, we can see that the definiteness of A guarantees that $a_i^j \neq 0$ for $j = 1, \cdots, s$, as in the standard GCR. Second, let A be indefinite with A^s definite; then $(r_{i-1}, Ap_{i-1}^s) = (r_{i-1}, A^s r_{i-1}) > 0$. Minimizing $\|r_{i+1}\|$ only along the direction p_i^s implies

$$a_i^s = (r_i, Ap_i^s)/(Ap_i^s, Ap_i^s) = (r_i, A^s r_i)/(Ap_i^s, Ap_i^s) > 0.$$

Now, since the step $x_{i+1} = x_i + P_i\underline{a}_i$ gives the minimum residual norm in the subspace P_i it is clear that $a_i^s \neq 0$. This can be easily checked if we use Gramm-Schmidt A^T A-orthogonalization of P_i starting with the vector p_i^s, and then obtain the steplengths a_i^j.

To prove (x) the norm of the residual is expanded as follows:

$$\|r_{i+1}\| = (r_0, r_0) - 2 \sum_{j=0}^{i} \sum_{l=1}^{s} a_j^l (r_0, Ap_j^l) + \sum_{j=0}^{i} \sum_{m=1}^{s} \sum_{l=1}^{s} a_j^l a_j^m (Ap_j^m, Ap_j^l).$$

Since $(r_0, Ap_j^l) = (r_j, Ap_j^l)$ by (vii), the above expression can be rewritten in matrix form:

$$\|r_{i+1}\| = (r_0, r_0) - 2 \sum_{j=0}^{i} \underline{a}_j^T \underline{m}_j + \sum_{j=0}^{i} \underline{a}_j^T W_j \underline{a}_j.$$

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Now it can be seen that minimizing $\|r_{i+1}\|$ over the affine subspace $x_0+\{P_0, \cdots, P_i\}$ is equivalent to solving the linear systems

$$W_j \underline{a}_j = \underline{m}_j, \qquad j=0, \cdots, i.$$

This is precisely the definition of $\underline{a}_j$ in s-GCR and (x) is proved. □

COROLLARY 5.1. *Under the assumptions of Theorem* 5.1 *the s-step* GCR *converges to the solution in at most* $\lceil n/s \rceil$ *iterations. If the matrix A is definite and* x_0 *is the same for* GCR *and s*-GCR *then* x_{si} *of* GCR *is the same (in exact arithmetic) as* x_i *of s*-GCR.

Proof. The first claim follows from Theorem 5.1 (iv) and (viii), and the second claim follows from (x). □

The following theorem, whose proof is completely analogous to Theorem 5.1, shows the relations satisfied by the vectors generated by s-Orthomin (k). This theorem shows that s-Orthomin (k) is a generalization of Orthomin (k) for A definite. Furthermore, the iteration does not break down for a class of nonsymmetric indefinite matrices.

THEOREM 5.2. *Let A be either definite or indefinite with* A^s *definite. The solution vectors* x_i *and the subspaces* R_i, P_i *generated by s-Orthomin* (k) *at the ith iteration satisfy the following relations provided that the degree of the minimal polynomial of* r_o *does not exceed* $s(i+1)$ *and* $s(i+1) \leqq n$.

(i) P_i *is* $A^T A$*-orthogonal to* P_j *for* $j=i-k, \cdots, i-1$, $i \geqq k$,

(ii) r_i *is orthogonal to* AP_j *for* $j=i-k-1, \cdots, i-1$, $i \geqq k+1$,

(iii) $(r_i, Ap_i^l)=(r_i, A^l r_i)$ *for* $l=1, \cdots, s$,

(iv) r_i *is orthogonal to* AR_{i-1},

(v) $(Ap_i^l, Ap_i^j)=(Ap_i^l, A^j r_i)$ *for* $1 \leqq j, l \leqq s$, $j=i-k, \cdots, i$, *and* $k \leqq i$.

(vi) $(r_j, Ap_j^l)=(r_{i-k}, Ap_i^l)$ *for* $1 \leqq l \leqq s$.

(vii) *If* $r_i \neq 0$, *then* $a_{i-1}^s \neq 0$.

(viii) x_{i+1} *minimizes* $\|r_{i+1}\|$ *over the space* $x_{i-k}+\{P_{i-k}, \cdots, P_i\}$.

REMARK 5.1. If A is indefinite and the assumptions of Theorem 3.1 hold, then A^2 is definite and Theorems 5.1 and 5.2 hold with $s=2$.

Next it is proved that s-Orthomin (k) converges but may require an infinite number of steps. The following theorem gives a bound on the norm of the residual error for all the s-step methods considered here. Theorem 5.3 and Proposition 5.1 are an adaptation of results on GCR and Orthomin (k) in [9].

THEOREM 5.3. *Let* $\{r_i\}$ *be the residual vectors generated by s-Orthomin* (k), *s*-GCR, *s*-MR *or* GMRES (s). *The following inequalities on the norm of the residual error hold. For A definite,*

$$\|r_{i+1}\|_2^2 \leqq \left[1-\frac{\lambda_n(M)^2}{\lambda_1(A^T A)}\right]^s \|r_i\|_2^2.$$

For A indefinite, A^s *definite, with s even,* $s \geqq 2$, *and under the hypothesis* (a) *or* (b) *of Theorem* 3.1,

$$\|r_{i+1}\|_2^2 \leqq [1-d^2/\lambda_1(A^{2T}A^2)]^{s/2} \|r_i\|_2^2.$$

Proof. Consider the s-step minimal residual method at the ith iterate x_i of s-Orthomin (k). The iterate and the residual given by s-MR are

$$\bar{x}_{i+1}=\bar{x}_i+a_i^1 r_i+\cdots+a_i^s A^{s-1} r_i,$$

$$\bar{r}_{i+1}=\bar{r}_i-a_i^1 A r_i-\cdots-a_i^s A^s r_i$$

where $P_i=\{r_i, \cdots, A^{s-1} r_i\}$ is the direction subspace of the s-dimensional steepest descent, and $W_i \underline{a}_i=\underline{m}_i$. The matrix W_i of inner products of the subspace P_i has the

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special form

$$W_i = [(A^{l+1}r_i, A^{k+1}r_i)], \qquad 1 \leqq l, k \leqq s,$$

and $\underline{m}_i = [(r_i, Ar_i), \cdots, (r_i, A^s r_i)]^T$. The matrix W_i of moments is positive definite as long as the degree of the minimal polynomial of r_i is greater than or equal to s. Since the residual r_{i+1} generated by GCR, s-Orthomin (k) ((iv) of Theorem 5.1, Theorem 5.2) is orthogonal to AR_i the inequality $\|r_{i+1}\|_2 \leqq \|\bar{r}_{i+1}\|_2$ follows.

If A is definite then the first iterate of s-MR is the same as the sth iterate of GCR. This is because the two methods minimize the same error functional on the same translated Krylov subspace $x_0 + \{r_0, \cdots, A^{s-1}r_o\}$. Using s iterations of 1-MR we obtain the bound for the definite case

$$\|r_{i+1}\|_2^2 \leqq \|\bar{r}_{i+1}\|_2^2 \leqq \|r_i\|_2^2 \left[1 - \frac{\lambda_n(M)}{\lambda_1(A^TA)}\right]^s.$$

Similarly, we obtain the bound for the indefinite case by use of Theorem 3.1 and $s/2$ iterations of 2-MR. □

Let Π denote the set of polynomials q_i of degree not exceeding $s(i+1)$ such that $q_i(0) = 1$. The spectrum of A is denoted by $\sigma(A)$. The Jordan canonical form of A is denoted by $J = T^{-1}AT$. The condition number of the nonsingular matrix T is defined as $k(T) = \|T\|_2 \|T^{-1}\|_2$.

PROPOSITION 5.1. *Let $\{r_i\}$ be the residual vectors generated by s*-GCR. *Then for A indefinite, A^s definite, with s even, $s \geqq 2$ and under the hypothesis* (a) *or* (b) *of Theorem* 3.1,

$$\|r_i\|_2^2 \leqq \min_{q_{s(i+1)} \in \Pi} \|q_{s(i+1)}(A)\|_2^2 \|r_0\|_2^2 \leqq [1 - d^2/\lambda_1(A^{2T}A^2)]^{s(i+1)/2} \|r_0\|_2^2.$$

If A has a complete set of eigenvectors then

$$\|r_i\|_2^2 \leqq \kappa(T)\Lambda_{s(i+1)} \|r_o\|_2^2$$

where

$$\Lambda_{s(i+1)} := \min_{q_{s(i+1)} \in \Pi} \max_{\lambda \in \sigma(A)} |q_{s(i+1)}(\lambda)|$$

If the matrix A is normal then $\|r_i\|_2^2 \leqq \Lambda_{s(i+1)} \|r_0\|_2^2$.

Proof. From $r_i = r_{i-1} - AP_{i-1}\underline{a}_{i-1}$ and Theorem 5.1 (ix) it follows that $r_i = q_{s(i+1)}(A)r_0$ for some polynomial $q_{s(i+1)}$ in Π. Theorem 5.1 (x) implies that $\|r_i\|_2^2 = \min_{q_{s(i+1)} \in \Pi} \|q_{s(i+1)}(A)r_0\|_2^2$ and the first inequality is proved.

The polynomial $q_2(\lambda) = 1 + \alpha\lambda^2$ is used to obtain

$$\min_{q_{s(i+1)} \in \Pi} \|q_{s(i+1)}(A)\|_2^2 \|r_0\|_2^2 \leqq \|[q_2(A)]^{s(i+1)/2}\|_2^2 \|r_0\|_2^2 \leqq \|q_2(A)\|_2^{s(i+1)/2} \|r_0\|_2^2.$$

Since

$$\|q_2(A)\|_2^2 = \max_{x \neq 0} \left[1 + 2\alpha \frac{(x, A^2x)}{(x, x)} + \alpha^2 \frac{(A^2x, A^2x)}{(x, x)}\right]$$

and

$$\frac{(A^2x, A^2x)}{(x, x)} \leqq \lambda_1(A^{2T}A^2),$$

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and by Theorem 3.1 the symmetric part of A^2 is either positive or negative definite and

$$\left|\frac{(x, A^2x)}{(x, x)}\right| \geqq \min_{k=1,\cdots,n} |\lambda_k(M^2+N^2)| \geqq d > 0.$$

Thus, the following inequality is true:

$$\|q_2(A)\|_2^2 \leqq 1 + 2\alpha d + \lambda_1(A^{2T}A^2)\alpha^2.$$

The right-hand side expression is minimized by $\alpha = d/\lambda_1(A^{2T}A^2)$, giving a minimum of $[1-(d^2/\lambda_1(A^{2T}A^2))$. This proves the second inequality. The third and fourth inequality can be easily proved by considering the Jordan decomposition of A. □

If the spectrum of A lies entirely in the positive or negative open half plane then an analysis by Manteuffel [15] shows that $\min_{q_{s(i+1)}\in\Pi}\|q_{s(i+1)}(A)\|_2^2$ and $\Lambda_{s(i+1)}$ approach zero as $i \to \infty$ which also implies convergence of s-GCR.

COROLLARY 5.2. *Let $\{r_i\}$ with $i = j(k+1)$ be the residual vectors generated by s-GCR (k). For A indefinite, A^s definite, with s even, $s \geqq 2$ and under the hypothesis* (a) *or* (b) *of Theorem* 3.1,

$$\|r_{j(k+1)}\|_2^2 \leqq \left[\min_{q_{s(k+1)}\in\Pi} \|q_{s(k+1)}(A)\|_2^2\right]^j \|r_0\|_2^2,$$

and hence

$$\|r_i\|_2^2 \leqq [1 - d^2/\lambda_1(A^{2T}A^2)]^{s(i+1)/2}\|r_0\|_2^2.$$

Thus, s-GCR (k) converges. If A has a complete set of eigenvectors then

$$\|r_{j(k+1)}\|_2^2 \leqq [\kappa(T)\Lambda_{s(k+1)}]^i \|r_0\|_2^2.$$

If the matrix A is normal then $\|r_{i(k+1)}\|_2^2 \leqq [\Lambda_{s(k+1)}]^i \|r_0\|_2^2$.

Proof. The proof follows from Theorem 5.1 and Proposition 5.1. □

Residual error bounds, which involve the spectral radius of the skew-symmetric part of A, are now given. The next lemma can be found in [9].

LEMMA 5.1. *For any real vector $x \neq 0$ and A positive definite,*

$$\frac{(x, Ax)}{(Ax, Ax)} \geqq \frac{\lambda_n(M)}{\lambda_n(M)\lambda_1(M) + \rho(N)^2} := c_1$$

where $\rho(N)$ is the spectral radius of the skew-symmetric part of A.

Proof. See [9]. □

If this lemma is applied to the matrix A^2 or $-A^2$ the following inequality is obtained.

COROLLARY 5.3. *If A is definite or indefinite under the hypothesis of Theorem* 3.1 *then the following inequality holds*:

$$\frac{(x, A^2x)}{(A^2x, A^2x)} \geqq \frac{d}{dd_1 + \rho(MN+NM)^2} := c_2$$

where $d_1 = \max_{k=1,\cdots,n} |\lambda_k(M^2+N^2)|\}$ and (M^2+N^2), $(MN+NM)$ is the symmetric and skew-symmetric part of A^2, respectively.

Proof. By the assumptions A^2 is positive or negative definite. The inequality follows by using Theorem 3.1 and by applying Lemma 5.1 to A^2 or $-A^2$. □

THEOREM 5.4. *Let $\{r_i\}$ be the residual vectors generated by s-*Orthomin (k), s-GCR, s-MR *and* GMRES (s). *Then for A definite*

$$\|r_{i+1}\|_2^2 \leqq [c_1]^s \|r_i\|_2^2,$$

and for A indefinite, A^s definite, with s even, $s \geqq 2$, and under the hypothesis (a) *or* (b) *of Theorem* 3.1,

$$\|r_{i+1}\|_2^2 \leqq [c_2]^{s/2} \|r_i\|_2^2.$$

Proof. As in Theorem 5.3 the proof is reduced to proving the inequalities for the s-MR case. Then by making use of Corollary 5.3 in a way similar to proving Theorem 3.1, the inequalities are proved. □

Next, it is shown that if the matrix is symmetric, skew-symmetric, or its symmetric part is the identity matrix, then s-Orthomin (1) is equivalent to s-GCR.

THEOREM 5.5. *If $A = M$, $A = N$, or $A = I - N$, with M and N symmetric and skew-symmetric, respectively, then* s-Orthomin (1) *is equivalent to* s-GCR.

Proof. It suffices to show that $\underline{b}_j^i = 0$ for $j \leqq i-1$. From Remark 3.1 this is true if $\underline{c}_j^i = [(Ar_{i+1}, Ap_j^1), \cdots, (A^s r_{i+1}, Ap_j^s)]^T = 0$ for $j \leqq i-1$.

It must be shown that

$$(A^\kappa r_{i+1}, Ap_j^\nu) = 0$$

for $\kappa, \nu = 1, \cdots, s$.

(i) For $A = M$, or $A = N$ this is equivalent to

$$(r_{i+1}, A^\kappa (Ap_j^\nu)) = 0$$

for $\kappa, \nu = 1, \cdots, s$ and $j \leqq i-1$; this is true from Theorem 5.1 (ii) and (vii).

(ii) For $A = I - N$, it follows that

$$(Ar_{i+1}, Ap_j^\nu) = (r_{i+1}, Ap_j^\nu) + (r_{i+1}, NAp_j^\nu) = -(r_{i+1}, A^2 p_j^\nu)) = 0.$$

Since $A^2 = I - 2N + N^2$ and $((I - 2N) r_{i+1}, Ap_j^\nu) = 0$ from the preceding cases, it follows that

$$(A^2 r_{i+1}, Ap_j^\nu) = (N^2 r_{i+1}, Ap_j^\nu) = (r_{i+1}, N^2 Ap_j^\nu) = (r_{i+1}, A^2 Ap_j^\nu) = 0.$$

The cases $(A^\kappa r_{i+1}, Ap_j^\nu) = 0$ for $\kappa = 3, \cdots, s$ follow inductively. □

COROLLARY 5.5. *For A indefinite and A^s definite, with s even and $s \geqq 2$, and under the assumptions of Theorem* 3.1, s-Orthomin (1) *converges in at most $\lceil n/s \rceil$ iterations.* □

Next, the s-step methods are compared to their one-step counterparts.

6. Work and storage comparison of s-step and one-step methods. In this section the computational work and storage of the s-step methods is compared to the standard ones. The vector work and storage for the single iteration of an s-step method is given in Table 6.1. For comparison of the mathematically equivalent methods GMRES (s)

TABLE 6.1
Vector operations for the jth iteration of the s-step (GCR, Orthomin (k), MR, GCR (k)), *and* GMRES (s); $s_1 = s(s+1)/2 + s$.

Vector operation	s-GCR	s-Orthomin (k)	s-GCR (k)	s-MR	GMRES (s)
Dotprods	$(j+1)s^2 + s_1$	$\min([(j+1)s^2 + s_1], [ks^2 + s_1])$	$(j \bmod (k) + 1)s^2 + s_1$	s_1	s_1
Vupdates	$2(j+1)s^2 + s$	$\min([2(j+1)s^2 + s], [2ks^2 + s])$	$2(j \bmod (k) + 1)s^2 + s$	$2s$	s_1
Matvecs	s	s	s	s	s
Storage	$2(j+1)s + 2$	$(2ks + s + 1)$	$(2ks + 2s + 1)$	$s + 2$	$s + 2$

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and s-MR the work for GMRES (s) is included. Note that the work for the s-Orthomin (k) is (a) the same as s-GCR if $j \leqq k-1$ and (b) the same as iteration $k-1$ of s-GCR if $(k-1)<j$. Storage (at the $(i-1)$-th iteration) includes the matrix A and the vectors: x_i, r_i, AR_i, $\{P_j\}_{j=j_i}^{j=i}$, $\{AP_j\}_{j=j_i}^{j=i}$; for s-GCR the vectors AR_i are stored in AP_{i+1}.

Next, the s-step methods are compared to the standard ones.

Remark 6.1. Let A be definite and let the s-step and the standard methods start with the same initial solution iterate x_0. The iterate x_i produced at the $i-1$ iteration of the s-step methods s-MR is the same as x_{si} produced at the $si-1$ iteration of GCR(s). Similarly, the iterate produced at the $i-1$ iteration of s-GCR, s-GCR (k) is the same as the iterate produced at the $si-1$ iteration of GCR, GCR$((k+1)s)$, respectively. The proof of this remark is derived from Theorem 5.1(ii).

From Theorems 4.1(b) in [9] and 5.2(ii) in this paper, it follows that the methods Orthomin $((k+1)s-1)$ and s-Orthomin (k), respectively, minimize the norm of the residual error on two different subspaces of the same dimension $(k+1)s$. This does not imply that the two methods produce (in exact arithmetic) the same solution iterates. Nevertheless, it seems useful to compare the work and storage of these two methods.

It is clear that in order to obtain (in exact arithmetic) the same iterate from the s-step methods and their equivalent standard ones the same matrix vector products are needed. However, the linear combinations (measured as vector updates) and the dotproducts may vary. Table 6.2 contains the total number of the dotproducts and vector updates for computing the iterate x_i of s-step GCR and Orthomin (k) and the iterate x_{si} of their one-step equivalent methods. The table entries for GCR and s-GCR can be easily derived from Tables 2.1 and 6.1.

TABLE 6.2
Vector operations to form x_{si} of GCR *and* Orthomin $((k+1)s-1)$ *or x_i of* s-GCR *and* s-Orthomin (k); $s_1 = s(s+1)/2+s$.

Vector operation	GCR	s-GCR	Orthomin $((k+1)s-1)$	s-Orthomin (k)
Dotprods	$(i^2s^2+5si)/2$	$(s^2i^2+3si)/2$	$si[(k+1)s+1]-$ $(k+1)s[k+1)s-5]/2$	$i(ks^2+s_1)-$ $s(k^2+3ks+1)/2$
Vupdates	i^2s^2+4si	$s^2i(i-1)+2si$	$2s^2i(k+1)-$ $(k+1)s[(k+1)s-5]-2$	$2iks^2-$ $s^2(k^2+3k-2)+2s(2s-1)$

The gap in vector computations in the case of GCR and s-GCR can be easily read off Table 6.2. For Orthomin $((k+1)s-1)$ and s-Orthomin (k), consider only the terms involving i and ignore the rest assuming that k and s are small. Then Orthomin $((k+1)s-1)$ requires $is(s-1)/2$ more inner products and $2s^2i$ more vector updates than the s-Orthomin (k). This is due to the fact that in s-step methods the directions within the s-dimensional subspaces P_i are not orthogonalized. Note that the storage for s-Orthomin (k) is increased by s vectors compared to the storage of Orthomin $((k+1)s-1)$.

7. Summary and future work. s-step generalizations of some Krylov subspace based iterative methods for nonsymmetric linear systems of equations have been derived. It is proved that the s-step GCR, s-step Orthomin (k) and s-step MR methods converge for all symmetric, nonsymmetric definite, and some nonsymmetric indefinite coefficient matrices. The GMRES(s) method in exact arithmetic gives the same solution iterate as the s-step MR method. Thus all the convergence theorems proved for s-MR apply

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for the GMRES(s) method. In [8] the s-step GMRES(m) method is derived and comparisons to the methods derived here are made on parallel vector computers.

Numerical tests [8] on problems arising in the discretization of elliptic partial differential equations suggest that they are stable for small s ($s \leqq 5$). The basic vector computations (inner products, vector updates, matrix vector products) are grouped together in the s-step methods and thus they are expected to have superior performance to the standard methods on parallel and vector computers. The implementation of these methods on parallel vector computers is the subject of work which will be published elsewhere.

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