SIAM J. NUMER. ANAL.
Vol. 24, No. 1, February 1987

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ORTHOGONAL ERROR METHODS*

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Abstract. In this paper we discuss the conjugate gradient method generalized to nonsymmetric matrices, constructing a class of algorithms that includes both the conjugate gradient algorithms as described in [12] and the orthogonal residual algorithms (cf. Elman [10]). We call this class orthogonal error algorithms and characterize the class of matrices for which finite term orthogonal error algorithms exist.

Key words. conjugate gradient, nonsymmetric, orthogonal residual

AMS(MOS) subject classification. 65F10

1. Introduction. The conjugate gradient method for symmetric positive definite matrices has proved very effective, especially when coupled with preconditioning techniques (cf. [2], [17], [21], [22], [25], [34]). A generalization of this method to nonsymmetric matrices has long been sought. One generalization, which we call the conjugate gradient method, involves optimizing at each step over a Krylov space in some inner product norm. In [12] we characterized the class, $CG(s)$, of matrices for which this iteration can be carried out using an s-term recursion. We showed that, except for a few anomalies, the class $CG(s)$ consists of matrices A for which conjugate gradient methods are already known.

In this paper we describe a generalization of conjugate gradient methods that we shall call orthogonal error methods. Given a bilinear form that does not include zero in its field of values, an algorithm can be constructed in which updates to the partial solution are chosen from the Krylov space of dimension i in such a way that the error is "orthogonal" to this same Krylov space. Such a bilinear form is an inner product if it is also positive and symmetric. If it is an inner product, then this algorithm is a conjugate gradient algorithm as defined in [12]. If it is not symmetric, then the concepts of orthogonal vectors, adjoint operators and normal operators must be modified. In this paper we characterize the class of matrices for which this iteration can be carried out using an s-term recursion.

In § 2 we show that if zero is not in the field of values of the bilinear form, an orthogonal error method exists and is uniquely defined. We establish a criterion for the existence of an s-term recursion. In § 3 we establish necessary and sufficient conditions for this criterion to be met. In so doing, we generalize the concept of normal operator from inner products to definite bilinear forms. In § 4 we discuss the implications of these results. We show that these results provide an easy way to prove the existence of known algorithms and demonstrate several new algorithms.

This paper is an extension of the work in [12]. The development is similar but now includes orthogonal residual methods (cf. Elman [10]) as well as conjugate gradient methods. These results suggest that to apply a three-term conjugate gradient-like algorithm to a linear system, one must find a preconditioning for which the preconditioned linear system has its spectrum on some straight line in the complex plane and a bilinear form for which the preconditioned system is normal and for which the parameters are computable.

* Received by the editors November, 1984; accepted for publication (in revised form) March 11, 1986.

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2. Orthogonal error methods. Given the linear system $A\mathbf{x}=\mathbf{b}$ and an initial guess $\mathbf{x}_0$, we consider iterations of the form

$$\mathbf{x}_{i+1}=\mathbf{x}_i+\sum_{j=0}^{1}\eta_{ij}\mathbf{r}_j,\qquad \mathbf{r}_j=\mathbf{b}-A\mathbf{x}_j, \tag{1}$$

that is, at each step the partial solution is incremented by some linear combination of the previous residual vectors (cf. Rutishauser [27], Engeli et al. [11]).

If $\eta_{ii}\neq 0$ for every i, then it is easy to show (cf. [12]) that the space spanned by the first i residuals is equal to the Krylov space of dimension i generated by A and $\mathbf{r}_0$; that is,

$$V_i=\{\mathbf{r}_0, A\mathbf{r}_0,\cdots, A^{i-1}\mathbf{r}_0\}=\{\mathbf{r}_0,\mathbf{r}_1,\cdots,\mathbf{r}_{i-1}\}. \tag{2}$$

The Cayley-Hamilton theorem (cf. Gantmacher [13, p. 83]) implies that if A is nonsingular, then A^{-1} can be written as a polynomial in A, and thus the initial error $\mathbf{e}_0=\mathbf{x}-\mathbf{x}_0$ can be written as

$$\mathbf{e}_0=A^{-1}\mathbf{r}_0\in V_d$$

for some d. Let the smallest such d be denoted by $d(\mathbf{r}_0)$. Since the residual vectors span the Krylov spaces, the proper choice of the η_{ij}'s in (1) will yield a solution after $d(\mathbf{r}_0)$ steps.

The problem, of course, is choosing the η_{ij}'s properly. One way is to enforce an optimality condition. Given an inner product, we may choose to minimize the error vector, $\mathbf{e}_i=\mathbf{x}-\mathbf{x}_i$, in the associated norm at every step. This is known as a conjugate gradient iteration and is discussed in [12]. Because the norm is minimized at each step, the solution will be reached in $d(\mathbf{r}_0)$ steps.

Another way to choose the η_{ij}'s so that the solution will be reached in $d(\mathbf{r}_0)$ steps is to force an orthogonality condition. Clearly, $\mathbf{e}_i\in V_d$ for every i. If we force $\mathbf{e}_i$ to be "orthogonal" to V_i, then $\mathbf{e}_d$ must be "orthogonal" to itself. This motivates the algorithm.

Suppose we are given a bilinear form such that

$$[\mathbf{x},\bar{\mathbf{x}}]\neq 0\quad\text{for every } \mathbf{x}\neq 0\quad\text{in } C^N. \tag{3}$$

We shall say that such a bilinear form is definite. By the Riesz Representation Theorem (cf. Royden [26, p. 121]) we know that there exists some matrix B such that

$$[\mathbf{x},\bar{\mathbf{y}}]=\langle B\mathbf{x},\mathbf{y}\rangle\quad\text{for every } \mathbf{x},\mathbf{y}\in C^N.$$

Here $\langle\cdot,\cdot\rangle$ is the standard inner product, $\langle\mathbf{x},\mathbf{y}\rangle=\sum x_i\bar{y}_i$. Let $F(B)=\{\langle B\mathbf{x},\mathbf{x}\rangle\,|\,\mathbf{x}\in C^N\}$ be the field of values of B (cf. Householder [14, pp. 37–57]). The expression (3) is equivalent to

$$0\notin F(B). \tag{4}$$

Note that (4) implies that B is nonsingular. Because a bilinear form that satisfies (4) is not necessarily symmetric, we shall consider a modified or one-sided orthogonality. Suppose we force

$$\langle B\mathbf{e}_i,\mathbf{z}\rangle=0\quad\text{for every } \mathbf{z}\in V_i \tag{5}$$

at every step i. If we write (1) as

$$\mathbf{x}_{i+1}=\mathbf{x}_i+\alpha_i\mathbf{p}_i, \tag{6}$$

where $\mathbf{p}_i \in V_{i+1}$, then

$$\mathbf{e}_{i+1} = \mathbf{e}_i - \alpha_i \mathbf{p}_i,$$

and by (5)

$$\langle B\mathbf{e}_{i+1}, \mathbf{z}\rangle = \langle B\mathbf{e}_i, \mathbf{z}\rangle - \alpha_i \langle B\mathbf{p}_i, \mathbf{z}\rangle = 0 \quad \text{for every } \mathbf{z} \in V_{i+1}. \tag{7}$$

In particular, let $\mathbf{z} = \mathbf{p}_i$ to get

$$\alpha_i = \frac{\langle B\mathbf{e}_i, \mathbf{p}_i\rangle}{\langle B\mathbf{p}_i, \mathbf{p}_i\rangle}. \tag{8}$$

Because $V_i \subseteq V_{i+1}$, (5) and (7) also yield

$$\alpha_i \langle B\mathbf{p}_i, \mathbf{z}\rangle = 0 \quad \text{for every } \mathbf{z} \in V_i. \tag{9}$$

We may conclude that (5) will be satisfied if we can find $\mathbf{p}_i \in V_{i+1}$ such that

$$\langle B\mathbf{p}_i, \mathbf{z}\rangle = 0 \quad \text{for every } \mathbf{z} \in V_i, \tag{10}$$

for every i. The following lemma demonstrates that (10) can be accomplished if $0 \notin F(B)$. Notice that this says that the denominator of (8) must be nonzero.

Before we prove the lemma, let us define $d(A)$ to be the degree of the minimal polynomial of A. We have

$$d(A) = \max_{\mathbf{p} \in C^N} d(\mathbf{p}).$$

LEMMA 1. *If B is such that $0 \notin F(B)$, then there exists a unique (up to constant multiplier) basis for V_d,*

$$V_d = \{\mathbf{p}_0, \cdots, \mathbf{p}_{d-1}\},$$

such that $\mathbf{p}_i \in V_{i+1}$ and

$$\langle B\mathbf{p}_i, \mathbf{z}\rangle = 0 \quad \textit{for every } \mathbf{z} \in V_i$$

for $i = 0, \cdots, d-1 = d(\mathbf{r}_0) - 1$.

Proof. The proof is both inductive and constructive. Let $\mathbf{p}_0 = \mathbf{r}_0$ and

$$\mathbf{p}_1 = A\mathbf{p}_0 - \beta_{00}\mathbf{p}_0, \beta_{00} = \frac{\langle BA\mathbf{p}_0, \mathbf{p}_0\rangle}{\langle B\mathbf{p}_0, \mathbf{p}_0\rangle}.$$

Because $0 \notin F(B)$, β_{00} exists. If $d(\mathbf{r}_0) > 1$, then $\mathbf{p}_1, \mathbf{p}_0$ are linearly independent and therefore span V_2. Uniqueness follows easily. Now assume the result for $j \leqq i$ and let

$$\mathbf{p}_{i+1} = A\mathbf{p}_i - \sum_{j=0}^{i} \beta_{ij}\mathbf{p}_j.$$

Taking inner products yields the system

$$\begin{pmatrix} \langle B\mathbf{p}_0, \mathbf{p}_0\rangle & & 0 \\ \langle B\mathbf{p}_0, \mathbf{p}_1\rangle & \langle B\mathbf{p}_1, \mathbf{p}_1\rangle & \\ \vdots & & \ddots \\ \langle B\mathbf{p}_0, \mathbf{p}_i\rangle & \cdots & \langle B\mathbf{p}_i, \mathbf{p}_i\rangle \end{pmatrix} \begin{pmatrix} \beta_{i0} \\ \beta_{i1} \\ \vdots \\ \beta_{ii} \end{pmatrix} = \begin{pmatrix} \langle BA\mathbf{p}_i, \mathbf{p}_0\rangle \\ \langle BA\mathbf{p}_i, \mathbf{p}_1\rangle \\ \vdots \\ \langle BA\mathbf{p}_i, \mathbf{p}_i\rangle \end{pmatrix}.$$

Because $0 \notin F(B)$, this is a nonsingular system and has a unique solution. If $i+1 < d(\mathbf{r}_0)$, then $A\mathbf{p}_i$ is independent of V_{i+1}, and so

$$V_{i+2} = \{\mathbf{p}_0, \cdots, \mathbf{p}_{i+1}\}.$$

Uniqueness is established by the standard orthogonality proof as follows. Assume $\tilde{\mathbf{p}}_{i+1} \in V_{i+2}$ and $\langle B\tilde{\mathbf{p}}_{i+1}, \mathbf{z}\rangle = 0$ for every $\mathbf{z} \in V_{i+1}$. Because the $\mathbf{p}$'s form a basis, we have

$$\tilde{\mathbf{p}}_{i+1} = \sum_{j=0}^{i+1} \alpha_j \mathbf{p}_j.$$

Taking inner products, starting with $\mathbf{p}_0$, yields $\alpha_0 = \alpha_1 = \cdots = \alpha_i = 0$. Thus $\tilde{\mathbf{p}}_{i+1} = \alpha_{i+1}\mathbf{p}_{i+1}$. This completes the proof. □

We summarize the above discussion by exhibiting the orthogonal error algorithm. Given a bilinear form, $[\cdot,\cdot] = \langle B\cdot,\cdot\rangle$, with $0 \notin F(B)$, and initial guess, $\mathbf{x}_0$, the linear system (1) can be solved in $d(\mathbf{r}_0)$ iterative steps as follows: Let

$$\mathbf{p}_0 = \mathbf{r}_0, \tag{11a}$$

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{p}_0, \qquad \alpha_0 = \frac{\langle B\mathbf{e}_0, \mathbf{p}_0\rangle}{\langle B\mathbf{p}_0, \mathbf{p}_0\rangle}, \tag{11b}$$

$$\mathbf{r}_1 = \mathbf{r}_0 - \alpha_0 A\mathbf{p}_0, \tag{11c}$$

and general step

$$\mathbf{p}_{i+1} = A\mathbf{p}_i - \sum_{j=0}^{i} \beta_{ij}\mathbf{p}_j, \tag{12a}$$

where

$$\begin{pmatrix} \langle B\mathbf{p}_0, \mathbf{p}_0\rangle & & & \\ \langle B\mathbf{p}_0, \mathbf{p}_1\rangle & \langle B\mathbf{p}_1, \mathbf{p}_1\rangle & & \\ \vdots & & \ddots & \\ \langle B\mathbf{p}_0, \mathbf{p}_i\rangle & & & \langle B\mathbf{p}_i, \mathbf{p}_i\rangle \end{pmatrix} \begin{pmatrix} \beta_{i0} \\ \beta_{i1} \\ \vdots \\ \beta_{ii} \end{pmatrix} = \begin{pmatrix} \langle BA\mathbf{p}_i, \mathbf{p}_0\rangle \\ \langle BA\mathbf{p}_i, \mathbf{p}_1\rangle \\ \vdots \\ \langle BA\mathbf{p}_i, \mathbf{p}_i\rangle \end{pmatrix}, \tag{12b}$$

$$\mathbf{x}_{i+2} = \mathbf{x}_{i+1} + \alpha_{i+1}\mathbf{p}_{i+1}, \qquad \alpha_{i+1} = \frac{\langle B\mathbf{e}_i, \mathbf{p}_i\rangle}{\langle B\mathbf{p}_i, \mathbf{p}_i\rangle}, \tag{12c}$$

$$\mathbf{r}_{i+2} = \mathbf{r}_{i+1} - \alpha_{i+1} A\mathbf{p}_{i+1}. \tag{12d}$$

Notice that if B is also Hermitian, then the bilinear form is an inner product. In this case the linear system that determines the β_{ij}'s will be diagonal. The orthogonality also implies optimality in the associated norm and the orthogonal error method becomes a conjugate gradient method. For example, if A is positive definite and symmetric, setting $B = A$ yields Hestenes and Stiefel's original algorithm (Hestenes and Stiefel [19]). If $B = A^*A$ then we have the conjugate gradient method that is often called the minimum or conjugate residual algorithm (cf. Chandra [4]).

If $B = A$, and $0 \notin F(A)$, then $B\mathbf{e}_i = \mathbf{r}_i$ and the above algorithm becomes the orthogonal residual algorithm described by Elman [10]. Whenever $B = CA$ with C Hermitian positive definite and $0 \notin F(CA)$, we shall call the resulting algorithm an orthogonal residual method.

Now let us consider under what conditions the calculation of the $\mathbf{p}_i$'s can be carried out using an s-term recursion; that is, under what conditions can (12a, b) be replaced by

$$\mathbf{p}_{i+1} = A\mathbf{p}_i - \sum_{j=i-s+2}^{i} \beta_{ij}\mathbf{p}_j. \tag{13}$$

Because the representation (12a, b) is essentially unique, (13) implies that $\beta_{ij}=0$ for $j+s-1\leqq i$. Examination of (12b) reveals that we must have

(14) $$\langle BA\mathbf{p}_i, \mathbf{p}_j\rangle = 0 \quad \text{for } j+s-1\leqq i,$$

for every i.

We must clarify a fine point here. Since V_{i+1} is of dimension $i+1$, if $d(\mathbf{p}_0)=i+1$, then it is not necessary to compute $\mathbf{p}_{i+1}$ because V_{i+1} contains the solution. Thus, β_{ij} need not be computed. With this in mind, we make the following definition:

An s-term orthogonal error iteration with respect to the definite bilinear form $\langle B\cdot,\cdot\rangle$ exists for the matrix A if and only if for every $\mathbf{p}_0$, $\langle BA\mathbf{p}_i, \mathbf{p}_j\rangle=0$ for every i, j such that $j+s-1\leqq i\leqq d(\mathbf{p}_0)-2$. We shall denote this as $A\in OE(s, B)$.

3. Characterization of $OE(s, B)$. In this section we shall characterize those matrices for which an s-term orthogonal error method exists. In the remainder of this paper we shall assume that the bilinear form is definite.

It is easy to see that if $d(A)\leqq s$, then $A\in OE(s, B)$. The condition in the definition is vacuously true for every $\mathbf{p}_0$ because $s-1>d(\mathbf{p}_0)-2$. The iteration converges in s or fewer steps.

Another sufficient condition is expressed by Lemma 2. Let A^* denote the adjoint of A with respect to the standard inner product. Then

$$\langle BA\mathbf{x}, \mathbf{y}\rangle = \langle BAB^{-1}B\mathbf{x}, \mathbf{y}\rangle = \langle B\mathbf{x}, (BAB^{-1})^*\mathbf{y}\rangle.$$

We let

(15a) $$A^\dagger = (BAB^{-1})^*$$

and say $A^\dagger$ is the right adjoint of A with respect to the definite bilinear form $[\cdot,\cdot]=\langle B\cdot,\cdot\rangle$. Similarly we have

$$\langle B\mathbf{x}, A\mathbf{y}\rangle = \langle A^*B\mathbf{x}, \mathbf{y}\rangle = \langle B(B^{-1}A^*B)\mathbf{x}, \mathbf{y}\rangle.$$

We let

(15b) $$A^x = (B^{-1}A^*B)$$

and say A^x is the left adjoint of A. Notice that $(A^x)^\dagger = (A^\dagger)^x = A$.

LEMMA 2. *If A is such that for every* $\mathbf{p}$, $A^\dagger\mathbf{p}\in\{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\}$, *then* $A\in OE(s, B)$.

Proof. Consider

$$\langle BA\mathbf{p}_i, \mathbf{p}_j\rangle = \langle B\mathbf{p}_i, A^\dagger\mathbf{p}_j\rangle.$$

Now $A^\dagger\mathbf{p}_j = q(A)\mathbf{p}_j$ for some polynomial $q(z)$ of degree $s-2$ or less. (Note that we cannot assume that the polynomial is independent of $\mathbf{p}_j$.) If $j+s-2<i$, then $q(A)\mathbf{p}_j\in V_{j+s-1}\subseteq V_i$. Since $\langle B\mathbf{p}_i, \mathbf{z}\rangle=0$ for every $\mathbf{z}\in V_i$, then $\langle BA\mathbf{p}_i, \mathbf{p}_j\rangle=0$. □

To characterize those matrices that satisfy the hypothesis of Lemma 2, we must first expand the concept of a normal matrix with respect to a definite bilinear form. We make the following definition:

The matrix A is normal with normal degree $n(A)=s$ with respect to the definite bilinear form $\langle B\cdot,\cdot\rangle$ if one of the following equivalent statements is true:

1. $A^\dagger = q_s(A)$, where q_s is a polynomial of degree s, and s is as small as possible.
2. A commutes with $A^\dagger$.
3. A and $A^\dagger$ have the same complete set of eigenvectors.
4. Any of the above is true with $A^\dagger$ replaced by A^*.

We shall prove the equivalence of the four statements in Theorem 4. First, let us establish some useful results that carry over from the case in which the definite bilinear form is an inner product.

LEMMA 3. *If λ is an eigenvalue of A, then $\bar{\lambda}$ is an eigenvalue of $A^\dagger$ and A^*. Let $\mathbf{v}_1$ be an eigenvector of A associated with λ_1. If $\mathbf{v}_2$ is an eigenvector of $A^\dagger$ associated with $\bar{\lambda}_2$, then*

$$(\lambda_1-\lambda_2)\langle B\mathbf{v}_1, \mathbf{v}_2\rangle=0.$$

If $\mathbf{v}_3$ is an eigenvector of A^x associated with $\bar{\lambda}_3$, then

$$(\bar{\lambda}_1-\bar{\lambda}_3)\langle B\mathbf{v}_3, \mathbf{v}_1\rangle=0.$$

Proof. From the definitions (15a) and (15b) we see that $A^\dagger$ and A^x are both similar to A^* and thus have the same eigenvalues as A^*. Now consider

$$\lambda_1\langle B\mathbf{v}_1, \mathbf{v}_2\rangle=\langle BA\mathbf{v}_1, \mathbf{v}_2\rangle=\langle B\mathbf{v}_1, A^\dagger\mathbf{v}_2\rangle=\lambda_2\langle B\mathbf{v}_1, \mathbf{v}_2\rangle,$$

which yields

$$(\lambda_1-\lambda_2)\langle B\mathbf{v}_1, \mathbf{v}_2\rangle=0.$$

The final result is proved in a similar fashion. □

LEMMA 4. *If $\mathbf{v}$ is an eigenvector of both A and $A^\dagger$, then $\mathbf{v}$ is a simple eigenvector of both. Further, if $A\mathbf{v}=\lambda\mathbf{v}$, then $A^\dagger\mathbf{v}=\bar{\lambda}\mathbf{v}$. The statements remain true if $A^\dagger$ is replaced by A^x.*

Proof. The last result follows directly from Lemma 3 and the assumption that the bilinear form is definite. Now, suppose A has a nonlinear elementary divisor associated with $\mathbf{v}$; then, there exists $\mathbf{w}\neq\mathbf{0}$ such that

$$(A-\lambda I)\mathbf{w}=\mathbf{v}\neq\mathbf{0}.$$

Taking inner products, we have

$$\langle B\mathbf{v}, \mathbf{v}\rangle=\langle BA\mathbf{w}, \mathbf{v}\rangle-\lambda\langle B\mathbf{w}, \mathbf{v}\rangle=\langle B\mathbf{w}, A^\dagger\mathbf{v}\rangle-\langle B\mathbf{w}, \bar{\lambda}\mathbf{v}\rangle=0.$$

Since the bilinear form is definite, $\langle B\mathbf{v}, \mathbf{v}\rangle=0$ implies $\mathbf{v}=\mathbf{0}$, which is a contradiction. The proof that $\mathbf{v}$ is a simple eigenvector of $A^\dagger$ is established in a similar manner. □

THEOREM 5. *The following statements are equivalent*:

(i) *$A^\dagger=q(A)$, for some polynomial $q(z)$.*

(ii) *A and $A^\dagger$ commute.*

(iii) *A and $A^\dagger$ have the same complete set of eigenvectors.*

(iv) *A and A^x commute.*

Proof. Assume (i); then clearly (ii) holds. Now assume (ii). Let $\mathbf{v}$ be an eigenvector of A with eigenvalue λ. We have

$$(A^\dagger)^kA\mathbf{v}=A(A^\dagger)^k\mathbf{v}=\lambda(A^\dagger)^k\mathbf{v} \quad \text{for every } k\geqq 0.$$

Consider the subspace $W=\{\mathbf{v}, A^\dagger\mathbf{v}, \cdots, (A^\dagger)^k\mathbf{v}, \cdots\}$. Every element of W is an eigenvector of A associated with λ. Since W is invariant with respect to $A^\dagger$, there is some $\mathbf{w}_1\in W$ that is an eigenvector of both A and $A^\dagger$. By Lemma 4, $\mathbf{w}_1$ is a simple eigenvector of $A^\dagger$ associated with $\bar{\lambda}$. Either $\mathbf{w}_1=\mathbf{v}$ or there is another eigenvector of $A^\dagger$, say $\mathbf{w}_2\in W$. Again by Lemma 4, $\mathbf{w}_2$ is a simple eigenvector of $A^\dagger$ associated with $\bar{\lambda}$. By elimination, every element of W is a simple eigenvector of $A^\dagger$ associated with $\bar{\lambda}$. Thus, $\mathbf{v}$ is a simple eigenvector of both A and $A^\dagger$ associated with λ and $\bar{\lambda}$, respectively.

Repeating this argument, we see that every eigenvector of A is an eigenvector of $A^\dagger$ and is simple. Thus, A and $A^\dagger$ have the same complete set of eigenvectors and (iii) is established.

Now assume (iii). We know A and $A^\dagger$ have the same complete set of eigenvectors. With the aid of Lemma 3 we may write

$$A=S\Lambda_1 S^{-1}, \quad \Lambda_1=\operatorname{diag}(\cdots,\lambda_i,\cdots), \quad A^\dagger=S\Lambda_2 S^{-1}, \quad \Lambda_2=\operatorname{diag}(\cdots,\bar{\lambda}_i,\cdots),$$

where the columns of S are eigenvectors of A and $A^\dagger$. Let $q(z)$ be the Lagrange interpolating polynomial such that

$$q(\lambda_i)=\bar{\lambda}_i \qquad i=1,\cdots,N.$$

We have

$$q(A)=Sq(\Lambda_1)S^{-1}=S\Lambda_2 S^{-1}=A^\dagger,$$

which establishes (i).

The equivalence of (iv) with (i), (ii) and (iii) is established by showing that (iv) is true if and only if (ii) is true. Assume (ii); then, we have

$$AA^\dagger=A^\dagger A;$$

substituting in the expression (15a), we have

$$A(B^{-1})^*A^*B^*=(B^{-1})^*A^*B^*A,$$

which is equivalent to

$$B^*A(B^{-1})^*A^*=A^*B^*A(B^{-1})^*.$$

If we take the adjoint with respect to the standard inner product, we have

$$AB^{-1}A^*B=B^{-1}A^*BA.$$

With the aid of (15b), we can see this is

$$AA^x=A^xA. \qquad \square$$

Theorem 5 establishes the equivalence of the four statements in the definition of normal. Clearly the roles of $A^\dagger$ and A^x can be interchanged in this theorem. We shall see below that if A is normal, then $A^\dagger=A^x$.

COROLLARY 6. *If A is normal with respect to the definite bilinear form $\langle B\cdot,\cdot\rangle$, then A can be decomposed as*

$$A=S\Lambda S^{-1}, \qquad \Lambda=\operatorname{diag}(\cdots,\lambda_i,\cdots),$$

with multiple eigenvalues grouped together. The matrix S can be chosen such that

$$D=S^*BS$$

is block diagonal, where each block corresponds to a distinct eigenvalue of A, each block is upper triangular, and each block has diagonal of modulus 1.

Conversely, if $A=S\Lambda S^{-1}$, $\Lambda=\operatorname{diag}(\cdots,\lambda_i,\cdots)$ and $D=S^*BS$ commutes with Λ, then A is normal with respect to the definite bilinear form $\langle B\cdot,\cdot\rangle$.

Proof. Let the columns of S be represented by $\mathbf{v}_i$. From Lemma 3 we see that if $\lambda_i\neq\lambda_j$, then $\langle B\mathbf{v}_i,\mathbf{v}_j\rangle=0$. Thus, D is block diagonal where each block corresponds to a set of multiple eigenvalues of A. From § 2 we know that a basis for the subspace associated with a multiple eigenvalue can be chosen such that $\langle B\mathbf{v}_i,\mathbf{v}_j\rangle=0$ if $i>j$. Finally, the eigenvectors can be scaled so that $|\langle B\mathbf{v}_i,\mathbf{v}_i\rangle|=1$. The converse is proved by noting that $A^\dagger=(BAB^{-1})^*=((S^{-1})^*DS^{-1}S\Lambda S^{-1}SD^{-1}S^*)^*=S\bar{\Lambda}S^{-1}$. Since A and $A^\dagger$ commute, we see that A is normal. $\square$

COROLLARY 7. *If A is normal, then $A^\dagger=A^x$.*

Proof. From Theorem 5 and Corollary 6 we see that if A is decomposed as $A=S\Lambda S^{-1}$, then

$$A^\dagger=S\bar{\Lambda}S^{-1}=A^x. \qquad \square$$

Before proceeding to the main result, let us discuss the implications of the above results. First, we note from Corollary 6 that if A is normal, then D and Λ must commute. Further, if A has distinct eigenvalues, then $|D| \equiv I$. If, in addition, the symmetric part of B is positive definite, then $D \equiv I$, B is a positive definite Hermitian matrix, and the bilinear form is an inner product. Finally, if A is normal, then $A^\dagger = S\bar{\Lambda}S^{-1} = A^x$. Since $A^* = (S^{-1})^*\bar{\Lambda}S^*$, we have $A^* = A^\dagger$ only if

$$(S^*S)\bar{\Lambda} = \bar{\Lambda}(S^*S).$$

If S^*S does not commute with $\bar{\Lambda}$, then $A^* \neq A^\dagger$. As an example let

$$D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_2 \end{bmatrix}.$$

If we let $B = D$ and $A = \Lambda$ we have a nonsymmetric definite bilinear form and a matrix A that is normal. Let S be any nonsingular matrix; then if $B = (S^{-1})^*DS^{-1}$ and $A = S\Lambda S^{-1}$, we still have a nonsymmetric definite bilinear form and a normal matrix A. In particular let

$$S = \begin{bmatrix} 1 & \frac{1}{2} & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

It is easy to see that S^*S does not commute with $\bar{\Lambda}$ and so $A^* \neq A^\dagger$. However, consider the inner product defined as $\langle \hat{B}\cdot, \cdot\rangle$, where $\hat{B} = (S^{-1})^*S^{-1}$. Then A is normal with respect to $\langle \hat{B}\cdot, \cdot\rangle$, and the adjoint of A with respect to $\langle \hat{B}\cdot, \cdot\rangle$ is the same as the adjoint with respect to $\langle B\cdot, \cdot\rangle$. Thus, if A is normal with respect to a definite bilinear form, then A is normal with respect to an inner product.

The following lemma characterizes as normal those matrices that satisfy the hypothesis of Lemma 2 and, therefore, are in $OE(s, B)$.

LEMMA 8. *A is such that for every* $\mathbf{p}$

$$A^\dagger\mathbf{p} \in \{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\}$$

if and only if A is normal with normal degree $n(A) \leqq s-2$.

Proof. If A is normal with $n(A) \leqq s-2$, then $A^\dagger = q_{s-2}(A)$, where $q_{s-2}(z)$ is a polynomial of degree $s-2$. Clearly,

$$A^\dagger\mathbf{p} = q_{s-2}(A)\mathbf{p} \in \{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\} \quad \text{for every } \mathbf{p}.$$

Now assume $A^\dagger\mathbf{p} \in \{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\}$, for every $\mathbf{p}$. Let $\mathbf{v}_i$ be an eigenvector of A associated with λ_i. Then $A^\dagger\mathbf{v}_i \in \{\mathbf{v}_i, A\mathbf{v}_i, \cdots, A^{s-2}\mathbf{v}_i\} = \{\mathbf{v}_i\}$, so $\mathbf{v}_i$ is an eigenvector of $A^\dagger$. From Lemma 4, $\mathbf{v}_i$ is a simple eigenvector of both A and $A^\dagger$ associated with λ_i and $\bar{\lambda}_i$, respectively.

By elimination, every eigenvector of A, $\mathbf{v}_i$ associated with λ_i, is simple and also an eigenvector of $A^\dagger$ associated with $\bar{\lambda}_i$. By Theorem 5, A is normal.

Since A has exactly $d(A)$ distinct eigenvalues, there is an interpolating polynomial, $q(z)$, of degree exactly $d(A)-1$ such that $q(\lambda_i) = \bar{\lambda}_i$, $i = 1, \cdots, d(A)$. Thus $n(A) \leqq d(A)-1$. If $d(A) = s-1$, then $n(A) \leqq s-2$.

Suppose $d(A) \geqq s$. Choose $\mathbf{p}$ with $d = d(\mathbf{p}) = d(A)$. The vectors $\{\mathbf{p}, A\mathbf{p}, \cdots, A^{d-1}\mathbf{p}\}$ are linearly independent. By hypothesis we know that

$$A^\dagger\mathbf{p} = q(A)\mathbf{p} \in \{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\}.$$

Thus, $q(x)$ must have degree $\leqq s-2$. $\square$

We have shown that sufficient conditions for $A \in OE(s, B)$ are $d(A) \leqq s$ or A is normal with normal degree $n(A) \leqq s-2$. We shall now show that these are necessary conditions as well. First we establish some results that will facilitate the proof.

Define the set

$$D = \{\mathbf{p}: d(\mathbf{p}) < d(A)\}.$$

This set is a union of subspaces of dimension at most $N-1$. Each subspace is generated by a proper divisor of the minimal polynomial of A. Thus there are a finite number of these subspaces. The set D is therefore a set of measure zero under the topology imposed by the standard inner product. Let us reconsider the calculation of the orthogonal basis of the Krylov space described in § 2 in the light of our more general setting. Given $\mathbf{p}$, let

$$\begin{aligned} \mathbf{p}_0 &= \mathbf{p}, \\ \mathbf{p}_1 &= A\mathbf{p}_0 - \beta_{00}\mathbf{p}_0, \\ &\vdots \\ \mathbf{p}_{i+1} &= A\mathbf{p}_i - \sum_{j=0}^{i} \beta_{ij}\mathbf{p}_j, \end{aligned}$$

where the β_{ij}'s are solutions to the lower triangular system of equations

$$\langle BA\mathbf{p}_i, \mathbf{p}_k\rangle = \sum_{j=0}^{k} \beta_{ij}\langle B\mathbf{p}_j, \mathbf{p}_k\rangle, \qquad k = 0, \cdots, i. \tag{16}$$

If $d(\mathbf{p}) > i$, then $\mathbf{p}_i$ can be considered as a function of $\mathbf{p}$. Let us extend this definition to all $\mathbf{p}$ by setting $\mathbf{p}_i = \mathbf{0}$ for $\mathbf{p}$ such that $d(p) \leqq i$. We now show that for all $i \leqq d(A)$, $\mathbf{p}_i$ is a continuous function of $\mathbf{p}$.

LEMMA 9. *If $\mathbf{p}_i$ is defined as above, then for all $i \leqq d(A)$, $\mathbf{p}_i$ is a continuous function of $\mathbf{p}$.*

Proof. Let

$$I(B) = \max \left| \frac{\langle \mathbf{q}, \mathbf{q}\rangle}{\langle B\mathbf{q}, \mathbf{q}\rangle} \right| \quad \text{for } \mathbf{q} \neq \mathbf{0}.$$

The proof proceeds by induction. Clearly, $\mathbf{p}_0 = \mathbf{p}$ is continuous. Now assume, as an induction hypothesis, that for $0 \leqq l \leqq i$ that $\mathbf{p}_l$ is a continuous function of $\mathbf{p}$ whose norm is bounded above by $\|\mathbf{p}\|$ times a polynomial in $\|A\|$, $\|B\|$, and $I(B)$ alone. We shall show that $\|\mathbf{p}_{i+1}\|$ has the same property. We have

$$\beta_{i0}\langle B\mathbf{p}_0, \mathbf{p}_0\rangle = \langle BA\mathbf{p}_i, \mathbf{p}_0\rangle,$$

which yields

$$|\beta_{i0}| \cdot \|\mathbf{p}_0\| = \frac{\langle BA\mathbf{p}_i, \mathbf{p}_0\rangle \|\mathbf{p}_0\|}{\langle B\mathbf{p}_0, \mathbf{p}_0\rangle} \leqq \frac{\|\mathbf{p}_0\|^2}{\langle B\mathbf{p}_0, \mathbf{p}_0\rangle} \cdot \|BA\mathbf{p}_i\| \leqq I(B) \cdot \|B\| \cdot \|A\| \cdot \|\mathbf{p}_i\|.$$

Thus, for $\mathbf{p}_0 \neq \mathbf{0}$, β_{i0} is continuous and bounded. Since the space upon which $\mathbf{p}_0 = \mathbf{0}$ is closed and of smaller dimension than the entire space, we can continuously extend the product $\beta_{i0}\mathbf{p}_0$ to the entire space.

Assume, as an induction hypothesis, that $\beta_{il}\mathbf{p}_l$ for $0 \leqq l \leqq k-1$ is a continuous function of $\mathbf{p}$ whose norm is bounded above by $\|\mathbf{p}\|$ times a polynomial in $\|A\|$, $\|B\|$, and $I(B)$ alone. We claim that $\beta_{ik}\mathbf{p}_k$ has the same property ($k \leqq i$). We have from (16)

$$\sum_{j=0}^{k} \beta_{ij}\langle B\mathbf{p}_j, \mathbf{p}_k\rangle = \langle BA\mathbf{p}_i, \mathbf{p}_k\rangle.$$

Thus

$$\beta_{ik}\langle B\mathbf{p}_k, \mathbf{p}_k\rangle = \langle BA\mathbf{p}_i, \mathbf{p}_k\rangle - \sum_{j=0}^{k-1} \beta_{ij}\langle B\mathbf{p}_j, \mathbf{p}_k\rangle,$$

so β_{ik} is a continuous function of $\mathbf{p}$ when $\mathbf{p}_k \neq \mathbf{0}$. Now for $k \leqq i$,

$$|\beta_{ik}| \leqq \frac{|\langle BA\mathbf{p}_i, \mathbf{p}_k\rangle| + \sum_{j=0}^{k-1} |\beta_{ij}|\,|\langle B\mathbf{p}_j, \mathbf{p}_k\rangle|}{\langle B\mathbf{p}_k, \mathbf{p}_k\rangle}$$

$$\leqq \frac{\langle \mathbf{p}_k, \mathbf{p}_k\rangle}{\langle B\mathbf{p}_k, \mathbf{p}_k\rangle}\left(\|BA\| \cdot \frac{\|\mathbf{p}_i\|}{\|\mathbf{p}_k\|} + \sum_{j=0}^{k-1} |\beta_{ij}| \cdot \|B\| \cdot \frac{\|\mathbf{p}_j\|}{\|\mathbf{p}_k\|}\right),$$

which yields

$$\|\beta_{ik}\mathbf{p}_k\| = |\beta_{ik}| \cdot \|\mathbf{p}_k\| \leqq I(B)\left(\|BA\| \cdot \|\mathbf{p}_i\| + \sum_{j=0}^{k-1} |\beta_{ij}| \cdot \|B\| \cdot \|\mathbf{p}_j\|\right).$$

Thus, for $\mathbf{p}_k \neq \mathbf{0}$, $\beta_{ik}\mathbf{p}_k$ is a continuous and bounded function of $\mathbf{p}$. The set upon which $\mathbf{p}_k = \mathbf{0}$ is closed and of smaller dimension than the entire space. We can continuously extend the product $\beta_{ik}\mathbf{p}_k$ to the entire space.

Finally, since

$$\mathbf{p}_{i+1} = A\mathbf{p}_i - \sum_{j=0}^{i} \beta_{ij}\mathbf{p}_j,$$

$\mathbf{p}_{i+1}$ is a sum of continuous functions, and so it is continuous and

$$\|\mathbf{p}_{i+1}\| \leqq \|A\| \cdot \|\mathbf{p}_i\| + \sum_{j=0}^{i} |\beta_{ij}| \cdot \|\mathbf{p}_j\|.$$

This completes the proof. □

We now prove the main result.

THEOREM 10. *$A \in OE(s, B)$ if and only if $d(A) \leqq s$ or A is normal with normal degree $n(A) \leqq s-2$.*

Proof. Sufficiency has been established above. We now assume that $A \in OE(s, B)$ and $d(A) > s$ and show that A is normal with normal degree $n(A) \leqq s-2$. The proof can be divided into four parts. First, we show that $\langle BA\mathbf{p}_{s-1}, \mathbf{p}\rangle = 0$ for all vectors $\mathbf{p}$. Second, if $d(\mathbf{p}) = s$ and $V_s = \{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-1}\mathbf{p}\}$ is the invariant subspace generated by $\mathbf{p}$, then the restriction $\tilde{A}$ of A to V_s has a complete set of mutually B-orthogonal eigenvectors. Third, we prove that A has a complete set of mutually B-orthogonal eigenvectors and thus that A is normal by Corollary 6. Fourth, we show that the normal degree $n(A) \leqq s-2$.

(I) Let $\mathbf{p}$ be any vector such that $d(\mathbf{p}) > s$. From the definition we know that

$$\langle BA\mathbf{p}_i, \mathbf{p}\rangle = 0, \qquad s-1 \leqq i \leqq d(\mathbf{p}) - 2.$$

In particular,

$$\langle BA\mathbf{p}_{s-1}, \mathbf{p}\rangle = 0.$$

Let $F(\mathbf{p}) = \langle BA\mathbf{p}_{s-1}, \mathbf{p}\rangle$ be considered as a function of $\mathbf{p}$. Since $\mathbf{p}_{s-1}$ is a continuous function of $\mathbf{p}$, then $F(\mathbf{p})$ is a continuous function of $\mathbf{p}$. We have $F(\mathbf{p}) = 0$ for every $\mathbf{p}$ such that $d(\mathbf{p}) > s$. Since $d(A) > s$, the set upon which $d(\mathbf{p}) \leqq s$ is closed and of smaller dimension. Therefore, $F(\mathbf{p}) = 0$ for all $\mathbf{p}$. This is trivially true for $d(\mathbf{p}) < s$ since $\mathbf{p}_{s-1} = \mathbf{0}$ for these $\mathbf{p}$. However, if $d(\mathbf{p}) = s$, then $\mathbf{p}_{s-1} \neq \mathbf{0}$.

(II) Let $\mathbf{p}$ be such that $d(\mathbf{p})=s$ and let

$$V_s=\{\mathbf{p}, A\mathbf{p}, \cdots, A^{s-1}\mathbf{p}\}$$

be the invariant subspace generated by $\mathbf{p}$. Let $\tilde{A}$ be the restriction of A to V_s. Suppose B maps V_s onto W_s. Let Q be the orthogonal projection with respect to $\langle\cdot,\cdot\rangle$ of W_s into V_s and let $\tilde{B}=QB$ restricted to V_s. For every $\mathbf{x}$ and $\mathbf{y}\in V_s$

$$\langle\tilde{B}\mathbf{x}, \mathbf{y}\rangle=\langle QB\mathbf{x}, \mathbf{y}\rangle=\langle B\mathbf{x}, \mathbf{y}\rangle,$$

and likewise

$$\langle\mathbf{x}, \tilde{B}^*\mathbf{y}\rangle=\langle\mathbf{x}, B^*\mathbf{y}\rangle.$$

Note, first, that since $\langle\tilde{B}\mathbf{x}, \mathbf{x}\rangle\neq 0$ for $\mathbf{x}\in V_s$, $\tilde{B}$ is not singular. Second, for every $\mathbf{x}$ and $\mathbf{y}\in V_s$,

$$\langle B\mathbf{x}, \tilde{A}^\dagger\mathbf{y}\rangle=\langle B\tilde{A}\mathbf{x}, \mathbf{y}\rangle=\langle\tilde{B}\tilde{A}\mathbf{x}, \mathbf{y}\rangle=\langle\tilde{B}\mathbf{x}, (\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{y}\rangle=\langle B\mathbf{x}, (\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{y}\rangle.$$

Thus, the right adjoint of $\tilde{A}$ with respect to $\langle B\cdot, \cdot\rangle$ is given by $\tilde{A}^\dagger=(\tilde{B}\tilde{A}\tilde{B}^{-1})^*$.

We have $d(\tilde{A})=s$. Let $\mathbf{p}$ be any generator of V_s; that is, let $\mathbf{p}\in V_s$ be such that $d(\mathbf{p})=s$. We know from above that

$$0=F(\mathbf{p})=\langle BA\mathbf{p}_{s-1}, \mathbf{p}\rangle=\langle\tilde{B}\tilde{A}\mathbf{p}_{s-1}, \mathbf{p}\rangle=\langle\tilde{B}\mathbf{p}_{s-1}, (\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p}\rangle.$$

Since $(\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p}=\sum_{l=0}^{s-1} a_l\mathbf{p}_l$,

$$0=\langle\tilde{B}\mathbf{p}_{s-1}, (\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p}\rangle=\sum_{l=0}^{s-1} a_l\langle\tilde{B}\mathbf{p}_{s-1}, \mathbf{p}_l\rangle=\alpha_{s-1}\langle\tilde{B}\mathbf{p}_{s-1}, \mathbf{p}_{s-1}\rangle,$$

so we must have $a_{s-1}=0$. Thus

$$(\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p}\in\{\mathbf{p}_0, \cdots, \mathbf{p}_{s-2}\}=\{\mathbf{p}, \tilde{A}\mathbf{p}, \cdots, \tilde{A}^{s-2}\mathbf{p}\},$$

for every $\mathbf{p}\in V_s$ such that $d(\mathbf{p})=s$.

Now consider

$$\mathrm{W}(\mathbf{p})=\mathbf{p}\wedge\tilde{A}\mathbf{p}\wedge\cdots\wedge\tilde{A}^{s-2}\mathbf{p}\wedge(\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p},$$

where $\wedge$ is the wedge product (cf. Mostow, Sampson and Meyer [24, pp. 553-560]). Since the wedge product is a multilinear function from one vector space into another, $W(\mathbf{p})$ is a continuous function of $\mathbf{p}$. For every $\mathbf{p}\in V_s$ such that $d(\mathbf{p})=s$, $W(\mathbf{p})=\mathbf{0}$ because the vectors are linearly dependent. The set $\{\mathbf{p}\in V_s\colon d(\mathbf{p})<s\}$ is a closed subset of smaller dimension; therefore, $W(\mathbf{p})=\mathbf{0}$ for every $\mathbf{p}\in V_s$. This is trivially true for $\mathbf{p}$ with $d(\mathbf{p})<s-1$ since the first $s-1$ vectors are linearly dependent. However, let $\mathbf{p}\in V_s$ have $d(\mathbf{p})=s-1$. Then, the first $s-1$ vectors are independent. This implies that if $d(\mathbf{p})=s-1$, then

$$(\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{p}\in\{\mathbf{p}, \cdots, \tilde{A}^{s-2}\mathbf{p}\}.$$

Now let $V_{s-1}^{(1)}\subseteq V_s$ be an invariant subspace of $\tilde{A}$ of dimension $s-1$. Since $d(\tilde{A})=s$, $V_{s-1}^{(1)}$ must be generated by a $\mathbf{p}$ with $d(\mathbf{p})=s-1$. This implies that $V_{s-1}^{(1)}$ has a basis, say $\mathbf{b}_1, \cdots, \mathbf{b}_{s-1}$, such that $d(\mathbf{b}_i)=s-1$, $i=1, \cdots, s-1$. From above we know that

$$\tilde{A}^\dagger\mathbf{b}_i\in V_{s-1}^{(1)}, \qquad i=1, \cdots, s-1.$$

Thus, $V_{s-1}^{(1)}$ is an invariant subspace of $\tilde{A}^\dagger$ as well. Let $\{\mathbf{b}_1, \cdots, \mathbf{b}_{s-1}\}$ be a basis for $V_{s-1}^{(1)}$ generated by starting with $\mathbf{b}_1$, $d(\mathbf{b}_1)=s-1$, and generated as we did the $\mathbf{p}_i$. Then $0=\langle B\mathbf{b}_i, \mathbf{b}_j\rangle$ for every $i>j$. Take any nonzero $\mathbf{q}$ in V_s orthogonal to $V_{s-1}^{(1)}$. Since $\tilde{B}$ is nonsingular, there exists a $\mathbf{q}_1\in V_s$ such that $\tilde{B}\mathbf{q}_1=\mathbf{q}$. Hence

$$\langle\tilde{B}\mathbf{q}_1, \mathbf{y}\rangle=0$$

for every $\mathbf{y} \in V_{s-1}^{(1)}$. Now $\tilde{B}\tilde{A}\mathbf{q}_1$ is orthogonal to $V_{s-1}^{(1)}$ because

$$\langle \tilde{B}\tilde{A}\mathbf{q}_1, \mathbf{y}\rangle = \langle \tilde{B}\mathbf{q}_1, (\tilde{B}\tilde{A}\tilde{B}^{-1})^*\mathbf{y}\rangle = 0.$$

Since $\mathbf{q}_1$ is unique (up-to-scale), we have

$$\tilde{A}\mathbf{q}_1 = \lambda_1 \mathbf{q}_1$$

for some λ_1. Now let $V_{s-1}^{(2)} \subseteq V_s$ be any invariant subspace of dimension $s-1$ such that $\mathbf{q}_1 \in V_{s-1}^{(2)}$. Using the same argument as above, we may let $\mathbf{q}_2 \in V_s$ be the unique (up-to-scale) vector such that $\tilde{B}\mathbf{q}_2$ is orthogonal to $V_{s-1}^{(2)}$. We have

$$\tilde{A}\mathbf{q}_2 = \lambda_2 \mathbf{q}_2$$

for some λ_2 and $\langle \tilde{B}\mathbf{q}_2, \mathbf{q}_1\rangle = 0$. If we continue in this fashion, we get $\{\mathbf{q}_1, \cdots, \mathbf{q}_s\}$ in V_s such that $\tilde{A}\mathbf{q}_i = \lambda_i \mathbf{q}_i$ and

$$\langle \tilde{B}\mathbf{q}_i, \mathbf{q}_j\rangle = 0 \quad \text{if } i > j.$$

Note that the eigenvalues λ_i are distinct since V_s was generated by a vector of degree s. Now let $\tilde{V}_{s-1}^{(1)} = \{\mathbf{q}_2, \cdots, \mathbf{q}_s\}$. As above, let $\tilde{\mathbf{q}}_1$ be the unique (up-to-scale) vector in V_s such that $\langle \tilde{B}\tilde{\mathbf{q}}_1, \mathbf{y}\rangle = 0$ for every $\mathbf{y} \in \tilde{V}_{s-1}^{(1)}$. As before, we have

$$\tilde{A}\tilde{\mathbf{q}}_1 = \bar{\lambda}_1 \tilde{\mathbf{q}}_1 \quad \text{and} \quad \langle \tilde{B}\tilde{\mathbf{q}}_1, \mathbf{q}_j\rangle = 0 \quad \text{for } 2 \leqq j \leqq s.$$

Since there are at most s eigenvectors in V_s, we must have $\tilde{\mathbf{q}}_1 = \mathbf{q}_1$. Repeating this argument yields

$$\langle B\mathbf{q}_i, \mathbf{q}_j\rangle = \langle \tilde{B}\mathbf{q}_i, \mathbf{q}_j\rangle = 0 \quad \text{for all } j \neq i.$$

(III) We now show that A has a complete set of mutually B-orthogonal eigenvectors. Suppose there exists $\mathbf{v}$ such that for some λ_i

$$(A - \lambda_i I)\mathbf{v} \neq \mathbf{0}, \qquad (A - \lambda_i I)^2 \mathbf{v} = \mathbf{0}.$$

Let $\mathbf{v}$ and $(A - \lambda_i I)\mathbf{v}$ be included in an invariant subspace, V, with $s-2$ eigenvectors associated with distinct eigenvalues. We know that there are at least s such eigenvectors from the argument above. V is an invariant subspace of dimension s. Let $\tilde{A}$ be the restriction of A to V. We have $d(\tilde{A}) = s$. Repeating the argument above, we see that V contains s B-orthogonal eigenvectors of A, which is a contradiction. Similarly if we assume that $\mathbf{q}_i$ and $\mathbf{q}_j$ are eigenvectors of A associated with distinct eigenvalues, we can include them in an invariant subspace of dimension s upon which $d(\tilde{A}) = s$. The above argument will yield $\mathbf{q}_i$ B-orthogonal to $\mathbf{q}_j$. Since A has a complete set of eigenvectors that are mutually B-orthogonal if they correspond to distinct eigenvalues, we may apply Corollary 6 and conclude that A is normal with respect to $\langle B\cdot, \cdot\rangle$.

(IV) We know that $A^\dagger = q(A)$ for some polynomial q. We now show that the degree of $q \leqq s-2$. Since A has $d(A)$ distinct eigenvalues, the degree of q is $\leqq d(A)-1$. From the definition of $OE(s, B)$ above, we know that if $d(\mathbf{p}) = d(A)$, then

$$F_i(\mathbf{p}) = \langle B\mathbf{p}_i, A^\dagger \mathbf{p}\rangle = 0, \qquad s-1 \leqq i \leqq d(A)-2.$$

Now $F_i(\mathbf{p})$ is a continuous function of $\mathbf{p}$, and so $F_i(\mathbf{p}) = 0$, $s-2 \leqq i \leqq d(A)-2$ for all $\mathbf{p}$. Since A is normal, every invariant subspace of A is an invariant subspace of $A^\dagger$; thus, if $f = d(\mathbf{p})$, then

$$A^\dagger \mathbf{p} \in \{\mathbf{p}, \cdots, A^{f-1}\mathbf{p}\} = \{\mathbf{p}_0, \cdots, \mathbf{p}_{f-1}\}.$$

If $d(\mathbf{p}) < d(A)$, then $f-1 \leqq d(A)-2$, so the orthogonality conditions yield

$$A^\dagger \mathbf{p} \in \{\mathbf{p}_0, \mathbf{p}_1, \cdots, \mathbf{p}_{s-2}\} = \{\mathbf{p}, \cdots, A^{s-2}\mathbf{p}\}.$$

Now let $d(\mathbf{p})=d(A)-1$. The polynomial p_k that annihilates $\mathbf{p}$ is the product of all but one factor $z-\lambda_k$ of the minimal polynomial of A. Let $d=d(A)$,

$$p_k(z)=\prod_{i\neq k}(z-\lambda_i)=z^{d-1}-\left(\sum_{i\neq k}\lambda_i\right)z^{d-1}+\cdots+\cdots$$

and let

$$q(z)=\gamma_{d-1}z^{d-1}+\gamma_{d-2}z^{d-2}+\cdots+\cdots.$$

We know that if $d(\mathbf{p})=d(A)-1$, then the vectors $\{\mathbf{p},\cdots,A^{d-2}\mathbf{p}\}$ are linearly independent. Now

$$A^{\dagger}\mathbf{p}=q(A)\mathbf{p}=\gamma_{d-1}A^{d-1}\mathbf{p}+\gamma_{d-2}A^{d-2}\mathbf{p}+\cdots.$$

Because $p_k(A)\mathbf{p}=\mathbf{0}$, we know

$$A^{d-1}\mathbf{p}=\left(\sum_{i\neq k}\lambda_i\right)A^{d-2}\mathbf{p}+\cdots+\cdots.$$

Thus,

$$A^{\dagger}\mathbf{p}=\left(\gamma_{d-1}\left(\sum_{i\neq k}\lambda_i\right)+\gamma_{d-2}\right)A^{d-2}\mathbf{p}+\cdots+\cdots,$$

but $A^{\dagger}\mathbf{p}\in\{\mathbf{p},\cdots,A^{s-2}\mathbf{p}\}$ implies

$$\left(\gamma_{d-1}\left(\sum_{i\neq k}\lambda_i\right)+\gamma_{d-2}\right)=0.$$

Since this is true for every k, we must have $\gamma_{d-1}=\gamma_{d-2}=0$. If $\gamma_{d-1}=0$, then we must have $\gamma_i=0, i>s-2$ since $\{\mathbf{p},\cdots,A^{d-2}\mathbf{p}\}$ are linearly independent and $A^{\dagger}\mathbf{p}\in\{\mathbf{p},\cdots,A^{s-2}\mathbf{p}\}$. Thus, $q(z)$ is of degree at most $s-2$. This completes the proof. □

4. Remarks and conclusions. In this section we discuss the implication of our results, some special details of the proof, and show how these results can be used to categorize known algorithms and suggest new algorithms.

The definition of $OE(s, B)$ requires the upper bound $i\leqq d(\mathbf{p}_0)-2$ (see § 2). If this were $i\leqq d(\mathbf{p}_0)-1$, the proof would be much less complicated. Although the conclusion is the same, it would be somewhat incomplete to use the easier assumption since the existence of an orthogonal error method does not require it.

As was pointed out in [12], there may be s-term recursions for $\mathbf{p}_{i+1}$ other than the one used in (13). In that paper a general class of s-term recursions was described that includes all commonly used recursion formulas. We conjecture that this general recursion is equivalent to (13) for some possibly larger s.

The results of this work assume that the bilinear form is fixed. A paper by Smolarski and Saylor [30] describes an algorithm in which the inner product depends upon the initial residual, $\mathbf{r}_0$. Like the results in [12], the results here can be extended to this case if the inner product depends continuously on $\mathbf{r}_0$.

Many of the results of this paper depend upon the assumption that the bilinear form is definite. If the bilinear form is indefinite, it is possible to have the misfortune of dividing by a near zero and taking a very large step. Work has been done on ways to avoid these catastrophies for symmetric indefinite systems (cf. Leuenberger [20]). However, it is unclear why one would want to perform an iteration whose iterates were not a priori bounded. If the form is definite, then by Lemma 9, each iterate is bounded by $\|\mathbf{x}_0\|$ plus $\|\mathbf{r}_0\|$ times a polynomial in $\|A\|$, $\|B\|$, and $I(B)$. If B is real and all arithmetic is real, then

$$|\langle B\mathbf{x}, \mathbf{x}\rangle| = |\langle \tfrac{1}{2}(B+B^*)\mathbf{x}, \mathbf{x}\rangle|.$$

Since $\frac{1}{2}(B+B^*)$ is symmetric and definite, there is a norm such that

$$\|\mathbf{x}\|^2 = |\langle B\mathbf{x}, \mathbf{x}\rangle|.$$

The orthogonal error method associated with a real positive definite B will not be optimal in this norm, nor will it be norm reducing at each step. However, the norm of each iterate will be bounded.

We have included the results on right and left adjoints with respect to a definite bilinear form for completeness. To our knowledge, they do not appear elsewhere. More importantly, they yield a complete understanding of the matrices that characterize $OE(s, B)$.

There are many orthogonal error algorithms that are not conjugate gradient algorithms in the sense that B need only be definite rather than Hermitian positive definite. However, the set of matrices for which some s-term orthogonal error algorithm exists is the same as the set for which some s-term conjugate gradient algorithm exists. In § 3 it was shown that if $A \in OE(s, B)$, then there is an associated Hermitian positive definite $\hat{B}$ such that $A \in OE(s, \hat{B})$. It may be much easier, however, to compute with B than to find $\hat{B}$.

It is true that $OE(3, B)$ is strictly contained in $OE(s, B)$ for $s > 3$, but in some sense the increase is trivial. It was shown in [12] that if $\eta(A) > 1$, then $d(A) \leqq \eta(A)^2$). Matrices with only a few distinct eigenvalues are not very prevalent in problems of interest. It was also shown in [12] that if $\eta(A) = 1$, the eigenvalues of A must lie on some straight line in the complex plane. A simple scaling will place the eigenvalues either on the real line or on the line $1 + iy$, $y \in R$. If the resulting systems are real, the algorithms for these matrices reduce to known methods as will be shown below.

Throughout this paper we have concerned ourselves only with the theoretical possibility of an s-term algorithm. The algorithm requires the computation of

$$\alpha_k = \frac{\langle B\mathbf{e}_k, \mathbf{p}_k\rangle}{\langle B\mathbf{p}_k, \mathbf{p}_k\rangle}, \qquad k = 0, \cdots, d(r_p) - 1.$$

Since $\mathbf{e}_k$ is not known, this quantity may not be computable. Recall that the choice of $\mathbf{x}_0$, A, and B uniquely determine the sequence of iterates. Here A represents the matrix with which the Krylov sequence is generated and could represent the product of several systems that result from scaling, preconditioning, or changing the basis of the original linear system. For the purposes of the following discussion, let us denote the original system by $\hat{A}\mathbf{x} = \hat{\mathbf{b}}$ and assume that $\hat{\mathbf{r}} = \hat{\mathbf{b}} - \hat{A}\mathbf{x}$ is the basic computable quantity. Since $\mathbf{e}_k$ is chosen to satisfy (5) and $\mathbf{p}_k$ can be expressed as in (13), we have

$$\alpha_0 = \frac{\langle B\mathbf{e}_0, \mathbf{r}_0\rangle}{\langle B\mathbf{r}_0, \mathbf{r}_0\rangle}, \tag{17a}$$

$$\alpha_k = \frac{\langle B\mathbf{e}_k, A\mathbf{p}_{k-1}\rangle}{\langle B\mathbf{p}_k, \mathbf{p}_k\rangle}, \qquad k \geqq 1. \tag{17b}$$

Below we outline some choices for A and B that result in computable algorithms and analyze the implications of Theorem 10.

1. Let $B = I$. The bilinear form is an inner product and the method becomes a conjugate gradient method. If we let

$$A = \hat{A}^* C \hat{A} \tag{18}$$

for any computable C, then (17a, b) are computable. Notice that A is self-adjoint with respect to $B=I$ if and only if C is self-adjoint with respect to $B=I$.

(a) Suppose $C=I$; then, $A=\hat{A}^*\hat{A}$. This was first described by Hestenes [18] and later mentioned by Reid [25].

(b) Suppose $C=(M^{-1})^*M^{-1}$, where M is a nonsingular preconditioning or splitting of $\hat{A}$. This method was examined by Kershaw [17] and Elman [10]. If we let $M=\frac{1}{2}(\hat{A}+\hat{A}^*)=A_s$, we have a method that closely resembles that of Concus and Golub [6] and Widlund [33].

(c) Let $\hat{A}$ be Hermitian and let $C=q(\hat{A})$, where q is a real polynomial. This method is being examined as a method for solving indefinite linear systems by Manteuffel and Saylor [23].

(d) Let $\hat{A}$ be normal with respect to $B=I$ with normal degree η, and let $C=q(\hat{A}, \hat{A}^*)$, where q is a real polynomial in $\hat{A}$ and $\hat{A}^*$. Then C will be normal with respect to $B=I$ with normal degree that depends upon q.

2. Let $B=\hat{A}$. Then, $\hat{A}$ must be definite. If we let

$$A=C\hat{A} \tag{19}$$

for any computable C, then (17a, b) are computable. The matrix A will be normal with respect to $B=\hat{A}$ with normal degree η if and only if

$$(C\hat{A})^\dagger=C^*\hat{A}^*=q(C\hat{A}) \tag{20}$$

for some polynomial q of degree η.

(a) Suppose $C=I$; then, $\hat{A}$ must be normal with respect to I. There are two interesting cases. For example, if $\hat{A}$ is Hermitian positive definite, then we have the conjugate gradient method first described by Hestenes and Stiefel [19]. If $\hat{A}=e^{i\Theta}(\lambda I+B)$ with λ real and $B=-B^*$, then this seems to be an algorithm which has been overlooked.

(b) Suppose we let $C=M^{-1}$, where M is a preconditioning or splitting of $\hat{A}$.

(i) If both $\hat{A}$ and M are Hermitian positive definite, then

$$(C\hat{A})^\dagger=C^*\hat{A}^*=(M^{-1})^*\hat{A}^*=M^{-1}\hat{A}=C\hat{A}. \tag{21}$$

Thus, $C\hat{A}$ is self-adjoint with respect to $B=\hat{A}$. This is the method described by Concus, Golub and O'Leary [5].

(ii) If, as in 1(b), we let $M=\frac{1}{2}(\hat{A}+\hat{A}^*)=A_s$ and $A_n=\frac{1}{2}(\hat{A}-\hat{A}^*)$, then

$$\begin{aligned}(C\hat{A})^\dagger=C^*\hat{A}^*&=A_s^{-1}(A_s=A_n)=I-A_s^{-1}A_n\\&=2I-A_s^{-1}\hat{A}=2I-C\hat{A}.\end{aligned} \tag{22}$$

Thus, $C\hat{A}$ is normal with respect to $B=\hat{A}$ with normal degree 1. This is the method described by Concus and Golub [6] and Widlund [33]. Eisenstat [8] pointed out that if $A_n\neq 0$, this is not a conjugate gradient method because the bilinear form is not an inner product.

(c) Suppose $\hat{A}$ is Hermitian and $C=q(\hat{A})$, where q is a real polynomial in $\hat{A}$ with $q(\hat{A})$ nonsingular. We have assumed that $\hat{A}$ was definite in setting $B=\hat{A}$, so without loss of generality we may assume that $\hat{A}$ is Hermitian positive definite. This method has been examined by Dubois, Greenbaum and Rodrique [7], and Johnson, Micchelli and Paul [16], among others.

(d) Suppose $\hat{A}$ and M are Hermitian positive definite and we let $C=q(M^{-1}\hat{A})M^{-1}$, where q is a real polynomial with $q(M^{-1}\hat{A})$ nonsingular. Again, $C\hat{A}$ is self-adjoint with respect to $B=\hat{A}$. This method was described by Adams [1].

3. Suppose we let $B=\hat{A}^*\hat{A}$. The bilinear form is again an inner product. If we let $A=C\hat{A}$, as in (19), the coefficients (17a, b) will be computable. The matrix A is normal with respect to B with normal degree η if and only if $\hat{A}C$ is normal with respect to I with degree η.
   (a) Let $C=I$; then, $\hat{A}$ must be normal with respect to I. If $\hat{A}$ is Hermitian, this becomes the minimal residual algorithm often used for indefinite systems (cf. Stiefel [31], Reid [25], Elman [10]). Again as in 2(a), if $\hat{A}$ has normal degree 1, this algorithm seems to have been overlooked.
   (b) Let $C=\hat{A}^*$. This corresponds to substituting $\hat{A}^*\hat{A}$ for $\hat{A}$ in 2(a); that is, performing Hestenes and Stiefel's [19] original algorithm on the normal equations.
   (c) Let $C=A_s^{-1}$ as in 1(b). For a finite-term recursion we must have $\hat{A}C$ normal with respect to I. If $\hat{A}$ is normal, then A_s commutes with $\hat{A}$ and $\hat{A}^*$ and so

$$(\hat{A}C)^*=A_s^{-1}(A_s-A_n)=I-A_s^{-1}A_n=I-A_nA_s^{-1}=2I-\hat{A}C. \tag{23}$$

   Thus, $\hat{A}C$ is normal with respect to I with normal degree 1, regardless of the degree of normality of $\hat{A}$.
   (d) Let $C=M^{-1}(M^{-1})^*\hat{A}^*$. Then $\hat{A}C$ is self-adjoint with respect to I. This corresponds to replacing $\hat{A}$ by $\hat{A}^*$ and M by M^*M in 2(b)(i).
4. Suppose we let $B=D\hat{A}$ for some D such that $D\hat{A}$ is definite. If we let $A=C\hat{A}$ for any computable C, then the coefficients in (17a, b) are computable. For an s-term recursion we need that $C\hat{A}$ is normal with respect to $D\hat{A}$, which implies that

$$(\hat{A}C)^*=D^*q(C\hat{A})(D^{-1})^* \tag{24}$$

   for some polynomial q. For example, let $D=C$; then, we have the requirement

$$(C\hat{A})^*=q(C\hat{A}), \tag{25}$$

   or that $C\hat{A}$ is normal with respect to I.
   (a) If $\hat{A}$ is Hermitian and $C=q(\hat{A})$, where q is a real polynomial such that $q(\hat{A})\hat{A}$ is positive definite, then a three-term conjugate gradient algorithm exists. This is similar to algorithms described in 1(c) and 2(c) but minimizes in a different norm. This method is being examined by Manteuffel and Saylor [23].
   (b) If C is any preconditioning that renders $C\hat{A}$ Hermitian positive definite, then this algorithm applies. Notice that the bilinear form is determined by $C\hat{A}$ and is thus an inner product. If C is a "good" preconditioning, then one would expect CA to be more like I than $\hat{A}$ or $\hat{A}^*\hat{A}$ are. If the standard inner product ($B=I$) is the norm of greatest interest but uncomputable, it may be preferable to minimize in the norm $B=C\hat{A}$ than norms based upon $\hat{A}$ or $\hat{A}^*\hat{A}$.

Finally, we remark that any of these methods that are computable may be applied to systems that do not yield a finite-term recursion by artificially truncating the recursion. Of course such an iteration will not be optimal. There are many ways to implement such a truncation (cf. Axelsson [3], Vinsome [32], Elman [10], Eisenstat, Elman and Schultz [9], Saad and Schultz [28], [29]). The measure of how well these truncated methods work may be a measure of how nearly normal these systems are.

5. Summary. In this paper we have defined a class of algorithms that includes the conjugate methods as well as orthogonal residual methods. We have shown that a choice of definite bilinear form $\langle B\cdot,\cdot\rangle$ and iteration matrix A completely determines the sequence of iterates. We have characterized the relationship between A and B that allows an s-term recursion. Finally, we have shown that the criteria of normality allows an easy way to prove the existence of known algorithms and to demonstrate several new algorithms.

Acknowledgments. We would like to express our appreciation to Wayne Joubert and David Young for pointing out errors in an earlier version of this paper. We also regret the omission of the important references [15], [35] and [36] from the body of this paper.

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