Necessary and Sufficient Conditions for the Simplification of Generalized Conjugate-Gradient Algorithms*

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ABSTRACT

Recent papers by Faber and Manteuffel characterize the cases where ORTHODIR, a generalized conjugate-gradient algorithm for solving complex non-Hermitian linear systems, can be defined by a short recurrence formula and thus simplified. In the present paper similar results are obtained for two other generalized conjugate-gradient algorithms, namely, ORTHOMIN and ORTHORES. Necessary and sufficient conditions on the coefficient matrix A are given so that simplification is possible. Illustrative examples are given.

1. INTRODUCTION

In this paper we are concerned with iterative methods for solving the linear system

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

where A is a given nonsingular square matrix and b is a given column vector.

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The conjugate-gradient method (CG method) developed by Hestenes and Stiefel [11] provides an effective tool for solving (1.1) in the *symmetrizable case* where ZA and Z are Hermitian and positive definite (HPD). Here Z is the auxiliary matrix used for the CG method.

A number of generalizations of the CG method have been proposed for handling the nonsymmetrizable case where Z and/or ZA need not be HPD. Young and Jea [21, 22] considered a procedure called the "idealized generalized conjugate-gradient acceleration procedure" (IGCG procedure). Given an initial guess $u^{(0)}$ to the true solution $\bar{u}$ of (1.1), the sequence $u^{(0)}, u^{(1)},\dots$ is defined by the condition

$$u^{(n)} - u^{(0)} \in K_n(r^{(0)}) \tag{1.2}$$

and by the Petrov-Galerkin condition

$$(v, Zr^{(n)}) = 0 \tag{1.3}$$

for all $v \in K_n(r^{(0)})$. Here $K_n(r^{(0)}) = K_n(r^{(0)}, A)$ is the *Krylov space of* $r^{(0)}$ *of degree n with respect to the matrix* A and is defined by

$$K_n(r^{(0)}) = \operatorname{span}\{r^{(0)}, Ar^{(0)},\dots, A^{n-1}r^{(0)}\}. \tag{1.4}$$

Here for $n = 0,1,2,\dots$ the residual vector $r^{(n)}$ is defined by

$$r^{(n)} = b - Au^{(n)}. \tag{1.5}$$

It can be shown (see, e.g., Daniel [4, 5] or Young and Jea [21]) that if ZA is HPD, then the condition (1.3) is equivalent to the minimization condition

$$\|u^{(n)} - \bar{u}\|_{(ZA)^{1/2}} \leqslant \|w - \bar{u}\|_{(ZA)^{1/2}} \tag{1.6}$$

for all w such that $w - u^{(0)} \in K_n(r^{(0)})$.

A matrix H is *positive real* (PR) if (v, Hv) is real and positive for all real nonzero vectors v. Similarly we can define *negative real* (NR) matrices. Following Faber and Manteuffel [10], we say that a matrix H is *definite* if $(v, Hv) \neq 0$ for all complex nonzero vectors v. It can be shown that if H is real, then it is definite if and only if it is either PR or NR; a proof of this is given in Appendix A. However, as shown in Appendix A, the concepts are not equivalent in the complex case. The definiteness condition is much more useful for the IGCG method in the complex case.

It can be shown (see for instance Householder [12]) that if A is definite, then $E(A)$, the convex hull of the eigenvalues of A, does not contain the origin. On the other hand, if A is normal and if $E(A)$ does not contain the origin, then A is definite.

The case where A and b of (1.1) are real was considered in [21]. It was shown that if ZA is PR, then the sequence $u^{(0)}, u^{(1)}, \dots$ is uniquely determined by (1.2) and (1.3) for $n \leqslant d$ and moreover that $u^{(d)} = \bar{u}$. Here $d = d(r^{(0)}) = d(r^{(0)}, A)$ is the smallest integer such that the vectors $r^{(0)}, Ar^{(0)}, \dots, A^d r^{(0)}$ are linearly dependent. Three procedures were considered in [21] for actually implementing the IGCG method. These variants were referred to as ORTHODIR, ORTHOMIN, and ORTHORES. The ORTHODIR variant converges if ZA is PR, and moreover $u^{(d)} = \bar{u}$. The other two variants may fail if one only assumes that ZA is PR. However, if both Z and ZA are PR, then ORTHOMIN and ORTHORES converge and moreover $u^{(d)} = \bar{u}$.

The ORTHODIR, ORTHOMIN, and ORTHORES algorithms are often not practical because in order to obtain a new iterate it is, in general, necessary to use all previous iterates. In some cases, however, the formulas for the methods reduce to short recurrences and thus simplify. This paper is concerned with necessary and sufficient conditions for such a simplification to occur.

We say that we have *condition* OD(s) if only s old vectors are needed to perform an iteration of ORTHODIR. Similarly *condition* OM(s) and *condition* OR(s) have corresponding meanings for ORTHOMIN and ORTHORES, respectively. If we have conditions OD$(s+1)$, OM(s), and OR(s), then we say that we have *condition* S(s).

A prime example of simplification is the *symmetrizable case*, where, as stated above, both Z and ZA are HPD. In this case S(1) holds; see, e.g., Hestenes and Stiefel [11], Engeli et al. [8], or Concus, Golub, and O'Leary [3].

As a generalization of the symmetrizable case, Jea [13], Jea and Young [14], and Young, Jea, and Kincaid [23] considered the case where A is real and for some nonsingular matrix K we have

$$KA = A^*K. \tag{1.7}$$

They showed if the auxiliary matrix Z satisfies (1.7), then S(1) holds. Moreover, they showed that for any nonsingular real matrix A there always exists a matrix K such that (1.7) holds. However, the determination of K is seldom practical. Even in cases where K can be determined, there is no guarantee that the methods will not break down. Nevertheless, this approach was used by Jea and Young [14] to give a new derivation of several variants of the method of Lanczos [16].

Jea and Young [14] showed that if a real PR matrix K exists which satisfies (1.7), then there also exists an HPD matrix $\hat{K}$ which satisfies (1.7). As shown by Young, Jea, and Kincaid [23], if we let $Z = A^*\hat{K}$, then we have S(1) and, moreover, ORTHODIR converges. (Actually one can also choose $Z = A^*K$, since $H = ZA = A^*KA$ is definite.) However, ORTHOMIN and ORTHORES may break down in this case.

A major breakthrough in this area was made by Faber and Manteuffel [9]. From their results it follows that if ZA is HPD and if

$$(ZAZ^{-1})^* = P_s(A) \tag{1.8}$$

for some polynomial $P_s(A)$ of degree s, then ORTHODIR converges and we have OD$(s+1)$. Moreover, except for certain special cases, the condition (1.8) is *necessary* as well as sufficient for OD$(s+1)$. Faber and Manteuffel also showed that the only general and useful simplification occurs when $s = 1$, and in that case A has a very special form and all eigenvalues of A lie on a straight line in the complex plane. In a subsequent paper, Faber and Manteuffel [10] extended their results to the case where ZA is definite.

The emphasis in this paper is primarily on the extension of the results of Faber and Manteuffel to ORTHOMIN and ORTHORES. This work is motivated by the fact that these methods are often preferred in practice to ORTHODIR in spite of the fact that ORTHODIR converges under more general conditions. In the first place, if all of the methods simplify, then ORTHOMIN and ORTHORES often require less work per iteration. Also, even if simplification does not occur, it is common practice to use truncated procedures obtained by discarding all but a few of the most recent vectors. Numerical experiments indicate that not only do the truncated versions of ORTHOMIN and ORTHORES require fewer operations per iteration than the truncated version of ORTHODIR, but they often have much better convergence properties as well.

Formulas for ORTHODIR for the complex case are given in Section 2, and formulas for ORTHOMIN and ORTHORES for the complex case are given in Section 3. The convergence results stated above for the real case can easily be extended to the complex case if we replace the "PR" condition by the "definite" condition.

In Sections 4 and 5 it is shown that if Z and ZA are definite and if we have OM(s) and OR(s), then except for special cases the condition (1.8) holds.

In Section 6 the case $s = 1$ is analyzed in detail, and procedures are given for choosing Z so that ORTHOMIN and ORTHORES, as well as ORTHODIR, will converge.

In Section 7 we discuss several conditions on the matrix A such that an auxiliary matrix Z exists which produces simplification and convergence. We also describe procedures for finding a suitable matrix Z corresponding to a given matrix A satisfying one of these conditions such that ORTHOMIN and ORTHORES, as well as ORTHODIR, simplify and converge.

In Section 8 we consider the application of the results to a number of special cases including many of those considered by Faber and Manteuffel [10]. These cases correspond to preconditionings of a given linear system, to the GCW method of Concus and Golub [2] and of Widlund [19], to polynomial preconditioning, and to certain generalized normal equations.

2. ORTHODIR

The ORTHODIR algorithm involves the choice of an auxiliary matrix Z, the generation of direction vectors $q^{(0)}, q^{(1)}, \dots,$ and the use of these vectors to determine the iterates $u^{(1)}, u^{(2)}, \dots$. Thus, with $u^{(0)}$ given, the direction vectors are determined by the following semiorthogonalization process:

$$\begin{aligned} &q^{(0)} = r^{(0)} \\ &q^{(n)} = Aq^{(n-1)} + \sum_{i=0}^{n-1} \beta_{n,i} q^{(i)}, \qquad n = 1,2,\dots, \end{aligned} \tag{2.1}$$

where

$$\beta_{n,i} = \frac{-\langle q^{(i)}, Aq^{(n-1)} \rangle - \sum_{j=0}^{i-1} \beta_{n,j} \langle q^{(i)}, q^{(j)} \rangle}{\langle q^{(i)}, q^{(i)} \rangle}. \tag{2.2}$$

The $\beta_{n,i}$ are chosen to make the $\{q^{(i)}\}$ semiorthogonal in the sense that

$$\langle q^{(i)}, q^{(n)} \rangle = 0 \qquad \text{for} \quad i < n. \tag{2.3}$$

Here we define the generalized inner product $\langle x, y \rangle$ by

$$\langle x, y \rangle = (x, Hy), \tag{2.4}$$

where $H = ZA$ and (u, v) is the standard inner product

$$(u, v) = \sum_{i=1}^{N} \bar{u}_i v_i. \tag{2.5}$$

It should be noted that the condition $\langle x, y\rangle = 0$ does not necessarily imply that $\langle y, x\rangle = 0$ unless H is Hermitian; hence the term "semiorthogonal" is used.

The direction vectors $q^{(0)}, q^{(1)}, \dots$ are used to update the iterates using

$$u^{(n+1)} = u^{(n)} + \hat{\lambda}_n q^{(n)}, \tag{2.6}$$

where

$$\hat{\lambda}_n = \frac{\left(q^{(n)}, Zr^{(n)}\right)}{\langle q^{(n)}, q^{(n)}\rangle}. \tag{2.7}$$

It is shown in [21] that $q^{(d)} = 0$ and $u^{(d)} = \bar{u}$, where $d = d(r^{(0)}, A)$, but that $u^{(n)} \neq \bar{u}$ if $n < d$.

For any given integer $s \geqslant 1$, we define the truncated method ORTHODIR(s) by requiring that $\beta_{n,i} = 0$ for $i < n - s$. Thus (2.1) becomes an $(s+1)$-term recurrence. Unfortunately, in the general case the truncated method does not have the desirable convergence properties of the nontruncated method.

We would like to know for what class of matrices A the formula for $q^{(n)}$ in the ORTHODIR algorithm automatically reduces to the $(s+1)$-term recurrence of ORTHODIR(s), for arbitrary b and $u^{(0)}$. For this to happen it is necessary and sufficient that $\beta_{n,i} = 0$ for $i < n - s$ and $n < d = d(r^{(0)})$. It is important to observe that as noted by Faber and Manteuffel [10], since $q^{(d)} = 0$ need not be computed, no condition need be placed on $\beta_{d,i}$.

These considerations suggest the following definition: given a matrix Z such that $H = ZA$ is definite, we will say $A \in$ OD(s, H) if, for any choice of $r^{(0)}$, the direction vectors $q^{(i)}$ generated by ORTHODIR, when applied to the linear system (1.1) with auxiliary matrix Z, satisfy $\langle q^{(i)}, Aq^{(n-1)}\rangle = 0$, with $H = ZA$, for $i < n - s$ and $n < d(q^{(0)})$. Thus OD(s, H) is the class of matrices for which ORTHODIR(s) $\equiv$ ORTHODIR(∞).

In order to characterize OD(s, H) we introduce the following definitions. Given a matrix A and a nonsingular matrix H, we define $A^{\dagger} = (HAH^{-1})^*$ to be the *adjoint of A with respect to H*. We note that $\langle u, Av\rangle = \langle A^{\dagger}u, v\rangle$ for all u, $v \in C^N$. We say that A is *normal with respect to H*, or that A is *H-normal*, if A and $A^{\dagger}$ commute. It can be shown (see Faber and Manteuffel [9, 10] and Drazin [6]) that if A is H-normal, and if H is definite, then A is normalizable (i.e., A is similar to a normal matrix) and there exists a polynomial P such that $A^{\dagger} = P(A)$. The *normal degree of A with respect to H*, denoted by $n(A, H)$, is defined as the degree of the polynomial P of lowest degree such that $A^{\dagger} = P(A)$. Since, as shown in Appendix B, $n(A, H)$ is independent of H, we let $n(A) = n(A, H)$. We will define $\bar{d}(A)$ to be the degree of the minimal polynomial of the matrix A.

We remark that A is H-normal if and only if A is Z-normal where $H = ZA$. This follows because $(ZAZ^{-1})^* = (HA^{-1}AAH^{-1})^* = (HAH^{-1})^*$.

The set $\mathrm{OD}(s, H)$ can be characterized by the following theorem.

THEOREM 2.1. *Let A be nonsingular and let H be definite. Then* $A \in \mathrm{OD}(s, H) \Leftrightarrow \bar{d}(A) \leqslant s + 1$ *or A is normal with respect to H with* $n(A) \leqslant s - 1$.

A proof of Theorem 2.1 is given by Faber and Manteuffel [9] for the case where H is HPD, and by Faber and Manteuffel [10] for the case where H is definite.

In the next two sections we will present similar results for ORTHOMIN and ORTHORES. For our study of these methods we will need to use a modification of Theorem 2.1. First, we define the set $\widetilde{\mathrm{OD}}(s, H)$ as follows. Given a matrix Z such that $H = ZA$ is definite, $A \in \widetilde{\mathrm{OD}}(s, H)$ if, for any choice of $r^{(0)}$, the direction vectors generated by ORTHODIR, when applied to the linear system (1.1) with auxiliary matrix Z, satisfy $\langle q^{(i)}, Aq^{(n-1)} \rangle = 0$ for $i < n - s$ and for $n \leqslant d(r^{(0)})$. Evidently $\widetilde{\mathrm{OD}}(s, H) \subset \mathrm{OD}(s, H)$.

The following theorem is suggested in [10]. A proof is given in Section 4 below.

THEOREM 2.2. *Let A be nonsingular and let H be definite. Then* $A \in \widetilde{\mathrm{OD}}(s, H) \Leftrightarrow \bar{d}(A) \leqslant s$ *or A is normal with respect to H with $n(A) \leqslant s - 1$.*

3. ORTHOMIN AND ORTHORES

For the ORTHOMIN and ORTHORES variants of the IGCG method we assume that Z and ZA are definite. The ORTHOMIN method is defined by

$$
\begin{aligned}
u^{(n+1)} &= u^{(n)} + \lambda_n p^{(n)}, \\
r^{(n+1)} &= r^{(n)} - \lambda_n A p^{(n)}, \\
p^{(0)} &= r^{(0)}, \\
p^{(n)} &= r^{(n)} + \sum_{i=0}^{n-1} \alpha_{n,i} p^{(i)}, \qquad n \geqslant 1,
\end{aligned}
\tag{3.1}
$$

where

$$\alpha_{n,i} = \frac{-\langle p^{(i)}, r^{(n)}\rangle - \sum_{j=0}^{i-1}\alpha_{n,j}\langle p^{(i)}, p^{(j)}\rangle}{\langle p^{(i)}, p^{(i)}\rangle}, \qquad i < n,$$
$$\lambda_n = \frac{\left(p^{(n)}, Zr^{(n)}\right)}{\langle p^{(n)}, p^{(n)}\rangle}. \tag{3.2}$$

Here, the $\alpha_{n,i}$'s are defined by the H-semiorthogonality condition

$$\langle p^{(i)}, p^{(n)}\rangle = 0 \qquad \text{for} \quad i < n. \tag{3.3}$$

The ORTHORES method is given by

$$u^{(n+1)} = \lambda_n r^{(n)} + \sum_{i=0}^{n} f_{n+1,i} u^{(i)},$$
$$r^{(n+1)} = -\lambda_n A r^{(n)} + \sum_{i=0}^{n} f_{n+1,i} r^{(i)}, \tag{3.4}$$

where

$$f_{n+1,i} = \lambda_n \sigma_{n+1,i} \qquad \text{for} \quad i \leqslant n,$$
$$\lambda_n = \left(\sum_{i=0}^{n} \sigma_{n+1,i}\right)^{-1},$$
$$\sigma_{n+1,i} = \frac{\langle r^{(i)}, r^{(n)}\rangle - \sum_{j=0}^{i-1}\sigma_{n+1,j}\left(r^{(i)}, Zr^{(j)}\right)}{\left(r^{(i)}, Zr^{(i)}\right)}. \tag{3.5}$$

The $\sigma_{n+1,i}$'s here are defined by the Z-semiorthogonality condition of the residuals:

$$\left(r^{(i)}, Zr^{(n+1)}\right) = 0 \qquad \text{for} \quad i < n+1. \tag{3.6}$$

It should be noted that for a given choice of the matrices A and Z and the vectors $u^{(0)}$ and b, the three algorithms ORTHODIR, ORTHOMIN, and ORTHORES generate the same iterates $u^{(1)}, u^{(2)}, \ldots$; see [21] for a proof for the real case. Moreover, the direction vectors $p^{(i)}$ for ORTHOMIN are nonzero scalar multiples of the direction vectors $q^{(i)}$ for ORTHODIR.

As in the case of ORTHODIR, it is possible to truncate ORTHOMIN to ORTHOMIN(s), which has an $(s+1)$-term recurrence formula for $p^{(n)}$, by forcing $\alpha_{n,i}=0$ for $i<n-s$. Likewise, ORTHORES may be truncated to ORTHORES(s), which has an $(s+2)$-term recurrence formula for $u^{(n+1)}$ and for $r^{(n+1)}$, by forcing $\sigma_{n+1,i}=0$ for $i<n-s$. Again, the convergence properties of the truncated methods are not the same as those of the nontruncated methods. Furthermore, the three truncated methods each give different iterates, in general.

As before, we define classes of matrices for which ORTHOMIN $\equiv$ ORTHOMIN(s) or ORTHORES $\equiv$ ORTHORES(s).

If Z and $H=ZA$ are definite, we will say that $A\in \mathrm{OM}(s,H)$ if, for any choice of $r^{(0)}$, the vectors $p^{(i)}$ generated by the ORTHOMIN algorithm for solving (1.1) with auxiliary matrix Z satisfy $\langle p^{(i)}, r^{(n)}\rangle=0$ for $i<n-s$ and $n<d(p^{(0)})$. We also say that $A\in \mathrm{OR}(s,H)$ if, for any choice of $r^{(0)}$, the vectors generated by the ORTHORES algorithm for solving (1.1) with auxiliary matrix Z satisfy $\langle r^{(i)}, r^{(n)}\rangle=0$ for $i<n-s$ and $n<d(r^{(0)})$.

4. CHARACTERIZATION OF $\widetilde{\mathrm{OD}}(s,H)$

Before we characterize the sets $\mathrm{OM}(s,H)$ and $\mathrm{OR}(s,H)$, it will be necessary to characterize the set $\widetilde{\mathrm{OD}}(s,H)$.

The proof of the characterization theorem for $\widetilde{\mathrm{OD}}(s,H)$ is similar to that of the characterization theorem for $\mathrm{OD}(s,H)$ found in [10]. It is included here for completeness. Throughout, it will be assumed that A is nonsingular and that H is definite.

LEMMA 4.1. $\bar{d}(A)\leqslant s \;\Rightarrow\; A\in\widetilde{\mathrm{OD}}(s,H)$.

Proof. The definition of $\widetilde{\mathrm{OD}}(s,H)$ is trivially satisfied, since for all $q^{(0)}$ we have $d(q^{(0)})\leqslant \bar{d}(A)\leqslant s$. ∎

LEMMA 4.2. *$A^{\dagger}p\in K_s(p,A)$ for all p* $\Rightarrow$ $A\in\widetilde{\mathrm{OD}}(s,H)$.

Proof. We know that $\langle q^{(i)}, Aq^{(n-1)}\rangle=\langle A^{\dagger}q^{(i)}, q^{(n-1)}\rangle$. But

$$A^{\dagger}q^{(i)}\in K_s\big(q^{(i)}\big)\subseteq K_{i+s}\big(q^{(0)}\big)=\operatorname{span}\{q^{(j)}\}_{j=0}^{i+s-1}.$$

Thus, if $i + s - 1 < n - 1$, then by the H-semiorthogonality condition on the $q^{(i)}$'s [Equation (2.3)], $\langle A^{\dagger} q^{(i)}, q^{(n-1)} \rangle = 0$. So, by definition, $A \in \widetilde{\text{OD}}(s, H)$. ∎

LEMMA 4.3. *$A^{\dagger} p \in K_s(p, A)$ for all p $\Leftrightarrow$ A normal, with $n(A) \leqslant s - 1$.*

Proof. See [10]. ∎

THEOREM 4.4. *The following are equivalent:*

(1) *$A^{\dagger} = P(A)$ for some polynomial P.*
(2) *A and $A^{\dagger}$ commute.*
(3) *A and $A^{\dagger}$ both have the same complete set of eigenvectors.*
(4) *Any of conditions* (1), (2), *or* (3) *hold, with the H-adjoint replaced by the H^*-adjoint.*

Proof. See [10]. ∎

COROLLARY 4.5. *If A is normal with respect to H, then for some nonsingular matrix Q we have $A = Q\Lambda Q^{-1}$, $\Lambda \equiv \text{diag}\{\lambda_i\}$, with repeated eigenvalues λ_i grouped together in Λ, and $D \equiv Q^*HQ$ is block diagonal, where the blocks correspond to the blocks of repeated eigenvalues in Λ, and the D blocks are upper triangular, with diagonal elements of modulus* 1. *Conversely, A is normal with respect to H if $A = Q\Lambda Q^{-1}$, $\Lambda = \text{diag}\{\lambda_i\}$, and $D \equiv Q^*HQ$ commutes with Λ.*

Proof. See [10]. ∎

Note, in particular, that this corollary implies that A is normal with respect to H if it is true that A has a complete set of eigenvectors, and eigenvectors associated with distinct eigenvalues of A are both H- and H^*-semiorthogonal.

THEOREM 4.6. *Let $\{q^{(i)}\}$ be the vectors generated by the* ORTHODIR *semiorthogonalization process. Then $q^{(i)}$ is a continuous function of $q^{(0)}$ for all i.*

Proof. See [10]. ∎

LEMMA 4.7. *If $\bar{d}(A) > s$ and $\langle q^{(0)}, Aq^{(s)}\rangle = 0$ for all $q^{(0)}$, then A is H-normal.*

Proof. This proof proceeds in a similar fashion to the proof of the normality of A in Theorem 10 of [10].

(1) *Defining an invariant subspace.* It is possible to pick $\tilde{p}$ such that $d(\tilde{p}) = s+1$. Let $K_{s+1} \equiv K_{s+1}(\tilde{p})$. Since $d(\tilde{p}) = s+1$, this subspace is $(s+1)$-dimensional and A-invariant.

(2) *Restricting to the subspace.* Let R be an $N \times (s+1)$ matrix whose columns are l^2-orthonormal and span K_{s+1}. Then $Q \equiv RR^*$ is the l^2-orthogonal projector onto K_{s+1}. Note that $Q^* = Q$. Let $\tilde{A} \equiv QAQ = AQ$, the l^2-projection of A onto K_{s+1}. Let $\tilde{H} \equiv QHQ$, considered as a map on K_{s+1}. Note that $\tilde{H}$ is nonsingular as a map on K_{s+1}: this follows from the fact that $(v, \tilde{H}v) = (v, Hv) \neq 0$ for all $v \in K_{s+1} \setminus \{0\}$. Then $\tilde{H}$ is invertible as a map on K_{s+1}. Now, let $\tilde{A}^{\dagger} \equiv (\tilde{H}\tilde{A}\tilde{H}^{-1})^*$, the $\tilde{H}$-adjoint of $\tilde{A}$ on K_{s+1}. It is easily verified that $\langle u, \tilde{A}v\rangle = \langle \tilde{A}^{\dagger}u, v\rangle$ for all $u, v \in K_{s+1}$. Note also that $d(v, A) = d(v, \tilde{A})$ and $K_n(v, A) = K_n(v, \tilde{A})$ for all $v \in K_{s+1}$.

(3) *Claim:* $\tilde{A}^{\dagger}q \in K_s(q) \subseteq K_{s+1}$ for all $q \in K_{s+1}$ such that $d(q) = s+1$. *Proof:* Note, for all $q \in K_{s+1}$,

$$0 = \langle q, Aq^{(s)}\rangle = \langle q, \tilde{A}q^{(s)}\rangle = \langle \tilde{A}^{\dagger}q, q^{(s)}\rangle,$$

writing $q^{(0)}$ as q. Now, $d(q) = s+1$ implies that $\{q^{(i)}\}_{i=0}^{s}$ span K_{s+1}. Thus, $\tilde{A}^{\dagger}q \in K_{s+1}$ equals $\sum_{i=0}^{s} a_i q^{(i)}$ for some $\{a_i\}$. Substituting,

$$0 = \langle \tilde{A}^{\dagger}q, q^{(s)}\rangle = \left\langle \sum_{i=0}^{s} a_i q^{(i)}, q^{(s)} \right\rangle = \sum_{i=0}^{s} \langle a_i q^{(i)}, q^{(s)}\rangle = a_s^* \langle q^{(s)}, q^{(s)}\rangle,$$

by the semiorthogonality of the $q^{(i)}$'s. Since $q^{(s)} \neq 0$ and H is definite, $a_s = 0$. Claim shown.

(4) *Claim:* $\tilde{A}^{\dagger}q \in K_s(q) \subseteq K_{s+1}$ for all $q \in K_{s+1}$ such that $d(q) = s$. *Proof:* Let

$$M(q^{(0)}) = \begin{pmatrix} q^{(0)} & q^{(1)} & \cdots & q^{(s-1)} & \tilde{A}^{\dagger}q^{(0)} \end{pmatrix},$$

an $N \times (s+1)$ matrix-valued function, again considering the $q^{(i)}$'s as functions of $q^{(0)}$. Now, let $W(q) = \det[M(q)^* M(q)]$. The map $W: K_{s+1} \to C$ is zero precisely when the columns of $M(q^{(0)})$ are linearly dependent. We showed above that $W(q)=0$ for all $q\in K_{s+1}$ such that $d(q)=s+1$. It can be shown that the set $\{q\in K_{s+1}: d(q)\neq s+1\}$ is of measure zero in the set K_{s+1}. Clearly, W is continuous (see Theorem 4.6). Thus, by continuity, W is zero on all of K_{s+1}. Now, when $d(q^{(0)})=s$, $\{q^{(i)}\}_{i=0}^{s-1}$ are linearly independent and span $K_s(q^{(0)})$. So $W(q^{(0)})=0$ implies that $\tilde{A}^{\dagger}q\in \operatorname{span}\{q^{(i)}\}_{i=0}^{s-1}=K_s(q^{(0)})$. Claim shown.

(5) *Claim:* $p_1\in K_{s+1}$ and $d(p_1)=s \Rightarrow K_s(p_1)$ is $\tilde{A}^{\dagger}$-invariant. *Proof:* Clearly, for such p_1, $K_s(p_1)$ is $\tilde{A}$-invariant. It can easily be shown that $K_s(p_1)$ has a basis $\{b_i\}$ such that $d(b_i)=s$ $\forall i$. But then $\tilde{A}^{\dagger}b_i\in K_s(b_i)=K_s(p_1)$ for every i, as shown in part (4) above. But since this is true on every basis vector, the whole subspace must be $\tilde{A}^{\dagger}$-invariant. Claim shown.

(6) *Extracting an eigenvector.* It can be easily seen that such a $p_1\in K_{s+1}$ with $d(p_1)=s$ actually exists. Also, we have seen that both K_{s+1} and $K_s(p_1)$ are $\tilde{A}$- and $\tilde{A}^{\dagger}$-invariant. Now, let $K_s(p_1)^{\perp_H}\equiv\{v\in K_{s+1}:\langle w,v\rangle=0\ \forall w\in K_s(p_1)\}$. *Claim:* $K_s(p_1)^{\perp_H}$ one-dimensional. *Proof:* Note that $\langle w,v\rangle=(w,\tilde{H}v)$ for all $w,v\in K_{s+1}$. Since $\tilde{H}$ is nonsingular as a map on K_{s+1}, we have $K_s(p_1)^{\perp}=\tilde{H}K_s(p_1)^{\perp_H}$, where $K_s(p_1)^{\perp}\equiv\{v\in K_{s+1}:(w,v)=0\ \forall w\in K_s(p_1)\}$. Since $K_s(p_1)^{\perp}$ is known to be one-dimensional and $\tilde{H}$ is nonsingular as a map on K_{s+1}, the claim is shown. Now, let q_1 be a nonzero vector in $K_s(p_1)^{\perp_H}$. *Claim:* $\tilde{A}q_1\in K_s(p_1)^{\perp_H}$. *Proof:* Clearly, $\tilde{A}q_1\in K_{s+1}$. But note also that if $w\in K_s(p_1)$, $\langle w,\tilde{A}q_1\rangle=\langle\tilde{A}^{\dagger}w,q_1\rangle=0$, since $K_s(p_1)$ is $\tilde{A}^{\dagger}$-invariant and $q_1\in K_s(p_1)^{\perp_H}$. Claim shown. Conclusion: q_1 is an eigenvector.

(7) *Extracting the rest of the eigenvectors from* K_{s+1}. It is possible to pick $p_2\in K_{s+1}$ such that $d(p_2)=s$ and $q_1\in K_s(p_2)$. Repeat the above process to obtain $q_2\in K_{s+1}$, an eigenvector, with $\langle q_1,q_2\rangle=0$. Repeat this process to obtain all the eigenvectors $\{q_i\}_{i=1}^{s+1}$ and associated eigenvalues $\{\lambda_i\}_{i=1}^{s+1}$ of K_{s+1}. Note that, since K_{s+1} has a complete set of eigenvectors, the λ_i's must all be distinct: otherwise, the minimal polynomial of $\tilde{p}$ would have degree less than $s+1$.

(8) Note that, by construction, the $\{q_i\}_{i=1}^{s+1}$ are H-semiorthogonal: $\langle q_i,q_j\rangle=0$ for $i<j$. Now, let $\tilde{p}_1$ be a linear combination from $\{q_i\}_{i=2}^{s+1}$ in which every vector has a nonzero component. Then the minimal polynomial of $\tilde{p}_1$ is given by $\prod_{i=2}^{s+1}(\lambda-\lambda_i)$. So $d(\tilde{p}_1)=s$, and $K_s(\tilde{p}_1)=\operatorname{span}\{q_i\}_{i=2}^{s+1}$. By repeating the argument above, there is an eigenvector in $(\operatorname{span}\{q_i\}_{i=2}^{s+1})^{\perp_H}$. But there are no more than $s+1$ eigenvectors in K_{s+1}. So this eigenvector is q_j for some j. But, by construction, $\langle q_j,q_i\rangle=0$ for $2\leqslant i\leqslant s+1$. Since H is definite, this eigenvector must be q_1. By repeating this argument, we see that the $\{q_i\}_{i=1}^{s+1}$ are H^*-semiorthogonal as well as H-semiorthogonal.

(9) *Claim:* A is normal. *Proof:* Otherwise, by Corollary 4.5, either A does not have a complete set of eigenvectors, or A has two eigenvectors associated with distinct eigenvalues which are not H- and H^*-semiorthogo-

nal. First, suppose there exists a v such that $(A-\lambda)v \neq 0$ and $(A-\lambda)^2 v = 0$. Now, let $\bar{p}$ be chosen so that $d(\bar{p}) = s+1$ and $v \in K_{s+1}(\bar{p})$. Such a $\bar{p}$ may be constructed from principal vectors of the matrix A. This subspace has all the properties shown above for subspace K_{s+1}—in particular, it contains $s+1$ eigenvectors. But, by construction, this new subspace has an incomplete set of eigenvectors. Contradiction. Similarly, consider any eigenvectors q_1, q_2 of A associated with distinct eigenvalues. These may be similarly included in a space like K_{s+1} and shown to be H- and H^*-semiorthogonal, by the above derivation. ■

THEOREM 4.8. *$A \in \widetilde{\text{OD}}(s, H)$ $\Leftrightarrow$ $\bar{d}(A) \leqslant s$ or A normal with respect to H with normal degree $n(A) \leqslant s-1$.*

Proof. $\Leftarrow$: Follows easily from Lemma 4.1, Lemma 4.2, and Lemma 4.3.
$\Rightarrow$: Suppose $A \in \widetilde{\text{OD}}(s, H)$ and $\bar{d}(A) > s$.

Consider the map $F_n : C^N \to C$, $F_n(q^{(0)}) = \langle q^{(0)}, Aq^{(n)} \rangle$, where $q^{(n)}$ is considered as a function of $q^{(0)}$. In particular, consider $F_s(q) = \langle q, Aq^{(s)} \rangle$, writing $q^{(0)}$ as q. Since $A \in \widetilde{\text{OD}}(s, H)$, by definition, we have $F_s(q) = 0$ for all $q \in C^N$.

By Lemma 4.7, A is normal with respect to H. By Theorem 4.4, there exists a polynomial P such that $A^{\dagger} = P(A)$. Since A has $\bar{d}(A)$ distinct eigenvalues, Lagrangian interpolation polynomials may be used to construct P such that $\deg P \leqslant \bar{d}(A) - 1$, i.e., $n(A) \leqslant \bar{d}(A) - 1$ (see [10]).

Recall $F_n(q) = \langle q, Aq^{(n)} \rangle$, writing $q^{(0)}$ as q. Since $A \in \widetilde{\text{OD}}(s, H)$, we have $F_n(q) = 0$ when $n > s-1$ for all $q \in C^N$. We have just seen $A^{\dagger}q \in K_{\bar{d}(A)}(q) = K_d(q) = \operatorname{span}\{q^{(i)}\}_{i=0}^{d-1}$, letting $d = d(q)$; thus $A^{\dagger}q = \sum_{i=0}^{d-1} c_i q^{(i)}$. But then

$$0 = \langle A^{\dagger}q, q^{(n)} \rangle = \left\langle \sum_{i=0}^{d-1} c_i q^{(i)}, q^{(n)} \right\rangle = \sum_{i=0}^{d-1} \bar{c}_i \langle q^{(i)}, q^{(n)} \rangle$$

for $n > s-1$. From the definiteness of H, we see that $c_{d-1} = c_{d-2} = \cdots = c_s = 0$. This implies $A^{\dagger}q \in K_s(q)$ for all q. By Lemma 4.3, A is H-normal, with normal degree $n(A) \leqslant s-1$. ■

5. CHARACTERIZATION OF OM(s, H) AND OR(s, H)

We will show in this section that $\text{OM}(s, H) = \text{OR}(s, H) = \widetilde{\text{OD}}(s+1, Z)$. We begin with several lemmas.

The following basic lemma concerns the definition of the vectors generated by the ORTHODIR semiorthogonalization process.

LEMMA 5.1. *Let A be nonsingular and H be definite. Let*

$$\gamma_n v^{(n)} = A v^{(n-1)} + \sum_{i=0}^{n-1} \gamma_{n,i} v^{(i)},$$

with $\gamma_{n,i}$ such that $(v^{(i)}, H v^{(n)}) = 0$ for $i < n$, and $\gamma_n \neq 0$ arbitrary. Let $v^{(0)} \neq 0$ be given. Then, the $v^{(i)}$'s are uniquely defined, and $v^{(n)} = 0$ if and only if $n \geqslant d(v^{(0)})$.

Proof. Let $d = d(v^{(0)})$. First, we will show by induction that $v^{(n)}$ is well defined and nonzero for $n < d$. Certainly this is true for $n = 0$. Suppose it is true for all $i < n$. Then the semiorthogonality condition implies that the $\gamma_{n,i}$'s satisfy

$$\begin{pmatrix} \langle v^{(0)}, v^{(0)} \rangle & \cdots & \langle v^{(0)}, v^{(n-1)} \rangle \\ \vdots & \ddots & \vdots \\ \langle v^{(n-1)}, v^{(0)} \rangle & \cdots & \langle v^{(n-1)}, v^{(n-1)} \rangle \end{pmatrix} \begin{pmatrix} \gamma_{n,0} \\ \vdots \\ \gamma_{n,n-1} \end{pmatrix}$$

$$= - \begin{pmatrix} \langle v^{(0)}, A v^{(n-1)} \rangle \\ \vdots \\ \langle v^{(n-1)}, A v^{(n-1)} \rangle \end{pmatrix}.$$

The semiorthogonality condition and the induction hypothesis imply that this matrix is lower triangular. By induction, $\{ v^{(i)} \}_{i=0}^{n-1}$ are all nonzero. Since H is definite, the diagonal elements of this matrix are nonzero, so the matrix is nonsingular. Thus, the $\gamma_{n,i}$'s are uniquely defined, and therefore $v^{(n)}$ is. Now, note that $\{ v^{(i)} \}_{i=0}^{n-1}$ are linearly independent: applying $\langle v^{(j)}, \cdot \rangle$ to $\sum_{i=0}^{n-1} a_i v^{(i)} \equiv 0$ for consecutive j's gives $a_j = 0$ for each j. Also, $v^{(n-1)}$ is not in $K_{n-1}(v^{(0)})$: else, $\{ v^{(i)} \}_{i=0}^{n-1} \subseteq K_{n-1}(v^{(0)})$ would be linearly dependent. Thus, $v^{(n-1)} = a A^{n-1} v^{(0)} + \tilde{v}$, for some scalar $a \neq 0$ and vector $\tilde{v} \in K_{n-1}(v^{(0)})$. Now, suppose $v^{(n)} = 0$. Then,

$$0 = v^{(n)} = A v^{(n-1)} + \sum_{i=0}^{n-1} \gamma_{n,i} v^{(i)} = a A^n v^{(0)} + A \tilde{v} + \sum_{i=0}^{n-1} \gamma_{n,i} v^{(i)}.$$

This implies that $A^n v^{(0)} \in K_n(v^{(0)})$. But this contradicts the fact that $n < d$. Thus, $v^{(n)} \neq 0$.

To complete the proof, we show that $v^{(n)} = 0$ for any $n \geqslant d$. Clearly, $v^{(n)} \in K_{n+1}(v^{(0)})$. But, for $n \geqslant d$, $\{v^{(i)}\}_{i=0}^{d-1}$ are a basis for $K_{n+1}(v^{(0)})$. So, $v^{(n)} = \sum_{i=0}^{n-1} a_i v^{(i)}$ for some scalars a_i. Applying $\langle v^{(j)}, \cdot \rangle$ for consecutive j's and invoking the semiorthogonality condition gives $a_j = 0$ for all j. Thus, $v^{(n)} = 0$ for $n \geqslant d$. ∎

The following lemma shows that scaling the new basis vector at each step of the semiorthogonalization process affects later vectors only by scaling them differently.

Lemma 5.2. *Let A be nonsingular and H be definite. Let*

$$\gamma_n v^{(n)} = A v^{(n-1)} + \sum_{i=0}^{n-1} \gamma_{n,i} v^{(i)},$$

$\gamma_{n,i}$ such that $(v^{(i)}, H v^{(n)}) = 0$, $i < n$, and $\gamma_n \neq 0$ arbitrary;

$$\tilde{\gamma}_n \tilde{v}^{(n)} = A \tilde{v}^{(n-1)} + \sum_{i=0}^{n-1} \tilde{\gamma}_{n,i} \tilde{v}^{(i)},$$

$\tilde{\gamma}_{n,i}$ such that $(\tilde{v}^{(i)}, H \tilde{v}^{(n)}) = 0$, $i < n$, and $\tilde{\gamma}_n \neq 0$ arbitrary. Let $\gamma_0 v^{(0)} = \tilde{\gamma}_0 \tilde{v}^{(0)} \neq 0$. Then $\tilde{v}^{(n)} = c_n v^{(n)}$ for some nonzero constants c_n.

Proof. If $n \geqslant d \equiv d(v^{(0)}) = d(\tilde{v}^{(0)})$, we are done, because $v^{(n)} = \tilde{v}^{(n)} = 0$ by Lemma 5.1. If $n < d$, then $\{v^{(i)}\}_{i=0}^{n}$ is a basis for $K_{n+1}(v^{(0)})$. Thus, $\tilde{v}^{(n)} = \sum_{i=0}^{n} a_i v^{(i)}$ for some a_i's. Applying $\langle v^{(j)}, \cdot \rangle$ for consecutive j's and using the semiorthogonality condition gives $a_i = 0$ for $i < n$; thus $\tilde{v}^{(n)} = a_n v^{(n)}$. Since $\tilde{v}^{(n)} \neq 0$, a_n is nonzero. ∎

Now we may characterize the set $\text{OR}(s, H)$.

Theorem 5.3. *Let Z, $H \equiv ZA$ be definite. Then $\text{OR}(s, H) = \widetilde{\text{OD}}(s+1, Z)$.*

Proof. Consider the following semiorthogonalization process:

$$\tilde{q}^{(0)} = r^{(0)};$$

$$\tilde{q}^{(n)} = A \tilde{q}^{(n-1)} + \sum_{i=0}^{n-1} \tilde{\beta}_{n,i} \tilde{q}^{(i)}, \qquad \text{imposing} \quad \left(\tilde{q}^{(i)}, Z \tilde{q}^{(n)}\right) \quad \text{for } i < n.$$

Now, the residuals of the ORTHORES algorithm are given by

$$\left(-\frac{1}{\lambda_n}\right) r^{(n+1)} = Ar^{(n)} + \sum_{i=0}^{n} (-\sigma_{n+1,i}) r^{(i)}$$

[see Equation (3.4)]. Comparing these $\tilde{q}^{(i)}$'s with the $r^{(i)}$'s of the ORTHORES algorithm which are defined by the Z-semiorthogonality condition [Equation (3.6)], we see that they are the same up to some nonzero scaling, by Lemma 5.2. Thus,

$$\begin{aligned} A \in \mathrm{OR}(s, H) &\Leftrightarrow (r^{(i)}, ZAr^{(n)}) = 0 \quad \text{for } i < n-s,\ n < d(r^{(0)}) \\ &\Leftrightarrow (\tilde{q}^{(i)}, ZA\tilde{q}^{(n)}) = 0 \quad \text{for } i < n-s,\ n < d(r^{(0)}) \\ &\Leftrightarrow (\tilde{q}^{(i)}, ZA\tilde{q}^{(n-1)}) = 0 \quad \text{for } i < n-(s+1),\ n \leqslant d(r^{(0)}) \\ &\Leftrightarrow A \in \widetilde{\mathrm{OD}}(s+1, Z). \qquad \blacksquare \end{aligned}$$

Now, we desire to characterize $\mathrm{OM}(s, H)$. We continue to assume Z, $H \equiv ZA$ definite.

THEOREM 5.4. $\mathrm{OM}(s, H) \subseteq \mathrm{OR}(s, H)$.

Proof.[1] Let $\theta(n) = \max\{0, n-s\}$. Now, suppose $A \in \mathrm{OM}(s, H)$, i.e., $\langle p^{(i)}, r^{(n)} \rangle = 0$ for $i < n-s$, $n < d(r^{(0)}) \equiv d$. Then $\alpha_{n,i} = 0$ for $i < n-s$, $n < d$. So we may write $p^{(n)} = r^{(n)} + \sum_{i=\theta(n)}^{n-1} \alpha_{n,i} p^{(i)}$. We seek to show that $(r^{(i)}, ZAr^{(n)}) = 0$ for $i < n-s$. Note that

$$\begin{aligned} r^{(n+1)} &= r^{(n)} - \lambda_n A p^{(n)} \\ &= r^{(n)} - \lambda_n A \left(r^{(n)} + \sum_{i=\theta(n)}^{n-1} \alpha_{n,i} p^{(i)} \right) \\ &= r^{(n)} - \lambda_n A r^{(n)} - \lambda_n \sum_{i=\theta(n)}^{n-1} \alpha_{n,i} A p^{(i)}. \end{aligned}$$

Now, suppose $n \geqslant d$. Then $r^{(n)} = 0$, since $u^{(d)} = \bar{u}$, and we are done.

[1] This proof is based on a technique used by Voevodin [17, 18].

Otherwise, $n < d$, so $\lambda_i \neq 0$ for $i \leqslant n$ $[(p^{(i)}, Zr^{(i)}) = (r^{(i)}, Zr^{(i)}) \neq 0$, since $r^{(i)} \neq 0$ and Z definite]. Thus

$$Ar^{(n)} = \frac{1}{\lambda_n}\left(r^{(n)} - r^{(n+1)}\right) - \sum_{i=\theta(n)}^{n-1} \alpha_{n,i} Ap^{(i)}$$

$$= \frac{1}{\lambda_n}\left(r^{(n)} - r^{(n+1)}\right) - \sum_{i=\theta(n)}^{n-1} \frac{\alpha_{n,i}}{\lambda_i}\left(r^{(i)} - r^{(i+1)}\right).$$

This implies $Ar^{(n)} \in \operatorname{span}\{r^{(j)}\}_{j=\theta(n)}^{n+1}$. Therefore,

$$\left(r^{(i)}, ZAr^{(n)}\right) = \left(r^{(i)}, Z\sum_{j=\theta(n)}^{n+1} a_j r^{(j)}\right) = 0 \quad \text{for} \quad i < \theta(n) \equiv \max\{0, n-s\},$$

by the Z-semiorthogonality of the residuals. Therefore we conclude that $A \in \text{OR}(s, H)$, by definition. ■

THEOREM 5.5. $\bar{d}(A) \leqslant s+1 \Rightarrow A \in \text{OM}(s, H)$.

Proof. $A \in \text{OM}(s, H) \Leftrightarrow \langle p^{(i)}, r^{(n)} \rangle = 0$ for $i < n-s$, $n < d(p^{(0)})$. But this requires that $n < d(p^{(0)}) \leqslant \bar{d}(A) \leqslant s+1$. Then it is never true that $i < n - s \leqslant 0$, so the definition is trivially satisfied. ■

THEOREM 5.6. *If A is Z-normal and $n(A) \leqslant s$ then $A \in \text{OM}(s, H)$.*

Proof. $n(A) \leqslant s \Rightarrow (ZAZ^{-1})^* = P_s(A)$ for some s-degree polynomial P. Then

$$\left(p^{(i)}, ZAr^{(n)}\right) = \left(p^{(i)}, ZAZ^{-1}Zr^{(n)}\right) = \left((ZAZ^{-1})^* p^{(i)}, Zr^{(n)}\right)$$

$$= \left(P_s(A)p^{(i)}, Zr^{(n)}\right) = 0 \qquad \text{for} \quad i+s<n,$$

by the Petrov-Galerkin condition. ■

THEOREM 5.7. $\text{OM}(s, H) = \text{OR}(s, H)$.

Proof. Using the previous results, we have

$$\begin{aligned} A \in \text{OM}(s,H) \quad &\Rightarrow \quad A \in \text{OR}(s,H) \quad \Leftrightarrow \quad A \in \widetilde{\text{OD}}(s+1, Z) \\ &\Leftrightarrow \quad \bar{d}(A) \leqslant s+1 \text{ or} \\ &\qquad\ A \text{ is } Z\text{-normal with } n(A) \leqslant s. \end{aligned}$$

But $\bar{d}(A) \leqslant s+1 \Rightarrow A \in \text{OM}(s, H)$, and likewise A is Z-normal with $n(A) \leqslant s$ $\Rightarrow A \in \text{OM}(s, H)$, by Theorems 5.5 and 5.6. ■

The previous theorems show that $\text{OM}(s, H) = \text{OR}(s, H) = \widetilde{\text{OD}}(s+1, Z)$ for A nonsingular and for Z and $H = ZA$ definite.[2]

Therefore, we know the following facts about generalized conjugate-gradient methods. Let $A \in C^{N\times N}$ be nonsingular, and consider auxiliary matrices Z and $H \equiv ZA$.

(1) For H definite, ORTHODIR$(s) \equiv$ ORTHODIR $\Leftrightarrow$ A has minimal polynomial of degree $\bar{d}(A) = s+1$, or A commutes with $(HAH^{-1})^*$ and there exists a polynomial P_{s-1} of degree $s-1$ such that $(HAH^{-1})^* = P_{s-1}(A)$.

(2) For Z, H definite, ORTHOMIN$(s) \equiv$ ORTHOMIN $\Leftrightarrow$ ORTHORES$(s) \equiv$ ORTHORES $\Leftrightarrow$ A has minimal polynomial of degree $\bar{d}(A) = s+1$, or A commutes with $(ZAZ^{-1})^*$ and there exists a polynomial P_s of degree s such that $(ZAZ^{-1})^* = P_s(A)$.

It is easily seen that for $H = ZA$, $(HAH^{-1})^* = (ZAZ^{-1})^*$; therefore $\widetilde{\text{OD}}(s+1, Z) = \widetilde{\text{OD}}(s+1, H)$. Thus we have

THEOREM 5.8. *Let A be nonsingular, with minimal polynomial of degree $\bar{d}(A) > s+2$. Furthermore, let the auxiliary matrix Z and the matrix $H = ZA$ be definite. Then* ORTHODIR$(s+1) \equiv$ ORTHODIR $\Leftrightarrow$ ORTHOMIN$(s) \equiv$ ORTHOMIN $\Leftrightarrow$ ORTHORES$(s) \equiv$ ORTHORES $\Leftrightarrow$ *A commutes with $(ZAZ^{-1})^*$ and there exists a polynomial P_s of degree s such that $(ZAZ^{-1})^* = P_s(A)$.*

This tells us that, for the cases of interest—i.e., when A has at least $s+3$ distinct eigenvalues—all three methods simplify, with no change in the iterates, for precisely the same matrices.

[2]An alternative proof of this result, which also applies to more general cases, has been developed by V. Faber and T. Manteuffel (private communication).

6. THE CASE $n(A)=1$

Faber and Manteuffel [9, 10] showed that if A is normal with respect to a matrix H, then for some HPD matrix $\hat{H}$, A is normal with respect to $\hat{H}$ and moreover $(HAH^{-1})^* = (\hat{H}A\hat{H}^{-1})^*$. They also showed that if $n(A)>1$ then

$$\sqrt{\bar{d}(A)} \leqslant n(A) \leqslant \bar{d}(A)-1.$$

This result suggests that the case $n(A)>1$ is not very useful, because it requires s to be at least $\sqrt{\bar{d}(A)}$. We conclude that, in general, in order that the formulas can be simplified to the point of computational usefulness, we must have $n(A)\leqslant 1$. From the results of Faber and Manteuffel [9, 10] we have

THEOREM 6.1. *If A is normalizable and if $n(A)\leqslant 1$, then for some HPD matrix $\hat{H}$, either A is a multiple of the identity, $A=(\hat{H}A\hat{H}^{-1})^*$, or $A = e^{i\theta}(B+irI)$, where r and θ are real and $(\hat{H}B\hat{H}^{-1})^* = B$.*

The third condition is equivalent to that given by Faber and Manteuffel [9], but is written here in a slightly different form.

We now give two theorems which give conditions on A so that a matrix $\hat{H}$ exists such that the second and third possibilities stated in Theorem 6.1 can occur. We also discuss cases where $\hat{H}$ and $Z=\hat{H}A^{-1}$ are definite so that ORTHOMIN and ORTHORES, as well as ORTHODIR, simplify.

THEOREM 6.2. *Let $A\in C^{N,N}$. There exists an HPD matrix $\hat{H}$ such that $(\hat{H}A\hat{H}^{-1})^* = A$ if and only if A is similar to a Hermitian matrix. Also, there exist HPD matrices Z and $\hat{H}$ such that $\hat{H}=ZA$ and $(\hat{H}A\hat{H}^{-1})^*=A$ if and only if A is similar to an HPD matrix.*

Proof. Suppose A is similar to a Hermitian matrix K, i.e., suppose $V^{-1}AV=K$ for some V. We let $\hat{H}=V^{-*}V^{-1}$. Since $A=VKV^{-1}$, we have $\hat{H}A\hat{H}^{-1}=V^{-*}KV^{*}=A^*$. On the other hand, if $A^*=\hat{H}A\hat{H}^{-1}$ for some HPD matrix $\hat{H}$, then $\hat{H}^{-1/2}A^*\hat{H}^{1/2}=\hat{H}^{1/2}A\hat{H}^{-1/2}$ and

$$\hat{H}^{1/2}A\hat{H}^{-1/2}=(\hat{H}^{1/2}A\hat{H}^{-1/2})^*.$$

Thus A is similar to the Hermitian matrix $\hat{H}^{1/2}A\hat{H}^{-1/2}$.

Suppose now that A is similar to an HPD matrix K, i.e., suppose $V^{-1}AV=K$ for some V. If we let $Z=V^{-*}V^{-1}$, then $\hat{H}=ZA=V^{-*}KV^{-1}$

and both Z and H are HPD. Moreover, $(\hat{H}A\hat{H}^{-1})^* = A$. Finally, if $(\hat{H}A\hat{H}^{-1})^* = A$ for some HPD matrix $\hat{H}$ with $Z = \hat{H}A^{-1}$ also HPD, then, as above, $\hat{H}^{1/2}A\hat{H}^{-1/2}$ is Hermitian. Since $\hat{H}A^{-1}$ is HPD, it follows that $\hat{H}^{-1/2}(\hat{H}A^{-1})\hat{H}^{-1/2} = \hat{H}^{1/2}A^{-1}\hat{H}^{-1/2}$ is HPD and $(\hat{H}^{1/2}A^{-1}\hat{H}^{-1/2})^{-1} = \hat{H}^{1/2}A\hat{H}^{-1/2}$ is HPD. ∎

From Theorem 6.2 it follows that if A is similar to a Hermitian matrix, then there exist Z and $\hat{H}$ such that $\hat{H} = ZA$, $\hat{H}$ is HPD, and we have OD(2). Also, if A is similar to an HPD matrix, there exist Z and $\hat{H}$ such that both Z and $\hat{H}$ are HPD, $\hat{H} = ZA$, and we have S(1). In Section 7 we will give some alternative choices for Z and $\hat{H}$ which can be used when A is similar to a Hermitian matrix or to an HPD matrix.

We now give a necessary and sufficient condition on A, stated by Faber and Manteuffel [9], for an HPD matrix $\hat{H}$ to exist such that the third possibility of Theorem 6.2 occurs.

THEOREM 6.3. *Let $A \in C^{N,N}$. There exists an HPD matrix $\hat{H}$ such that*

$$A = e^{i\theta}(B + irI), \tag{6.1}$$

where r and θ are real and such that

$$B = (\hat{H}B\hat{H}^{-1})^* \tag{6.2}$$

if and only if A is similar to a diagonal matrix and the eigenvalues of A lie on a straight line.

Proof. If A has the form (6.1) where B satisfies (6.2), then $\tilde{B}^* = \tilde{B}$, where $\tilde{B} = \hat{H}^{1/2}B\hat{H}^{-1/2}$. Evidently

$$\tilde{A} = \hat{H}^{1/2}A\hat{H}^{-1/2} = e^{i\theta}(\tilde{B} + irI). \tag{6.3}$$

Since the eigenvalues of $\tilde{B}$ are real, the eigenvalues λ of $\tilde{A}$, and hence those of A, have the form $\lambda = e^{i\theta}(x + ir)$, where x, r, and θ are real. Thus each eigenvalue lies on the straight line in the complex z-plane obtained by rotating the line $\operatorname{Im} z = r$ about the origin through a suitable angle θ.

Suppose now that A is similar to a diagonal matrix and that all eigenvalues of A lie on a straight line. Clearly, for some real x, r, and θ, each eigenvalue λ of A can be written in the form $\lambda = e^{i\theta}(x + ir)$. Thus the Jordan canonical form of A has the form

$$D_1 = e^{i\theta}(D + irI),$$

where D is a real diagonal matrix. Therefore, for some nonsingular matrix V we have

$$A = VD_1V^{-1} = e^{i\theta}(B + irI), \tag{6.4}$$

where

$$B = VDV^{-1}. \tag{6.5}$$

If we let $\hat{H} = V^{-*}V^{-1}$, then $\hat{H}$ is HPD and $(\hat{H}B\hat{H}^{-1})^* = VDV^{-1} = B$. Thus A and B satisfy (6.1) and (6.2). ■

Suppose now that A is similar to a diagonal matrix and that the eigenvalues of A lie on a straight line. By Theorem 6.3 and (6.3), A has the form (6.1) where B is similar to a Hermitian matrix. Let V be any matrix such that

$$V^{-1}BV = K, \tag{6.6}$$

where K is Hermitian. Evidently, by (6.4), $V^{-1}AV = e^{i\theta}(K + irI)$. We consider various choices of Z and H, namely,

$$Z_1 = V^{-*}V^{-1}A^{-1}, \qquad H_1 = V^{-*}V^{-1},$$

$$Z_2 = A^*V^{-*}V^{-1}, \qquad H_2 = A^*V^{-*}V^{-1}A,$$

$$Z_3 = V^{-*}V^{-1}, \qquad H_3 = V^{-*}V^{-1}A.$$

In each case we can verify that for all three choices

$$A^\dagger = (ZAZ^{-1})^* = (HAH^{-1})^* = e^{-2i\theta}A - 2irIe^{-i\theta},$$

which is a polynomial of degree one in A.

In the general case H_1 and H_2 are definite and ORTHODIR converges and simplifies for the first two choices. Let us now further assume that K is Hermitian definite. It can be shown that in this case Z and H are definite for all three choices. Thus, for example, consider Z_1. We have

$$Z_1 = V^{-*}V^{-1}A^{-1} = V^{-*}(V^{-1}A^{-1}V)V^{-1}$$

$$= V^{-*}(V^{-1}AV)^{-1}V^{-1}.$$

To show that Z_1 is definite we show $V^{-1}AV$ is definite. But by (6.1) and (6.6) we have

$$\begin{aligned} V^{-1}AV &= V^{-1}\{e^{i\theta}(B+irI)\}V \\ &= e^{i\theta}(K+irI), \end{aligned}$$

where K is Hermitian definite. Thus for any vector x we have

$$(x,(K+irI)x) = (x,Kx) + ir(x,x).$$

The first term is real and does not vanish for $x \neq 0$ if K is definite. The second term is purely imaginary and does not vanish unless $r = 0$. Thus, since either K is definite or else $r \neq 0$, $V^{-1}AV$ is definite. From this it follows that Z^{-1} and hence Z is definite.

It follows from the above analysis that if A has the form (6.4) where B is similar to a Hermitian definite matrix K, then, with the above choices of Z and H, ORTHOMIN and ORTHORES, as well as ORTHODIR, converge and simplify. Moreover, we have S(1).

7. CONDITIONS FOR SIMPLIFICATION

From the previous discussion it follows that for some auxiliary matrix Z the generalized CG methods simplify under each of the following conditions:

CONDITION α. There exists Z such that H is definite and $(ZAZ^{-1})^* = P(A)$.

CONDITION β. There exists Z such that Z and H are definite and $(ZAZ^{-1})^* = P(A)$.

CONDITION γ. There exists Z such that H is definite and $(ZAZ^{-1})^* = A$.

CONDITION δ. There exists Z such that Z and H are definite and $(ZAZ^{-1})^* = A$.

Here $P(A)$ is a polynomial and $H = ZA$. As we have seen, ORTHODIR converges for suitable Z when Condition α or γ holds, and all three variants converge when Condition β or δ holds.

In this section we formulate four other conditions, Conditions a, b, c, and d, on the matrix A, and we show that they imply Conditions α, β, γ, and δ, respectively. We also give procedures for choosing Z when Condition a, b, c, or d holds. We then study the question as to whether Conditions α, β, γ, and δ imply Conditions a, b, c, and d, respectively. Counterexamples are given for some cases.

We now consider the following conditions on the matrix A:

Condition a. A is similar to a normal matrix (normalizable).

Condition b. A is similar to a normal definite matrix.

Condition c. A is similar to a Hermitian matrix.

Condition d. A is similar to a Hermitian definite (HD) matrix.

Evidently Conditions a, b, c, and d imply that the Jordan canonical form of A is diagonal, diagonal definite, real diagonal, and real diagonal definite, respectively.

Let us now consider alternative choices of the auxiliary matrix Z corresponding to a given linear system (1.1) where A is normal. We consider the following choices:

Choice I: $Z = I$, $H = A$ (conjugate gradient),

Choice II: $Z = A^*$, $H = A^*A$ (conjugate residual),

Choice III: $Z = A^{-1}$, $H = I$ (minimum error).

We remark that Choice III is in general not practical. However, if (1.1) is derived from another system of the form

$$\hat{A}u = \hat{b}$$

and if $A = \hat{A}^*C\hat{A}$, $b = \hat{A}^*C\hat{b}$, where C is chosen so that A is normal, then the conjugate gradient procedures with Choice III can be carried out; see Faber and Manteuffel [10, Section D]. We remark that this choice of A corresponds to the use of generalized normal equations.

Since A is normal, $A^* = P(A)$ for some polynomial $P(A)$. If A is Hermitian then $P(A) = A$. In any case for each choice we have

$$(ZAZ^{-1})^* = (HAH^{-1})^* = P(A). \tag{7.1}$$

If A is definite, then Z and H are both definite and we have Condition β—or, if $P(A) = A$, Condition δ—for Choices I, II, and III.

Suppose now that A is normalizable. That is, suppose that for some nonsingular matrix V we have

$$V^{-1}AV = K, \tag{7.2}$$

where K is normal. We can consider the modified system

$$\text{Ⓐ}\,\text{ⓤ} = \text{ⓑ}, \tag{7.3}$$

where

$$\text{Ⓐ} = V^{-1}AV, \qquad \text{ⓑ} = V^{-1}b, \qquad \text{ⓤ} = V^{-1}u. \tag{7.4}$$

We now apply the generalized conjugate-gradient methods with auxiliary matrix Z to (7.3). One can verify from the formulas for ORTHODIR, ORTHOMIN, and ORTHORES given in Sections 2 and 3 that this is equivalent to applying the methods to the original system (1.1) with

$$Z = V^{-*}\,\text{Ⓩ}\,V^{-1}. \tag{7.5}$$

Thus Choices I, II, and III correspond to the following choices:

Choice I*: $\quad Z = V^{-*}V^{-1}, \qquad H = V^{-*}V^{-1}A$
$\qquad\qquad\qquad\qquad\qquad\qquad\quad = V^{-*}KV^{-1},$

Choice II*: $\quad Z = A^{*}V^{-*}V^{-1} \qquad H = A^{*}V^{-*}V^{-1}A,$
$\qquad\qquad\qquad = V^{-*}K^{*}V^{-1},$

Choice III*: $\quad Z = V^{-*}V^{-1}A^{-1} \qquad H = V^{-*}V^{-1}.$
$\qquad\qquad\qquad = V^{-*}K^{-1}V^{-1},$

We now show that if we let $Z = Z_1 = V^{-*}V^{-1}$ then $(ZAZ^{-1})^{*} = P(A)$. Here P is a polynomial of degree $n(A)$ such that $K^{*} = P(K)$. Since $A = VKV^{-1}$, we have

$$\begin{aligned}(ZAZ^{-1})^{*} &= (V^{-*}V^{-1}AVV^{*})^{*} = (V^{-*}KV^{*})^{*}\\ &= VK^{*}V^{-1} = VP(K)V^{-1}\\ &= P(VKV^{-1}) = P(A).\end{aligned}$$

Similar proofs can be given for the other choices of Z. If K is Hermitian as well as normal, then $(ZAZ^{-1})^* = A$ for all three choices of Z. We have thus shown that Condition a implies Condition α and that Condition c implies Condition γ.

Suppose now that A is similar to a normal definite matrix K (Condition b) and that $K = V^{-1}AV$. With the choices of Z given above, both Z and H are definite and (7.1) holds; thus we have Condition β. Similarly, if A is similar to a Hermitian definite (HD) matrix K (Condition d) then $V^{-1}AV = K$ for some V. Evidently both Z and H are definite for all three choices and $ZA = A^*Z$. Thus we have Condition δ.

From the above discussion it follows that Conditions a, b, c, and d imply Conditions α, β, γ, and δ, respectively. We now consider the converse questions. The fact that Condition α implies Condition a follows from a result of Faber and Manteuffel [10] which states that if A is H-normal for some definite H, then A is similar to a diagonal matrix. The fact that Condition γ implies Condition c follows from Theorem 6.2.

We now show that Condition δ implies Condition d in a limited sense. Indeed, we prove

THEOREM 7.1. *If A is real and if there exists a real matrix Z such that $(ZAZ^{-1})^* = A$ and such that Z and H are definite, then A satisfies Condition* d.

Proof. Since $(ZAZ^{-1})^* = A$, we have $A^*Z^* = Z^*A$ and $ZA = A^*Z$. Therefore

$$(Z + Z^*)A = A^*(Z + Z^*).$$

Since Z is real and definite, $Z_1 = Z + Z^*$ is HD. Also, since $H = ZA$, we have $H^*A = A^*H^*$. [Note that $(ZA)^*A - A^*(ZA)^* = A^*(Z^*A - A^*Z^*) = 0$.] Also we can show that $H_1A = A^*H_1$, where $H_1 = H + H^*$ is HD. Moreover

$$H_1 = H + H^* = ZA + (ZA)^* = ZA + A^*Z^*$$
$$= ZA + Z^*A = Z_1A.$$

Thus $A = Z_1^{-1}H_1$. Without loss of generality we may assume H_1 to be HPD. Evidently A is similar to

$$H_1^{1/2}AH_1^{-1/2} = H_1^{1/2}Z_1^{-1}H_1^{1/2},$$

which is definite since Z_1 is. Thus A satisfies Condition d. ∎

We also prove

THEOREM 7.2. *If* $(ZAZ^{-1})^* = A$ *for some matrix* Z *such that* Z *and* $H = ZA$ *are definite and such that* Z *or* H *is HPD, then* A *satisfies Condition* d.

Proof. Since $ZA = H$, we have $A = Z^{-1}H$. If H is HPD, then A is similar to the matrix $H^{1/2}Z^{-1}H^{1/2} = H^{1/2}AH^{-1/2}$. Since $H^{1/2}Z^{-1}H^{1/2}$ is definite, A is similar to a definite matrix. A similar argument can be given if Z is HPD. ■

The following counterexample shows that in the general case Condition δ does not necessarily imply Condition d. Indeed, let

$$A = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, \qquad H = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}.$$

Note that Z and H are definite, $H = ZA$, and

$$HA = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} = A^*H.$$

Hence Condition δ holds. On the other hand, A is not similar to a definite matrix, since $E(A)$, the convex hull of the eigenvalues of A, contains the origin.

The above example, of course, also shows that Condition β does not imply Condition b. However, we now show that Condition β does imply Condition b in a limited sense.

THEOREM 7.3. *If there exists a definite matrix* Z *such that* $H = ZA$ *is definite,* H *or* Z *is HPD, and* A *is* H*-normal, then* A *is similar to a normal definite matrix.*

Proof. Suppose that a matrix Z exists such that the specified properties hold, with H HPD. Then $A = Z^{-1}H$ is similar to the matrix $\hat{A} = H^{1/2}Z^{-1}H^{1/2}$, which is definite, since Z is definite. Therefore $E(\hat{A})$, the convex hull of the eigenvalues of $\hat{A}$, which is the same as $E(A)$, does not contain the origin. Also, since A is similar to a normal matrix, it is similar to a diagonal matrix D. Moreover, the diagonal elements of D are the same as the eigenvalues of A and also of $Ⓐ$. Since $E(A) = E(D)$ does not contain the origin, D is normal definite. Therefore A is similar to a normal definite matrix.

The proof for the case where Z is HPD and H is definite is similar. We omit the details. ∎

We now show that under certain circumstances where $n(A) = 1$, Condition β does imply Condition b.

THEOREM 7.4. *If Condition β holds, if A and Z are real, if $n(A) = 1$, and if not all of the eigenvalues of A are purely imaginary, then Condition* b *holds.*

Proof. Since Z is definite and A is Z-normal with $n(A) = 1$, it follows from Theorem 6.3 that all eigenvalues of A lie in a straight line. Since A is real, then unless A has a single real eigenvalue (in which case $A = cI$ for some real constant c), the line either is the real axis or is parallel to the imaginary axis.

If all of the eigenvalues of A are real, then for some real diagonal matrix D, A is similar to D and $D^* = D$. Hence by Theorem B.1, Appendix B, $(ZAZ^{-1})^* = A$. Since Z and ZA are definite and since A and Z are real, as we have shown previously, A is similar to a definite matrix. Hence D is Hermitian definite. Thus A is similar to a Hermitian definite matrix and Condition b holds.

Suppose now that all eigenvalues lie on a line parallel to the imaginary axis. Unless the line is the imaginary axis itself, then D, a diagonal matrix whose diagonal elements are the eigenvalues of A, is definite as well as normal; hence A is similar to a normal definite matrix and again Condition b holds. ∎

The following example shows that Condition b need not hold if all of the eigenvalues of A are purely imaginary. Thus consider the case

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad Z = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad H = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

Evidently $ZA = -A^*Z$, and Z and H are definite, since $Z + Z^T = H + H^T = 2I$. Thus Condition β holds. However, Condition b does not hold, since A has eigenvalues $\pm i$ and is therefore not similar to a definite normal matrix.

8. SPECIAL CASES

Let us now assume that the system

$$Au = b \tag{8.1}$$

has been obtained from another system

$$\hat{A}u = \hat{b} \tag{8.2}$$

by multiplying both sides of (8.2) by Q^{-1}. Thus, we have

$$A = Q^{-1}\hat{A}, \qquad b = Q^{-1}\hat{b}. \tag{8.3}$$

The matrix Q is often referred to as the *preconditioning matrix*, and (8.1) is often referred to as the *preconditioned system*.

We now consider the application of the results of previous sections to various special cases involving certain assumptions on Q and $\hat{A}$. Our analysis will include most of the cases studied by Faber and Manteuffel [10] as well as other cases. In our studies we are particularly concerned with cases where ORTHOMIN and ORTHORES, as well as ORTHODIR, converge. We will consider four classes of cases, namely, the general case, the GCW method, polynomial preconditioning, and generalized normal equations.

General Case

Q HPD, $\hat{A}$ Hermitian. Here A is similar to the Hermitian matrix $V^{-1}AV = Q^{-1/2}\hat{A}Q^{-1/2}$, where $V = Q^{-1/2}$. We consider two choices of Z, namely, $Z_1 = Q$, $H_1 = \hat{A}$ and $Z_2 = \hat{A}$, $H_2 = \hat{A}Q^{-1}\hat{A}$. If $\hat{A}$ is HPD, all three methods converge with both choices. Otherwise ORTHODIR converges for the second choice.

Q HPD, $Q^{-1/2}\hat{A}Q^{-1/2}$ Normal. Here A is similar to the normal matrix $Q^{1/2}(Q^{-1}\hat{A})Q^{-1/2} = Q^{-1/2}\hat{A}Q^{-1/2}$. Again we consider two choices of Z, namely, $Z_1 = Q$, $H_1 = \hat{A}$ and $Z_2 = \hat{A}^*$, $H_2 = \hat{A}^*Q^{-1}\hat{A}$. If $Q^{-1/2}\hat{A}Q^{-1/2}$ is definite, then both Z and H are definite for both choices and all three methods can be used. Otherwise ORTHODIR converges for the second choice.

$Q^{-1}\hat{A}$ Similar to a Hermitian Matrix. Let V be any nonsingular matrix such that $V^{-1}AV = K$, where K is Hermitian. We consider the choices $Z_1 = V^{-*}V^{-1}$, $H_1 = V^{-*}V^{-1}A = V^{-*}KV^{-1}$ and $Z_2 = A^*V^{-*}V^{-1} =$

$V^{-*}K^*V^{-1}$, $H_2 = A^*V^{-*}V^{-1}A$. If K is definite, then Z and H are definite with both choices and all three variants converge. Otherwise ORTHODIR converges for the second choice.

$Q^{-1}\hat{A}$ *Similar to a Normal Matrix.* Let V be any nonsingular matrix such that $V^{-1}AV = K$, where K is normal. We consider the choices $Z_1 = V^{-*}V^{-1}$, $H_1 = V^{-*}V^{-1}A = V^{-*}KV^{-1}$ and $Z_2 = A^*V^{-*}V^{-1} = V^{-*}K^*V^{-1}$, $H_2 = A^*V^{-*}V^{-1}A$. If K is definite, then Z and H are definite with both choices and all three variants converge. Otherwise ORTHODIR converges for the second choice.

The GCW Method

Let us now assume that $\hat{A} + \hat{A}^*$ is HPD. Following Concus and Golub [2] and Widlund [19], we consider the use of the splitting matrix

$$Q = \frac{\hat{A} + \hat{A}^*}{2}.$$

Evidently

$$\hat{A} = Q - R,$$

where

$$R = \frac{\hat{A}^* - \hat{A}}{2}$$

and $R^* = -R$. Moreover, $A = Q^{-1}\hat{A}$ is similar to $Q^{1/2}AQ^{-1/2}$, and

$$\begin{aligned} Q^{1/2}AQ^{-1/2} &= Q^{-1/2}\hat{A}Q^{-1/2} \\ &= K. \end{aligned}$$

Evidently $K = I - Q^{-1/2}RQ^{-1/2}$ and

$$\begin{aligned} K^* &= I - Q^{-1/2}R^*Q^{-1/2} \\ &= I + Q^{-1/2}RQ^{-1/2} \\ &= 2I - K. \end{aligned}$$

Thus $K = Q^{-1/2}\hat{A}Q^{-1/2}$ is normal with normal degree 1. Moreover $A = I - Q^{-1}R$ has the form (6.1) with $\theta = \frac{3}{2}\pi$, $r = 1$, $B = iQ^{-1}R$, and $\hat{H} = \hat{A}^*Q^{-1}\hat{A}$.

We consider two choices of Z and H, namely $Z_1 = Q$, $H_1 = \hat{A}$ and $Z_2 = \hat{A}^*$, $H_2 = \hat{A}^* Q^{-1}\hat{A}$. Since $\hat{A} + \hat{A}^*$ is HPD, it follows from Theorem A.2, Appendix A, that $\hat{A}$ is definite. Thus Z and H are definite for both choices, and all three variants converge. The first choice corresponds to Case 2b(ii) considered by Faber and Manteuffel [10]. They also considered as Case 3c the choice $Z = \hat{A}^* Q$, $H = \hat{A}^*\hat{A}$. They assumed $\hat{A}$ to be normal. It can easily be shown that if $\hat{A}$ is normal, then $QR = RQ$, $Q\hat{A} = \hat{A}Q$, and $Q\hat{A}^* = \hat{A}^* Q$. Therefore

$$
\begin{aligned}
(HAH^{-1})^* &= (\hat{A}^*\hat{A}Q^{-1}\hat{A}\hat{A}^{-1}\hat{A}^{-*})^* \\
&= Q^{-1}\hat{A}^* = I + Q^{-1}R \\
&= 2I - A.
\end{aligned}
$$

Thus simplification occurs. To show that $Z = \hat{A}^* Q$ is definite, we have

$$
\begin{aligned}
Z + Z^* &= \hat{A}^* Q + (\hat{A}^* Q)^* \\
&= Q\hat{A}^* + Q\hat{A} \\
&= Q(\hat{A}^* + \hat{A}).
\end{aligned}
$$

Evidently $Z + Z^*$ is similar to the matrix $Q^{-1/2}(Z + Z^*)Q^{1/2} = Q^{1/2}(\hat{A}^* + \hat{A})Q^{1/2}$, which is HPD, since $\hat{A}^* + \hat{A}$ is HPD. Therefore $Z + Z^*$ has positive eigenvalues and hence is HPD. Since $Z + Z^*$ is HPD, it follows that Z is definite by Theorem A.2, Appendix A.

Let us now consider the possibility of relaxing the assumption that $\hat{A} + \hat{A}^*$ is HPD. If we assume instead that $\hat{A}$ is definite, then by Theorem A.3, Appendix A, there exists a real number β and an HPD matrix K such that $Ke^{i\beta}\hat{A} + (Ke^{i\beta}\hat{A})^*$ is HPD. Thus if $\hat{A}$ is definite, we can apply the GCW method to the modified system

$$
e^{i\beta}K\hat{A}u = e^{i\beta}Kb.
$$

In general, of course, it may not be feasible to find β and K.

Polynomial Preconditioning

Let us now consider the case where $Q^{-1} = q(\hat{A})$, where $q(\hat{A})$ is polynomial with real coefficients such that $q(\hat{A})$ is nonsingular. This choice of Q corresponds to polynomial preconditioning; see [7], [15], and [1]. We also assume $\hat{A}$ is Hermitian, so that $q(\hat{A})$ is Hermitian. Moreover, $A = q(\hat{A})\hat{A}$ is Hermitian and nonsingular. We can use the choices $Z_1 = I$, $H_1 = A$ and $Z_2 = A$, $H_2 = A^2$. The first choice was considered by Faber and Manteuffel [10] as Case 4a. If A is HPD, then Z and H are definite with both choices and hence all three variants converge. Otherwise ORTHODIR converges with the second choice.

Faber and Manteuffel [10] considered as Case 2c the choice $Z = q(\hat{A})^{-1}$, $H = \hat{A}$. If $\hat{A}$ is HPD, then H is definite and ORTHODIR converges. Simplification occurs: because q has real coefficients, $(HAH^{-1})^* = (\hat{A}q(\hat{A})\hat{A}\hat{A}^{-1})^* = q(\hat{A})\hat{A} = A$.

Next, let us consider the case where $Q^{-1} = q(M^{-1}\hat{A})M^{-1}$, where $\hat{A}$ is Hermitian and M is HPD. Again we assume $q(M^{-1}A)M^{-1}$ is nonsingular and q has real coefficients. This preconditioning was considered by Adams [1]. Evidently $A = Q^{-1}\hat{A} = q(M^{-1}\hat{A})M^{-1}\hat{A}$ is similar to the matrix

$$M^{1/2}AM^{-1/2} = M^{1/2}q(M^{-1}\hat{A})M^{-1}\hat{A}M^{-1/2}$$

$$= q(M^{-1/2}\hat{A}M^{-1/2})M^{-1/2}\hat{A}M^{-1/2},$$

which is Hermitian, since $M^{-1/2}\hat{A}M^{-1/2}$ is Hermitian. We can use the choices $Z_1 = M$, $H_1 = MA$ and $Z_2 = A^*M$, $H_2 = A^*MA$. We note that if A is HPD, then Z is definite and ORTHOMIN and ORTHORES converge. This follows because, as we now show, $q(\hat{A})$ is HPD. Thus, A is similar to the matrix $\hat{A}^{-1/2}q(\hat{A})\hat{A}^{1/2} = q(\hat{A})$, and therefore the Hermitian matrix $q(\hat{A})$ has positive eigenvalues, and is therefore HPD, since A has positive eigenvalues. Thus we have S(1) with the choices $Z_1 = M$, $H_1 = MA$ and $Z_2 = A^*M$, $H_2 = A^*MA$. Evidently ORTHODIR converges for the second choice in the general case. If MA is HPD, then all three variants converge for both choices.

Faber and Manteuffel [10] considered, as Case 2d, the choice $Z = Mq(M^{-1}\hat{A})^{-1}$, $H = \hat{A}$ with the assumption that $\hat{A}$ is HPD. Evidently ORTHODIR converges. We now show that if MA is HPD, then all three variants converge. Since

$$MA = Mq(M^{-1}\hat{A})M^{-1}\hat{A}$$

$$= M^{-1/2}q(M^{-1/2}\hat{A}M^{-1/2})M^{-1/2}\hat{A},$$

we have

$$M^{-1/2}(MA)M^{-1/2} = q(M^{-1/2}\hat{A}M^{-1/2})(M^{-1/2}\hat{A}M^{-1/2}).$$

Also

$$M^{-1/2}ZM^{-1/2} = \left[M^{1/2}q(M^{-1}\hat{A})M^{-1/2}\right]^{-1}$$
$$= \left[q(M^{-1/2}\hat{A}M^{-1/2})\right]^{-1}.$$

As above, we can show that $q(M^{-1/2}\hat{A}M^{-1/2})$ is HPD, since $M^{-1/2}\hat{A}M^{-1/2}$ is HPD and since MA and hence $M^{-1/2}(MA)M^{-1/2}$ is HPD. Thus $M^{-1/2}ZM^{-1/2}$ and hence Z is HPD.

Generalized Normal Equations

First we let $Q^{-1} = \hat{A}^*C$, where C is Hermitian. Evidently $A = \hat{A}^*C\hat{A}$ is Hermitian. We consider the three choices $Z_1 = I$, $H_1 = A$; $Z_2 = A$, $H_2 = A^2$; and $Z_3 = A^{-1}$, $H_3 = I$. If C is HPD, then A is HPD and Z and H are definite in all cases. Thus all three variants converge. If C is Hermitian, ORTHODIR converges for the second and third choices.

Suppose now that $Q^{-1} = M^{-1}M^{-*}\hat{A}^*$. Evidently $A = Q^{-1}\hat{A} = M^{-1}M^{-*}\hat{A}^*\hat{A}$ is similar to $MAM^{-1} = M^{-*}\hat{A}^*\hat{A}M^{-1}$, which is HPD. We can consider the three choices $Z_1 = M^*M$, $H_1 = \hat{A}^*\hat{A}$, $Z_2 = A^*M^*M$, $H_2 = A^*M^*MA$ and $Z_3 = M^*MA^{-1} = M^*M\hat{A}^{-1}\hat{A}^{-*}M^*M$, $H_3 = M^*M$. Evidently H and Z are definite for all three choices, and all three variants converge.

APPENDIX A. DEFINITE MATRICES AND RELATED MATRICES

The matrix H is *definite* if $(v, Hv) \neq 0$ for all $v \neq 0$. The matrix H is *positive real* (PR) or *negative real* (NR) if for all real $v \neq 0$ we have $(v, Hv) > 0$ or $(v, Hv) < 0$, respectively. We now show that if H is real, then H is definite if and only if H is either PR or NR.

THEOREM A.1. *If H is real, then H is definite if and only if H is PR or NR.*

Proof. Suppose H is definite. For any real v we have

$$2(v, Hv) = \left(v, (H + H^T)v\right).$$

Since $H + H^T$ is real and symmetric, it has real eigenvalues and a corresponding set of mutually orthogonal real eigenvectors. If all eigenvalues of $H + H^T$ are positive (negative), then $(v, Hv) > 0$ (< 0) for all real v and hence H is PR (NR). Evidently no eigenvalue can vanish; otherwise $H + H^T$ would be singular and hence not definite. Moreover, if there exist eigenvalues $\mu_1 > 0$ and $\mu_2 < 0$ and real eigenvectors v_1 and v_2 such that $(H + H^T)v_i = \mu_i v_i$, $i = 1,2$, $(v_1, v_1) = (v_2, v_2) = 1$, and $(v_1, v_2) = 0$, then $(v,(H + H^T)v) = 0$ for $v = v_1 + \sqrt{-\mu_1/\mu_2}\,v_2$. This contradicts the assumption that $(v, Hv) \neq 0$. Thus H is PR or NR.

Suppose now that H is PR or NR. Since H is definite if and only $-H$ is definite, we can, without loss of generality, assume that H is PR. Let $v \in C^N \backslash \{0\}$, and let $v = u + iw$, where u and w are real. Evidently

$$\begin{aligned}(v, Hv) &= (u + iw, H(u + iw)) \\ &= [(u, Hu) + (w, Hw)] + i[(u, Hw) - (w, Hu)].\end{aligned}$$

Since H is PR and since u and w do not both vanish, the real part is positive. Hence $(v, Hv) \neq 0$. ∎

We note that a real matrix H is PR or NR if and only if its symmetric part $(H + H^T)/2$ is Hermitian definite (HD).

It is worth noting that the above characterization does not carry over to complex definite matrices. For instance, the matrix

$$\begin{pmatrix} 1 & 10i \\ -10i & 1 \end{pmatrix}$$

is PR but not definite, and the diagonal matrix iI is definite but neither PR nor NR.

In the complex case if $H + H^*$ is HPD, then H is definite but not conversely. Thus we have

THEOREM A.2. *Let H be a matrix such that $H + H^*$ is HD. Then H is definite.*

Proof. For any $x \neq 0$ we have

$$\begin{aligned}0 \neq (x,(H + H^*)x) &= (x, Hx) + (Hx, x) \\ &= (x, Hx) + \overline{(x, Hx)} = 2\,\mathrm{Re}(x, Hx).\end{aligned}$$

Therefore $(x, Hx) \neq 0$ and H is definite. ∎

The converse of Theorem A.2 does not hold. Thus consider the case $H = iI$. Evidently $H^* = -iI = -H$, so that $H + H^* = 0$. However, we can prove the following.

THEOREM A.3. *If H is a definite matrix, there exists a real number β and an HPD matrix K such that*

$$Ke^{i\beta}H + (Ke^{i\beta}H)^*$$

is HPD.

Proof. If H is definite, then $E(H)$, the convex hull of the set of eigenvalues of H, does not contain the origin; see, e.g., Householder [12]. Consequently for some real β all eigenvalues of $e^{i\beta}H$ lie in the right half plane, and hence $e^{i\beta}H$ is N-stable; see, e.g., Young [20]. The result follows from a theorem of Lyapunov.[3]

APPENDIX B. THE NORMAL DEGREE OF A NORMALIZABLE MATRIX

In Section 2 we defined the adjoint of a matrix A with respect to a nonsingular matrix H as $A^\dagger = (HAH^{-1})^*$. We also defined the concept of an H-normal matrix A (where $A^\dagger A = AA^\dagger$) and the normal degree $n(A, H)$ of A with respect to H. In this appendix we show that $n(A, H)$ is independent of H for any definite matrix H.

Faber and Manteuffel [10] showed that if A is H-normal for some definite matrix H, then A is normalizable, i.e., A is similar to a normal matrix. Let V be any nonsingular matrix such that $V^{-1}AV = K$ for some normal matrix K. We show that A is H-normal, where H is the HPD matrix $H = V^{-*}V^{-1}$. It follows from a result of Drazin [6] (see also Faber and Manteuffel [9]) that $K^* = P(K)$ for some polynomial $P(K)$. Therefore

$$\begin{aligned} A^\dagger &= (HAH^{-1})^* = VK^*V^{-1} \\ &= VP(K)V^{-1} = P(VKV^{-1}) = P(A). \end{aligned}$$

Since $A^\dagger A = AA^\dagger$, it follows that A is H-normal.

[3]See, e.g., Young [20] for a statement and proof of the Lyapunov theorem for the case where H is real. The extension to the case where H is complex is straightforward.

We now prove

THEOREM B.1. *Let A be a normalizable matrix, and let the diagonal matrix D be a Jordan canonical form of A. Let H be a definite matrix such that A is H-normal. For any polynomial P, $D^* = P(D)$ if and only if*

$$A^\dagger = (HAH^{-1})^* = P(A).$$

Proof. Since A is H-normal and H is definite, there exists an HPD matrix $\hat{H}$ such that $(\hat{H}A\hat{H}^{-1})^* = (HAH^{-1})^*$; see Faber and Manteuffel [10]. Since A is H-normal, A is $\hat{H}$-normal and

$$(\hat{H}A\hat{H}^{-1})^* A = A(\hat{H}A\hat{H}^{-1})^*.$$

Hence $\textcircled{A} = \hat{H}^{1/2}A\hat{H}^{-1/2}$ is normal. Therefore there exists a unitary matrix W such that $W\textcircled{A}W^{-1} = D_1$ where D_1 is a diagonal matrix. Since D_1 is similar to A, as well as to $\textcircled{A}$, it follows that D_1 is a Jordan canonical form of A. Therefore, since D and D_1 are Jordan canonical forms of A, $D_1 = TDT^{-1}$ for some (unitary) permutation matrix T. Thus we have

$$D = T^{-1}W^{-1}\textcircled{A}WT$$

and, since $W^*W = T^*T = I$,

$$D^* = T^{-1}W^{-1}\textcircled{A}^*WT.$$

Evidently, for any polynomial P, $D^* = P(D)$ if and only if

$$\begin{aligned} T^{-1}W^{-1}\textcircled{A}^*WT &= P\left(T^{-1}W^{-1}\textcircled{A}WT\right) \\ &= T^{-1}W^{-1}P\left(\textcircled{A}\right)WT. \end{aligned}$$

Therefore $D^* = P(D)$ if and only if $\textcircled{A}^* = P(\textcircled{A})$. But $\textcircled{A}^* = P(\textcircled{A})$ if and only if $A^\dagger = (\hat{H}A\hat{H}^{-1})^* = P(A)$. ∎

From Theorem B.1 it follows that $n(A, H) = n(A)$, where $n(A)$ is the degree of the polynomial P of lowest degree such that $D^* = P(D)$. Thus $n(A, H)$ depends only on A and not on H.

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