Simultaneous Iteration for the Matrix Eigenvalue Problem*

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ABSTRACT

Let B be a given positive definite Hermitian matrix, and assume the matrix P satisfies the "normality" condition $PB^{-1}P^HB = B^{-1}P^HBP$, where P^H denotes the Hermitian of P. In this paper, we develop an accelerated version of simultaneous iteration for partial solution of the eigenproblem $Px = \lambda x$. Convergence together with sharp error bounds is obtained. The results are then applied to the solution of the symmetric eigenproblem $Ax = \lambda Bx$, where the algorithms are shown to be improvements over existing techniques.

1. INTRODUCTION

Since the development of Bauer's [2] simultaneous iteration method for solution of the classical matrix eigenvalue problem

$$Px = \lambda x, \tag{1}$$

a few variants have been developed [3,4,6,7] that improve the general convergence characteristics of the iteration. In application to a given matrix, the accelerated convergence can often be dramatic, particularly when a clustering of the dominant eigenvalues occurs. Simultaneous iteration and its variants are natural extensions of the power method, which on the other hand is plagued by slow convergence in the presence of clustering. These techniques attempt to capitalize on the assets of the power method while at the same time overcoming its major handicap.

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In this paper we develop a generalization of the method of Rutishauser [6] that applies when the symmetry condition on P is relaxed. (See Assumption below.) Although the generalization that we will study has interest in its own right, it has important applications to problems that are described in terms of a given metric. To illustrate, consider the generalized eigenproblem

$$Ax = \lambda Bx, \tag{2}$$

where the matrices A and B are Hermitian and B is positive definite. The usual approach for its solution involves the use of the Cholesky decomposition $B = LL^H$ to transform (2) into the equivalent Hermitian eigenproblem

$$L^{-1}AL^{-H}y = \lambda y. \tag{3}$$

This is often unsatisfactory, since the Cholesky decomposition of B is not always desirable, particularly when inverse iteration is used to solve (3). In fact, the decomposition may not even be feasible, as is the case when B is large, sparse, and not banded. The algorithm treated here allows us to avoid computing the Cholesky factorization of B by applying the technique formally to the matrices $P_1 = B^{-1}A$ and $P_2 = A^{-1}B$. The essential feature of P_1 and P_2 is the "B-orthogonality" of their eigenvectors, and this is the basic property for our generalization.

In the next section we introduce the algorithm, Sec. 3 is devoted to obtaining convergence results, and some concluding remarks are made in Sec. 4.

Matrices will be denoted by upper case letters; vectors and scalars by lower case letters. Our analysis will deal solely with vectors and operators of the unitary space C^n. We let B denote a Hermitian positive definite matrix and define the B inner product by

$$\langle x, y \rangle_B = \langle x, By \rangle.$$

Norms that are used include the vector norms:

$$\|x\|^2 = \langle x, x \rangle,$$

$$\|x\|_B^2 = \langle x, x \rangle_B,$$

and the induced matrix norms:

$$\|A\| = \sup_{\|x\|=1} \|Ax\|,$$

$$\|A\|_B = \sup_{\|x\|_B=1} \|Ax\|_B.$$

A matrix P that satisfies $\langle Px,y\rangle_B = \langle x,Py\rangle_B$ will be called B-Hermitian. The quantity $\langle Px,x\rangle_B/\langle x,x\rangle_B$ will be referred to as the generalized Rayleigh quotient of P. Finally, for any rectangular matrix X, the subspace spanned by the columns of X will be denoted by span(X).

2. THE ALGORITHM

ASSUMPTION. *The matrix is B-normal in the sense that P is normal in the B inner product, or, equivalently,*

$$PB^{-1}P^HB = B^{-1}P^HBP.$$

Thus, P is nondefective and there exists a B-orthonormal basis for C^n *consisting of eigenvectors of P.*

Let $1 \leqslant p \leqslant n$. (Typically, $1 < p \ll n$.) Then the algorithm begins with an initial $n \times p$ matrix X_0 satisfying

$$X_0^HBX_0 = I. \tag{4}$$

This can be accomplished by choosing linearly independent initial guesses and employing the Gram-Schmidt process as it is defined in the B inner product. The successive $n \times p$ matrices X_k, $k = 1,2,\ldots$, whose columns represent approximations to eigenvectors of P, are computed using the iteration

$$\begin{aligned} &1.\ Z_k = PX_k,\ S_k = Z_k^HBZ_k; \\ &2.\ \text{A unitary matrix } Q_k \text{ is determined so that} \\ &Q_k^HS_kQ_k = D_k^2, \text{ where } D_k \text{ is a real, diagonal matrix;} \\ &3.\ X_{k+1} = Z_kQ_kD_k^{-1}. \end{aligned} \tag{5}$$

Here we recommend that step 2 be carried out by Jacobi's method, with the stipulation that the diagonal entries of D_k be arranged in decending order by modulus. Note that the iteration maintains the B-orthonormality condition

$$X_{k+1}^H B X_{k+1} = I. \tag{6}$$

Note also that when P is B-Hermitian (5) is actually a Ritz process applied to the subspaces span(PX_k). This is true because the eigenproblem for S_k results from the B-orthogonal projection of the eigenproblem for P^{-2} onto span(PX_k).

Theorems 4, 5, and 6 of the next section establish the convergence of iteration (5) together with sharp error bounds. In particular, the diagonal entries of D_k yield the moduli of the eigenvalues of P, and the corresponding columns of X_k provide a basis for the subspaces that correspond to the eigenvalues of equal modulus. Thus, eigenvalues of the same modulus cannot be distinguished by this algorithm. However, the occurence of unequal eigenvalues of the same modulus is signaled by distinct Rayleigh quotients of the corresponding columns of X_k. A remedy is provided by solving the projected eigenproblem

$$X^H P X y = \lambda y, \tag{7}$$

where X is the matrix formed from the columns of X_k that correspond to equal diagonal entries of D_k. Observe that the columns whose Rayleigh quotients equal the corresponding entries of D_k are in fact eigenvectors of P and may therefore be excluded from this process. Also note that (7) is related to the acceleration step used by Stewart [7].

The description of the algorithm is not meant to privide more than the theoretical structure. There are many other considerations that must accompany effective implementation. However, all of the comments made in [6,9] apply here with a few obvious modifications, so, for the most part, we will be content with establishing some important theoretical results.

3. CONVERGENCE THEOREMS

The essence of the method described in the previous section is that the iterates X_{k+1} act as a basis for $\text{span}(PX_k) = \text{span}(P^k X_0) = P^k \text{span}(X_0)$. Thus, the method is actually a form of the power method applied to the subspaces span(X_k). Assuming that the eigenvalues of P can be written

$$|\lambda_1| \geqslant |\lambda_2| \geqslant \cdots \geqslant |\lambda_p| > |\lambda_{p+1}| \geqslant \cdots \geqslant |\lambda_n|, \tag{8}$$

we conclude (cf. [5]) that the iterates will converge to the dominant p-dimensional invariant subspace of P.

Let $\Lambda_1 = \operatorname{diag}(\lambda_1, \ldots, \lambda_p)$ and $\Lambda_2 = \operatorname{diag}(\lambda_{p+1}, \ldots, \lambda_n)$ and suppose U_1 and U_2 are $n \times p$ and $n \times (n-p)$ matrices, respectively, of eigenvectors of P satisfying

$$\begin{aligned} P(U_1; U_2) &= (U_1; U_2)\operatorname{diag}(\Lambda_1, \Lambda_2), \\ (U_1; U_2)^H B (U_1; U_2) &= I. \end{aligned} \tag{9}$$

Then the nondefectiveness of P implies the existence of $p \times p$ and $(n-p) \times p$ matrices E_k and F_k, respectively, satisfying

$$X_k = U_1 E_k + U_2 F_k. \tag{10}$$

Note that

$$X_{k+1} = U_1 \Lambda_1 E_k Q_k D_k^{-1} + U_2 \Lambda_2 F_k Q_k D_k^{-1} \tag{11}$$

The feasibility of (5) depends on the nondefectiveness of S_k and the invertibility of D_k for each k. These issues are treated in the first theorem. Note that the sufficiency condition is that X_0 is not deficient in $\operatorname{span}(U_1)$, i.e., that E_0 is nonsingular. This condition is also necessary.

THEOREM 1. *Suppose E_0 is nonsingular. Then, for each k, S_k is Hermitian positive definite. Moreover, the E_k and D_k are nonsingular, and D_k may be chosen with positive entries on the diagonal. Finally,*

$$\|E_k\|, \|F_k\| \leqslant 1. \tag{12}$$

Proof. S_k is clearly Hermitian and nonnegative definite. If $S_0 y = 0$, then $PX_0 y = 0$ and it follows that

$$\begin{aligned} y &= E_0^{-1} \Lambda_1^{-1} \Lambda_1 E_0 y \\ &= E_0^{-1} \Lambda_1^{-1} U_1^H B P X_0 y \\ &= 0. \end{aligned}$$

S_0 and D_0 therefore satisfy the conclusions of the theorem. From (10) and

(11) it is easy to obtain the identities

$$E_k = \Lambda_1^k E_0 C_k,$$
$$F_k = \Lambda_2^k F_0 C_k, \tag{13}$$

where $C_k = \prod_{i=0}^{k-1} Q_i D_i^{-1}$ is nonsingular by induction. The first conclusions of the theorem for all k are immediate. To prove (12), it is convenient to make use of the Cholesky factorization $B = LL^H$. First note that (9) and (10) imply

$$E_k = U_1^H B X_k,$$
$$F_k = U_2^H B X_k.$$

Hence,

$$\begin{aligned} \|E_k\| &= \|U_1^H B X_k\| \\ &= \|(L^H U_1)^H (L^H X_k)\| \\ &\leqslant 1, \end{aligned}$$

since both of the matrices in parenthesis have orthonormal columns. The same is true of F_k and the theorem is proved. ■

The convergence of X_k, together with appropriate rates, can be obtained by relating (1) to an equivalent problem with $B = I$ and proceeding as in [6]. However, the theoretical results in [6] are asymptotic, establishing only the order of convergence. We will obtain more concrete bounds for convergence. It should be noted that the results are similar to those obtained by Stewart [7] for a related version of simultaneous iteration, although the bounds given here are sharper.

The next theorem, among other things, establishes the expected convergence rate of the subspaces span(X_k) to span(U_1). The proof is a direct consequence of (13) and will be omitted.

THEOREM 2. *Suppose E_0 is nonsingular. Then $F_k E_k^{-1}$ tends to zero as governed by the inequality*

$$\|F_k E_k^{-1}\| \leqslant |\lambda_{p+1}\lambda_p^{-1}|^k \|F_0 E_0^{-1}\|. \tag{14}$$

Note that (14) is true for any of the variants of simultaneous iteration. Its implications are clear, particularly when $|\lambda_p| \gg |\lambda_{p+1}|$, regardless of how the basis X_k is selected. The significance of the accelerated version treated here is that the convergence of the ith approximations is actually governed by $|\lambda_{p+1}\lambda_i^{-1}|^k$. We first treat the eigenvalues. To do so, we will require the Poincaré separation theorem:

THEOREM 3. *Let T be an $n \times n$ Hermitian matrix with eigenvalues*

$$\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n.$$

Let the $n \times m$ matrix R have orthonormal columns, and suppose the eigenvalues of $R^H TR$ are written

$$\nu_1 \geqslant \nu_2 \geqslant \cdots \geqslant \nu_m.$$

Then

$$\nu_i \leqslant \mu_i \qquad (i = 1, \ldots, m), \tag{15}$$

$$\nu_{m-i+1} \geqslant \mu_{n-i+1} \qquad (i = 1, \ldots, m). \tag{16}$$

THEOREM 4. *Let d_{ik} denote the diagonal entries of D_k. Let I_i denote the $p \times i$ matrix consisting of the first i columns of the $p \times p$ identity matrix. Then the d_{ik} satisfy*

$$|\lambda_i|^2\left(1 + \varepsilon_{ik}^2\right)^{-1} \leqslant d_{ik}^2 \leqslant |\lambda_i|^2, \tag{17}$$

where $\varepsilon_{i0} = \|F_0 E_0^{-1} I_i\|$ and $\varepsilon_{ik} = |\lambda_{p+1}\lambda_i^{-1}|^k \varepsilon_{i0}$.

Proof. We first establish the right inequality in (17). Note that

$$S_k = X_k^H P^H B P X_k = \left(L^H X_k\right)^H (L^{-1} P^H L)(L^H P L^{-H})\left(L^H X_k\right).$$

The columns of $L^H X_k$ are orthonormal. So the inequality follows from (15), since d_{ik}^2 and $|\lambda_i|^2$ are the eigenvalues of S_k and $(L^{-1}P^H L)(L^H P L^{-H})$, respectively.

To establish the left inequality, observe that

$$S_k = E_k^H \Lambda_1^H \Lambda_1 E_k + F_k^H \Lambda_2^H \Lambda_2 F_K$$

and that the last term is a nonnegative definite matrix. Hence, the eigenvalues d_{ik}^2 of S_k are upper bounds for the eigenvalues of $E_k^H \Lambda_1^H \Lambda_1 E_k$, which we shall call α_{ik}. That is,

$$d_{ik}^2 \geqslant \alpha_{ik} \qquad (i = 1, \ldots, p). \tag{18}$$

Now from

$$\det\left(E_k^H \Lambda_1^H \Lambda_1 E_k^H - \alpha_{ik} I\right) = 0,$$

and the fact that $E_k^H E_k + F_k^H F_k = I$, there follows

$$\det\left[\Lambda_1^{-H}\left(I + W_k^H W_k\right)\Lambda_1^{-1} - \alpha_{ik}^{-1} I\right] = 0,$$

where $W_k = F_k E_k^{-1}$. If we fix i and let β_{ik} denote the dominant eigenvalue of $I_i^H \Lambda_1^{-H}(I + W_k^H W_k)\Lambda_1^{-1} I_i$, then (16) of Theorem 3 together with (18) yields

$$\beta_{ik} \geqslant \alpha_{ik}^{-1} \geqslant d_{ik}^{-2}.$$

An upper bound for β_{ik} is furnished by

$$\begin{aligned}
\beta_{ik} &= \sup_{\|z\|=1} \left(\|\Lambda_1^{-1} I_i z\|^2 + \|W_k \Lambda_1^{-1} I_i z\|^2\right) \\
&= \sup_{\|z\|=1} \left(\|\Lambda_1^{-1} I_i z\|^2 + \|W_k I_i \left(\Lambda_1^{-H} I_i\right)^H I_i z\|^2\right) \\
&\leqslant \sup_{\|z\|=1} \|\Lambda_1^{-1} I_i z\|^2 \left(1 + \|W_k I_i\|^2\right) \\
&= |\lambda_i|^{-2}\left(1 + \|W_k I_i\|^2\right).
\end{aligned}$$

Equation (17) now follows from noting

$$\begin{aligned}
\|W_k I_i\| &= \|F_k E_k^{-1} I_i\| \\
&\leqslant |\lambda_{p+1}\lambda_i^{-1}|^k \|F_0 E_0^{-1} I_i\|,
\end{aligned}$$

and the theorem is proved. ■

Observe that the multiplicity of the eigenvalues is not a factor in the convergence rates obtained in this theorem. This contrasts with the remaining two theorems, which deal with the eigenvectors.

THEOREM 5. *Suppose, for* $1 \leqslant i \leqslant j \leqslant p$, *that*

$$|\lambda_{i-1}| > |\lambda_i| = \cdots = |\lambda_j| > |\lambda_{j+1}|.$$

Let u *denote any eigenvector of* P *belonging to* λ_μ $(i \leqslant \mu \leqslant j)$ *with* $\|u\|_B = 1$. *Then there exists a linear combination,* v, *of columns* i *through* j *of* X_{k+1} *such that*

$$\|v - u\|_B \leqslant \gamma_k. \tag{19}$$

Here, $\gamma_k = [|\lambda_1\lambda_i^{-1}|(|\lambda_i|^2 - |\lambda_{p+1}|^2)\|F_k\|\alpha_{ik}^{-1} + |\lambda_{p+1}\lambda_i^{-1}|]\varepsilon_{ik}$, *where* $\alpha_{ik} = \min\{|d_{\nu k}^2 - |\lambda_i|^2| : \nu = 1, 2, \ldots, i-1, j+1, \ldots, p\}$ *and* ε_{ik} *is as in Theorem* 4.

Proof. We represent $u = U_1 s$ for $s \in C^p$, noting that s is a unit vector such that $s_\nu = 0$ for $\lambda_\nu \neq \lambda_\mu$. Denote the columns of the matrix Q_k by q_ν, and let $\bar{Q} = (q_i, \ldots, q_j)$ and $\hat{Q} = (q_1, q_2, \ldots, q_{i-1}, q_{j+1}, \ldots, q_p)$. We now establish the theorem by determining a vector t in span$(\bar{Q})$ so that (19) is satisfied for $v = \lambda_\mu^{-1} P X_k t$. In fact, if we let $t = \bar{Q}\bar{Q}^H E_k^{-1} s$, it is easy to see that v is a linear combination of columns i through j of X_{k+1}. To prove (19), we first note that

$$\begin{aligned}
\|v - u\|_B &= \|\lambda_\mu^{-1} P X_k t - U_1 s\|_B \\
&\leqslant \|\lambda_\mu^{-1} P\left(X_k t - X_k E_k^{-1} s\right)\|_B + \|\lambda_\mu^{-1} P\left(X_k E_k^{-1} - U_1\right)s\|_B \\
&\leqslant |\lambda_1\lambda_1^{-1}| \cdot \|X_k\left(t - E_k^{-1} s\right)\|_B + |\lambda_{p+1}\lambda_i^{-1}| \cdot \|U_2 W_k s\|_B \\
&\leqslant |\lambda_1\lambda_i^{-1}| \cdot \|t - E_k^{-1} s\| + |\lambda_{p+1}\lambda_i^{-1}|\epsilon_{ik}.
\end{aligned} \tag{20}$$

Concentrating on the first term in the last line of (20), note that

$$\begin{aligned}
\|t - E_k^{-1} s\| &= \|(\bar{Q}\bar{Q}^H - I)E_k^{-1} s\| \\
&= \|\hat{Q}\hat{Q}^H E_k^{-1} s\| \\
&= \|\hat{Q}^H E_k^{-1} s\|.
\end{aligned} \tag{21}$$

It suffices to provide the appropriate bound for $\|\hat{Q}^H E_k^{-1} s\|$, which we do in two steps. First, observe that

$$\begin{aligned}\left\|\hat{Q}^H\left(S_k-|\lambda_i|^2 I\right)E_k^{-1}s\right\| &\leqslant \left\|\left(S_k-|\lambda_i|^2 I\right)E_k^{-1}s\right\| \\ &= \left\|\left[E_k^H\Lambda_1^H\Lambda_1+F_k^H\Lambda_2^H\Lambda_2 W_k-|\lambda_i|^2\left(E_k^H+F_k^H W_k\right)\right]s\right\| \\ &\leqslant \left\|F_k^H\left(\Lambda_2^H\Lambda_2-|\lambda_i|^2\right)W_k s\right\| \\ &\leqslant \|F_k\|\left(|\lambda_i|^2-|\lambda_{p+1}|^2\right)\varepsilon_{ik}.\end{aligned}$$

Second, with $\hat{D}=\operatorname{diag}(d_{1k},\ldots,d_{i-1k},\ d_{j+1k},\ldots,d_{pk})$, from (5) there follows

$$\begin{aligned}\left\|\hat{Q}^H\left(S_k-|\lambda_i|^2 I\right)E_k^{-1}s\right\| &= \left\|\left(\hat{D}^2-|\lambda_i|^2 I\right)\hat{Q}^H E_k^{-1}s\right\| \\ &\geqslant \alpha_{ik}\|\hat{Q}^H E_k^{-1}s\|.\end{aligned}$$

Combining these two inequalities yields

$$\|\hat{Q}^H E_k^{-1}s\| \leqslant \left(|\lambda_i|^2-|\lambda_{p+1}|^2\right)\alpha_{ik}^{-1}\|F_k\|\varepsilon_{ik}. \tag{22}$$

Equation (19), and the theorem, now follow from (20), (21), and (22). ■

According to Theorems 1 and 2, and since $\|F_k\| \leqslant \|F_k E_k^{-1}\|$, we have $\|F_k\| \leqslant \varepsilon_{pk}$. Thus, for large k, γ_k is certainly smaller than ε_{ik}. This is to be expected, since by Theorem 4 the error in the approximate eigenvalues is no larger than ε_{ik}^2.

Theorem 5 describes how close each individual eigenvector of P is to the subspace of approximations. Although there is asymptotically no difference, we consider the opposing question in our last theorem.

THEOREM 6. *Under the assumptions and notation of Theorem* 5, *suppose* k *is so large that* $(j-i+1)\gamma_k^2<1$. *Then, for each* $m=i,\ldots,j$, *there exists a linear combination,* u_m, *of the eigenvectors whose corresponding eigenvalues have modulus* $|\lambda_i|$ *such that*

$$\|X_k e_m-u_m\|_B \leqslant \gamma_k\sqrt{\frac{j-i+1}{1-(j-i+1)\gamma_k^2}}\ . \tag{23}$$

Proof. For convenience we let X and U denote the matrices consisting of columns i through j of x_{k+1} and U_1, respectively. Let P_X denote the B-orthogonal projector of C^n onto span(X), and for each $m = i, \ldots, j$, let t_m be such that $Xt_m = P_X U_1 e_m$. Then Xt_m is the linear combination of columns i through j of X_{k+1} closest to the eigenvector $U_1 e_m$. So from Theorem 5 it follows that

$$\|Xt_m - U_1 e_m\|_B \leqslant \gamma_k. \tag{24}$$

Thus, for $m \neq \nu$, we have

$$\begin{aligned}
|\langle t_m, t_\nu \rangle| &= |\langle Xt_m, Xt_\nu \rangle_B| \\
&= |\langle P_X U_1 e_m, P_X U_1 e_\nu \rangle_B| \\
&= |\langle U_1 e_m, P_X U_1 e_\nu \rangle_B| \\
&= |\langle U_1 e_m, (P_X - I) U_1 e_\nu \rangle_B| \\
&= |\langle (P_X - I) U_1 e_m, (P_X - I) U_1 e_\nu \rangle_B| \\
&\leqslant \|Xt_m - U_1 e_m\|_B \cdot \|Xt_\nu - U_1 e_\nu\|_B \\
&\leqslant \gamma_k^2.
\end{aligned}$$

Moreover, since $|\langle u_m, P_X u_m \rangle_B - \langle u_m, u_m \rangle_B| \leqslant \gamma_k^2$, then $1 \geqslant \langle t_m, t_m \rangle \geqslant 1 - \gamma_k^2$, and we may write $T^H T = I + V$, where $T = (t_i, \ldots, t_j)$ and $|v_{m\nu}| \leqslant \gamma_k^2$.

Since $(j - i + 1)\gamma_k^2 < 1$, it is easy to see that T is nonsingular. From (24) we may therefore conclude that

$$\|XT - U\|_B^2 \leqslant (j - i + 1)\gamma_k^2.$$

Hence,

$$\|X - UT^{-1}\|_B^2 \leqslant (j - i + 1)\gamma_k^2 \|T^{-1}\|^2. \tag{25}$$

It is clear that $\|T^{-1}\|^2 \leqslant [1 - (j - i + 1)\gamma_k^2]^{-1}$. Equation (23) now follows from (25), and the proof is complete. ■

It is important to note that the accuracy of the algorithm treated here does not directly involve the conditioning of B, provided, of course, that we measure the error in terms of the B-norm. On the other hand, if the errors of the eigenvector approximations are measured in the Euclidean norm, then as expected the square root of the condition number of B appears as a factor.

4. CONCLUDING REMARKS

There are two ways of applying the shifted power method form of simultaneous iteration to (2). First is the popular approach that focuses on the reduced eigenproblem (3), namely:

INDIRECT METHOD (cf. [9]). Compute the Cholesky decomposition $B = LL^H$. Let the spectral shift ρ be given, and replace P and B in (5) by $L^{-1}AL^{-H} - \rho I$ and I, respectively. Note in step 1 that Z_k is easily computed via

$$\begin{aligned} L^H V_k &= X_k, \\ LZ_k &= (A - \rho B)V_k. \end{aligned} \tag{26}$$

Note also that $S_k = Z_k^H Z_k$.

A more versatile approach is described as follows:

DIRECT METHOD. Define $P = B^{-1}(A - \rho B)$, and apply the procedure as in (5). Note that step 1 now requires the solution of

$$BZ_k = (A - \rho B)X_k. \tag{27}$$

This method has the advantage that iterative as well as other factorization methods may be used to determine Z_k when computation of the Cholesky factors is not feasible (e.g., when B is very large and not banded). Note the importance of stationary iterative methods to economize when computing for each column of Z_k in (27). In fact, even when the Cholesky factors are computable, it is more effective to use them in the direct method to solve (27), since this approach is less sensitive to the conditiong of B than is the indirect one. This occurs because the errors introduced into $S_k = Z_k^H B Z_k$ are attributable only to the *residual* of the computed solution of (27). For the indirect method, the errors in $S_k = Z_k^H Z_k$ can be much larger, since they depend on the *actual* errors incurred in the computed solution of (26).

A significant improvement over existing methods for solving (2) can be realized from (5) by choosing $P = (A - \rho B)^{-1}B$. The resulting process corresponds to inverse iteration with spectral shift ρ, and is particularly useful when eigenvalues near a given ρ are required. Computation of the Cholesky factorization of B is avoided, yet we are now confronted with the need to

solve the indefinite linear systems

$$(A-\rho B)Z_k = BX_k. \tag{28}$$

Even though the computation of the first column of X_{k+1} is numerically stable, there is reason to suspect the accuracy of the remaining columns when ρ is very near an eigenvalue of (1). Although this is an open theoretical question, a series of numerical tests indicate that this is not a problem. On the contrary, the procedure appears to be remarkably stable for such values of ρ and exhibits the rapid convergence guaranteed in the previous theorems.

The algorithm developed by Stewart [7] could just as well have been the object of our generalization. However, although the disadvantages are not major, Stewart's algorithm requires a little more storage and does not naturally incorporate a power iteration in the acceleration step. In attempting to extend Stewart's algorithm, the storage requirements would be similar to those of the algorithm presented in this paper. But, depending upon how the algorithm extension is made, either an additional orthonormalization step will be required, or else the acceleration phase will involve the solution of a reduced generalized eigenproblem (cf. [1]). The difficulty with the latter is that it excludes the use of the Jacobi method, which is effective in this connection.

With some modifications, the results of this paper are valid under weaker assumptions on the matrix P. Specifically, the B-normality of P can be replaced by the nondefectiveness of the dominant p eigenvalues and the B-orthonormality of the corresponding eigenvectors. Note that this allows for the defectiveness of the eigenvalues λ_i, $i=p+1,\ldots,n$. The results are modified by replacing $|\lambda_{p+1}|^k$ by the quantity $\mu_k = \sup\{\|P^k z\|_B : \|z\|_B = 1, U_1^H B z = 0\}$ and requiring k so large that $\mu_k < |\lambda_p|^k$. The asymptotic results are therefore the same, since $\lim_{k\to\infty} (\mu_k)^{1/k} = |\lambda_{p+1}|$.

An efficient working FORTRAN version of (5) in its general form, which includes RITZIT as a special case, has been developed by Dr. Paul J. Nikolai of the Applied Mathematics Group, Air Force Flight Dynamics Laboratory, Wright-Patterson Air Force Base, Ohio. It is currently being prepared for publication.

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