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GENERALIZED RAYLEIGH METHODS WITH APPLICATIONS TO FINDING EIGENVALUES OF LARGE MATRICES

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Section 1. Introduction

Since the development of the Sturm sequence method [10] and, later, the QR algorithm [2], the computational problem of finding the eigenvalues and eigenvectors of a symmetric matrix A is essentially solved --provided A is not too large. In both of these methods, the matrix is first reduced to tri-diagonal form. If A is extremely large, this preliminary reduction may not be computationally feasible for several reasons. First of all, it requires the use of the entire matrix in a series of transformations and no use can be made of sparseness or bandedness --two characteristics of most large matrices which occur in applications. Secondly, if only a few eigenvalues and eigenvectors are required (as is usually the case), the reduction may take more time than is reasonable. Finally, it often happens that physical considerations can provide rough approximations to some of the eigenvalues or eigenvectors. The above-mentioned methods cannot make much use of such information.

In [4], I. Erdelyi proposed a method for finding p eigenvalues and eigenvectors of an $n \times n$ matrix A, where n is large and $p << n$. An important feature of this method is that the only operation which involves the matrix A itself is matrix-vector multiplication. Hence, A can be stored on magnetic tape (or other auxilliary storage) and sparseness and bandedness can be taken into account to reduce the amount of computation. A major drawback, however, is the necessity of finding the roots of a polynomial of degree p; a difficult problem for even moderate sizes of p.

In this paper, we present a theory of generalized Rayleigh quotients which can be used to develop methods, such as Erdelyi's, for calculating some of the eigenvalues and eigenvectors of large matrices. If X is an approximation to an eigenvector of an $n \times n$ symmetric matrix A, then the Rayleigh Quotient

$$\lambda_R = \frac{X^T A X}{X^T X} \tag{1.1}$$

is an approximation to an eigenvalue of A. Our generalization of this concept involves the construction of a $p \times p$ matrix B, where usually $p << n$. The eigenvalues of B will be used to approximate the eigenvalues of A. These eigenvalues are, in fact, Rayleigh quotients of A corresponding to certain approximate eigenvectors which are determined by the eigenvectors of B. The matrix B is obtained by restricting A to a p-dimensional subspace H. If H is invariant under A, then the eigenvalues of B are also eigenvalues of A. In general, of course, H will not be invariant, and the accuracy of the approximations will depend on how "nearly" invariant H is. This leads to the problem of constructing subspaces which are nearly invariant, and the related problem of estimating how close a subspace is to being invariant.

The problem of constructing invariant subspaces can be solved using Bauer's Treppeniteration [1] or the method of Collar and Jahn [3]. (See [8] for a description of these techniques.) Both of these methods, however, employ a series of transformations which use the entire matrix A and hence suffer from the same disadvantages, for large matrices, as does the reduction to tri-diagonal form.

In Section 2, the eigenvalues and eigenvectors, which are determined by a matrix A and a subspace H, are defined. We then consider a quantity $V_A(H)$ which provides a measure of how nearly invariant H is, with respect to A. Using this measure, in Section 3, we derive error bounds for the approximate eigenvalues and eigenvectors. Finally, in the last section, two methods are discussed for finding subspaces which are nearly invariant, and hence give good approximations. The first method is a modification of Erdelyi's method while the second is an inverse iteration method. Both can be used effectively on very large matrices.

Most of the discussion is restricted to symmetric matrices. Methods for non-symmetric matrices, as well as numerical results, will be discussed in later papers.

Section 2. Approximate Eigenvalues and Eigenvectors

Let $Y_1,\ldots,Y_p$ be any set of $p < n$ orthonormal vectors in E^n, Euclidean n-space. If H is the subspace spanned by these vectors, and $(Y_1\ldots Y_p)$ denotes the $n\times p$ matrix whose i-th column is Y_i, then the restriction of an $n\times n$ matrix A to H (which Householder, [8] calls the section of A determined by H) is given by

$$B = (Y_1\ldots Y_p)^T A (Y_1\ldots Y_p) \ . \tag{2.1}$$

If A is Hermitian, with eigenvalues $\lambda_1 \geq \lambda_2 \geq\cdots\geq \lambda_n$, then B is also Hermitian, with eigenvalues $\mu_1 \geq\cdots\geq \mu_p$ which satisfy

$$\lambda_n \leq \mu_p = \min_{z\varepsilon H} \frac{Z^TAZ}{Z^TZ} \leq \lambda_p \tag{2.2}$$

and

$$\lambda_1 \geq \mu_1 = \max_{z\varepsilon H} \frac{Z^TAZ}{Z^TZ} \geq \lambda_{n-p+1} \ . \tag{2.3}$$

(See Householder [8], pages 75-76.) Furthermore, if the corresponding eigenvectors of B are $Z_1, Z_2,\ldots,Z_p$, and we let

$$\tilde{X}_i = (Y_1\ldots Y_p)Z_i$$

then

$$\frac{\tilde{X}_i^T A \tilde{X}_i}{\tilde{X}_i^T \tilde{X}_i} = \frac{Z_i^T (Y_1\ldots Y_p)^T A (Y_1\ldots Y_p) Z_i}{Z_i^T (Y_1\ldots Y_p)^T (Y_1\ldots Y_p) Z_i}$$

$$= \frac{Z_i^T B Z_i}{Z_i^T Z_i} = \mu_i, \ i = 1,2,\ldots p \ .$$

If we are given a p-dimensional subspace H, the above ideas suggest the following definition.

Definition 2.1. Let H be a p-dimensional subspace of E^n, $p < n$, and let $Y_1,\ldots,Y_p$ be any set of linearly independent vectors in H. The $p \times p$ matrix B which satisfies

$$(Y_1 \ldots Y_p)^T (Y_1 \ldots Y_p) B = (Y_1 \ldots Y_p)^T A (Y_1 \ldots Y_p) \tag{2.4}$$

is called the restriction of A to H. The eigenvalues $\mu_1,\ldots,\mu_p$ of B are called H-approximate eigenvalues of A, and if Z is an eigenvector of B, then $\tilde{X} = (Y_1 \ldots Y_p) Z$ is an H-approximate eigenvector of A.

Note that (2.4) has a solution, since the Gram matrix [6] $(Y_1 \ldots Y_p)^T (Y_1 \ldots Y_p)$ is non-singular whenever $Y_1,\ldots,Y_p$ are linearly independent. Clearly, the matrix B depends on the choice of the basis for H. In fact, if this basis is orthonormal, then (2.4) becomes (2.1). Our first result shows, however, that the H-approximate eigensystem depends only upon the subspace H.

Theorem 2.1. The H-approximate eigensystem does not depend upon the particular vectors in H which are used to define the restricted matrix B.

Proof: Let $\{Y_1,\ldots,Y_p\}$ and $\{\tilde{Y}_1,\ldots,\tilde{Y}_p\}$ be two linearly independent sets of vectors in H. Without loss of generality, we can assume that the first set is orthonormal. Let T be the $p \times p$ non-singular matrix such that $(\tilde{Y}_1 \ldots \tilde{Y}_p) = (Y_1 \ldots Y_p) T$. If $\tilde{B}$ is the matrix defined by (2.4) using $\{\tilde{Y}_1,\ldots,\tilde{Y}_p\}$, then

$$(\tilde{Y}_1 \ldots \tilde{Y}_p)^T (\tilde{Y}_1 \ldots \tilde{Y}_p)\tilde{B} = (\tilde{Y}_1 \ldots \tilde{Y}_p)^T A (\tilde{Y}_1 \ldots \tilde{Y}_p)$$

hence

$$\begin{aligned} T^T T\tilde{B} &= T^T (Y_1 \ldots Y_p)^T A (Y_1 \ldots Y_p) T \\ &= T^T (Y_1 \ldots Y_p)^T (Y_1 \ldots Y_p) B T \\ &= T^T B T \end{aligned}$$

so

$$\tilde{B} = T^{-1} B T \ .$$

Thus B and $\tilde{B}$ have the same eigenvalues, and their eigenvectors, Z_i and $\tilde{Z}_i$, are related by $T\tilde{Z}_i = Z_i$. Hence,

$$(Y_1 \ldots Y_p) Z_i = (Y_1 \ldots Y_p) T\tilde{Z}_i = (\tilde{Y}_1 \ldots \tilde{Y}_p)\tilde{Z}_i$$

which implies that B and $\tilde{B}$ produce the same H-approximate eigenvectors.

A consequence of this theorem is that any H-approximate eigensystem can be obtained using an orthonormal basis for H. In particular, for A Hermitian, formulas (2.2) and (2.3) must always hold, and furthermore, we can assert that the H-approximate eigenvalues and eigenvectors satisfy

$$\mu_i = \frac{X_i^T A X_i}{X_i^T X_i} \ . \tag{2.5}$$

In order to derive error estimates for these approximations, we introduce the following notion.

Definition 2.2. Let A be an $n \times n$ matrix, H a p-dimensional subspace of E^n, $p < n$, $\{Y_1, \ldots, Y_p\}$ an orthonormal basis for H, and P the projection of E^n onto H. The variation of H under A is the non-negative number

$$V_A(H) = \{\sum_{k=1}^{p} \|\varepsilon_k\|^2\}^{1/2}$$

where

$$\varepsilon_k = (I-P)AY_k, \quad k = 1, \ldots, p \; . \tag{2.6}$$

(The norm we use here, and throughout this paper, is the Euclidean norm

$$\|x\| = (x^T x)^{1/2} \qquad .)$$

We will occasionally omit the reference to A and write simply $V(H)$.

In order for this to be a proper definition, $V_A(H)$ should not change if we use another orthonormal basis for H.

Lemma 2.1. The value of $V_A(H)$ does not depend upon the choice of orthonormal bases for H.

Proof: Let $\{Y_1, \ldots, Y_p\}$ and $\{\tilde{Y}_1, \ldots, \tilde{Y}_p\}$ be two orthonormal bases for H. Let ε_k and $\tilde{\varepsilon}_k$ be the corresponding vectors defined by (2.6). Then there is a $p \times p$ orthogonal matrix $T = (t_{ij})$ such that

$$Y_i = \sum_{j=1}^{p} t_{ij}, \tilde{Y}_j,$$

hence

$$\sum_{k=1}^{p} \|\varepsilon_k\|^2 = \sum_{k=1}^{p} \varepsilon_k^T \varepsilon_k$$

$$= \sum_{k=1}^{p} Y_k^T A^T (I-P) A Y_k$$

$$= \sum_{k=1}^{p} \{ \sum_{j=1}^{p} t_{kj} \tilde{Y}_j^T \} A^T (I-P) A \{ \sum_{i=1}^{p} t_{ki} \tilde{Y}_i \}$$

$$= \sum_{j=1}^{p} \sum_{i=1}^{p} (\sum_{k=1}^{p} t_{kj} t_{ki}) \tilde{Y}_j^T A^T (I-P) A \tilde{Y}_i$$

$$= \sum_{j=1}^{p} \tilde{Y}_j^T A^T (I-P) A \tilde{Y}_i$$

$$= \sum_{j=1}^{p} \|\tilde{\varepsilon}_j\|^2 .$$

Thus, the two bases produce the same value for $V_A(H)$.

An alternative expression for ε_k, which uses the restriction of A to H, is given by the following lemma.

Lemma 2.2. Let $Y_1, \ldots, Y_p$ be an orthonormal basis for H. Then equation (2.6) can be replaced by

$$\varepsilon_k = AY_k - \sum_{i=1}^{p} b_{ik} Y_i \tag{2.7}$$

where $\{b_{ik}\}$ are the elements of the matrix defined by (2.1). That is,

$$b_{ik} = Y_i^T A Y_k .$$

<u>Proof</u>:

$$AY_k - \sum_{i=1}^{p} b_{ik} Y_i = AY_k - \sum_{i=1}^{p} (Y_i^T A Y_k) Y_i$$

$$= AY_k - \sum_i Y_i Y_i^T A Y_k$$

$$= (I - \sum_i Y_i Y_i^T) A Y_k$$

$$= (I-P) A Y_k = \varepsilon_k \; .$$

Formula (2.7) can also be written in matrix form as

(2.8) $$A(Y_1 \ldots Y_p) = (Y_1 \ldots Y_p) B + (\varepsilon_1 \ldots \varepsilon_p) \; .$$

Section 3. Error Estimates

The classical Ritz method for finding the eigenvalues of a self-adjoint linear operator L, on a Hilbert space X, involves finding a sequence of finite dimensional subspaces $X_1, X_2, \ldots$, with

$$X_1 \subset X_2 \subset \ldots \subset X$$

and $X_k \to X$. If the restriction of L to X_k has eigenvalues $\lambda_1^{(k)} \geq \lambda_2^{(k)} \geq \ldots \geq \lambda_k^{(k)}$, and L has eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots$ then it can be shown (see Gould [7], page 133) that

$$\lim_{k\to\infty} \lambda_i^{(k)} = \lambda_i .$$

For a fixed k, however, it is difficult to obtain bounds on the error $|\lambda_i^{(k)}-\lambda_i|$. Our next theorem gives a result of this type, for the simpler case of $X = E^n$.

Throughout this section, let A be an $n\times n$ symmetric matrix, H a p-dimensional subspace, and $Y_1, \ldots, Y_p$ an orthonormal basis for H.

<u>Theorem 3.1</u>. Let $\mu_1, \ldots, \mu_p$ be H-approximate eigenvalues. For each k, $1 \leq k \leq p$, there is an eigenvalue λ_k of A with

$$|\lambda_k - \mu_k| \leq V_A(H) . \tag{3.1}$$

<u>Proof</u>: Using (2.8) we have

$$\begin{aligned} A\tilde{X}_k = A(Y_1 \ldots Y_p)Z_k &= (Y_1 \ldots Y_p)BZ_k + (\varepsilon_1 \ldots \varepsilon_p)Z_k \\ &= \mu_k(Y_1 \ldots Y_p)Z_k + (\varepsilon_1 \ldots \varepsilon_p)Z_k \\ &= \mu_k\tilde{X}_k + (\varepsilon_1 \ldots \varepsilon_p)Z_k , \end{aligned}$$

hence

$$(A-\mu_k I)\tilde{X}_k = (\varepsilon_1 \dots \varepsilon_p) Z_k \quad . \tag{3.2}$$

By a well-known estimation theorem ([9], page 141) there is an eigenvalue λ_k of A with

$$|\lambda_k - \mu_k| \leq \frac{\|(\varepsilon_1 \dots \varepsilon_p) Z_k\|}{\|\tilde{X}_k\|} \quad . \tag{3.3}$$

Now, we may assume $\|Z_k\| = 1$, in which case, letting $Z_k = (\xi_1, \dots, \xi_p)^T$, we obtain

$$\|\tilde{X}_k\|^2 = \|(Y_1 \dots Y_p) Z_k\|^2 = \|\sum_{i=1}^{p} \xi_i Y_i\|^2 = \sum_{i=1}^{p} \xi_i^2 = |Z_k|^2 = 1 \ .$$

Furthermore, if $\varepsilon_i = (\varepsilon_{i1}, \dots, \varepsilon_{in})^T$, $i = 1, \dots, p$, then

$$\begin{aligned} \|(\varepsilon_1 \dots \varepsilon_p) Z_k\|^2 &= \sum_{i=1}^{n} (\sum_{j=1}^{p} \varepsilon_{ji} \xi_j)^2 \\ &\leq \sum_{i=1}^{n} (\sum_{j=1}^{p} \varepsilon_{ji}^2 \sum_{j=1}^{p} \xi_j^2) \\ &= \sum_{j=1}^{p} (\sum_{i=1}^{n} \varepsilon_{ji}^2) \cdot \sum_{j=1}^{p} \xi_j^2 = \sum_{j=1}^{p} |\varepsilon_j|^2 = V(H)^2 \ . \end{aligned}$$

Combining this with (3.3) proves the theorem.

A corresponding result for H-approximate eigenvectors is not possible, since it is known that error bounds for eigenvectors must depend upon the separation of the eigenvalues. Using a standard theorem as given, for example, in Isaacson and Keller [9], page 142, together with the inequality

$$\|(A-\mu_k I) X_k\| \leq V(H)$$

obtained in the previous proof, we can state the following result.

Theorem 3.2. Let A have eigenvalues $\lambda_1,\dots,\lambda_n$ and let $d = \min\{|\lambda_i-\lambda_j| : \lambda_i \neq \lambda_j\}$. Then for each H-approximate eigenvector $\tilde{X}_i$ there is an eigenvector X_i of A with

$$\|\tilde{X}_i - X_i\| \leq \frac{V(H)}{d}.$$

If d is of the same magnitude as $V(H)$, then clearly this bound is not of much use. In the next section, we will consider two methods for finding sequences of p-dimensional subspaces H_1, $H_2,\dots$ for which $V(H_k) \to 0$. The above theorem can then be used to conclude that the H_k-approximate eigenvectors converge to eigenvectors of A. In order to gain some insight into the rates of convergence of the approximate eigenvectors and eigenvalues, we next consider some asymptotic error estimates.

We will say that a vector $Y(\varepsilon)$ is an $O(\varepsilon^k)$ approximation to X if

$$|Y(\varepsilon)-X| \leq c\varepsilon^k$$

for all small $\varepsilon > 0$, where c is a constant.

A simple rephrasing of Theorem 3.2 results in:

Theorem 3.3. If $V_A(H) = O(\varepsilon)$, then the H-approximate eigenvectors are $O(\varepsilon)$ approximations to eigenvectors of A.

The converse of this theorem is also true.

Theorem 3.4. If $Y_1,\dots,Y_p$ are $O(\varepsilon)$ approximations to p distinct eigenvectors of A, and if H is the subspace spanned by $Y_1,\dots,Y_p$ then $V_A(H) = O(\varepsilon)$.

Proof: Let $Y_i = X_i + W_i$ where $AX_i = \lambda_i X_i$ and $\|W_i\| = O(\varepsilon)$. Then by formula (2.6),

$$\varepsilon_i = (I-P)AY_i = (I-P)(\lambda_i X_i + AW_i)$$

$$= (I-P)(\lambda_i Y_i - \lambda_i W_i + AW_i)$$

$$= (I-P)(A-\lambda_i I)W_i \ .$$

But then

$$V_A(H) = \{\sum_{i=1}^{p} \|(I-P)(A-\lambda_i I)W_i\|^2\}^{1/2}$$

$$\leq \|I-P\| \{\sum_{i=1}^{p} \|A-\lambda_i I\|^2 \|W_i\|^2\}^{1/2}$$

$$= \|I-P\| \{\sum_{i=1}^{p} \|A-\lambda_i I\|^2\}^{1/2} \ O(\varepsilon) = O(\varepsilon) \ .$$

For the H-approximate eigenvalues, we can obtain a better result. In fact, it is known (see Fox [5], pp. 279-280) that if $\tilde{X}$ is an $O(\varepsilon)$-approximation to an eigenvector of A, then the corresponding Rayleigh quotient is an $O(\varepsilon^2)$-approximation to an eigenvalue. We have shown in Section 2 that the H-approximate eigenvalues are Rayleigh quotients corresponding to the H-approximate eigenvectors. Combining this with the previous theorem gives our final estimate.

Theorem 3.5. If $V_A(H) = O(\varepsilon)$, then the H-approximate eigenvalues are $O(\varepsilon^2)$-approximations to eigenvalues of A.

Section 4. Methods for Finding Invariant Subspaces

In this section, we consider two methods for finding a sequence of subspaces $H_0, H_1, \ldots,$ such that $V_A(H_k) \to 0$. The first is a modification of the following method, proposed by I. Erdelyi [4], for finding the p eigenvalues of largest moduli and the corresponding eigenvectors.

Let Y_0 be an arbitrary vector, and let $Y_k = AY_{k-1}$, $k=1,2,\ldots,p$. If Y_0 is contained in a p-dimensional invariant subspace H, then $Y_0,\ldots,Y_p$ are in H, hence they will be linearly dependent and there will exist constants $a_0,a_1,\ldots,a_p$, not all zero, such that

$$a_0Y_0 + a_1Y_1 + \ldots + Y_p = 0 . \tag{4.1}$$

The polynomial

$$P(x) = a_0 + a_1x + \ldots + x^p \tag{4.2}$$

is an annihilating polynomial for A, hence is a divisor of the characteristic polynomial. The roots $\lambda_1,\ldots,\lambda_p$ of (4.2) are eigenvalues of A, and the corresponding eigenvectors are given by

$$\hat{X}_i = \alpha_0Y_0 + \alpha_1Y_1 + \ldots + \alpha_{p-1}Y_{p-1} \tag{4.3}$$

where $\alpha_0,\ldots,\alpha_{p-1}$ are defined by

$$\frac{P(x)}{x-\lambda_i} = \alpha_0 + \alpha_1x + \ldots + \alpha_{p-1}x^{p-1} .$$

If Y_0 does not lie in an invariant subspace, we will not be able to satisfy (4.1). In this case, determine $a_0,\dots,a_{p-1}$ to minimize the expression

$$(4.4) \qquad ||a_0Y_0 + a_1Y_1 + \dots + Y_p|| .$$

This leads to the p×p linear system

$$(4.5) \qquad a_0Y_i^TY_0 + a_1Y_i^TY_1 + \dots + Y_i^TY_p = 0, \; i=1,\dots,p .$$

The solution to this system is then used to form the polynomial (4.2). The relation of this method to our previous discussion is given in the following theorem.

Theorem 4.1. Let Y_0 be an arbitrary vector, and let $Y_k = AY_{k-1}$, $k = 1,\dots,p$. If H is the subspace spanned by $Y_0,\dots,Y_{p-1}$, then the H-approximate eigenvalues are identical with the approximations obtained from Erdelyi's method. Moreover, aside from a scalar factor, the corresponding approximate eigenvectors are also identical.

Proof: The restricted matrix B, defined by (2.4) can be shown to have the form

$$B = \begin{pmatrix} 0 & 0 & \dots & 0 & b_0 \\ 1 & 0 & \dots & 0 & b_1 \\ 0 & 1 & \dots & 0 & b_2 \\ & & & & \\ 0 & 0 & \dots & 1 & b_{p-1} \end{pmatrix}$$

where $(b_0,\dots,b_{p-1})$ is the solution to

$$Y_i^T Y_0 b_0 + Y_i^T Y_1 b_1 + \ldots + Y_i^T Y_{p-1} b_{p-1} = Y_i^T A Y_{p-1} = Y_i^T Y_p$$

$$i=0,1,\ldots p-1 \ .$$

Thus, $b_i = -a_i$, $i = 0,\ldots,p-1$ where $a_0,\ldots,a_{p-1}$ are defined by (4.5) Moreover, the matrix B is in companion form and hence its characteristic polynomial is

$$-b_0 - b_1 x - \ldots - b_{p-1} x^{p-1} + x^p = 0$$

which is identical with the polynomial obtained by Erdelyi. To show that the two methods produce the same eigenvectors, let $\tilde{X}_i = (Y_0,\ldots,Y_{p-1})Z_i$ where $BZ_i = \mu_i Z_i$. Then

$$\begin{aligned}
(A-\mu_i I)\tilde{X}_i &= (A-\mu_i I)(Y_0 \ldots Y_{p-1})Z_i \\
&= (Y_1 Y_2 \ldots Y_p)Z_i - \mu_i (Y_0 \ldots Y_{p-1})Z_i \\
&= (Y_1 Y_2 \ldots Y_p)Z_i - (Y_0 \ldots Y_{p-1})BZ_i \\
&= (Y_1 Y_2 \ldots Y_p)Z_i - (Y_1 Y_2 \ldots Y_{p-1} \tilde{Y}_p)Z_i
\end{aligned}$$

where $\tilde{Y}_p = b_0 Y_0 + b_1 Y_1 + \ldots + b_{p-1} Y_{p-1}$. Hence,

$$\begin{aligned}
(A-\mu_i I)\tilde{X}_i &= \xi_{ip}[Y_p - b_0 Y_0 - \ldots - b_{p-1} Y_{p-1}] \\
&= \xi_{ip}(a_0 Y_0 + a_1 Y_1 + \ldots + Y_p)
\end{aligned}$$

where ξ_{ip} is the p-th coordinate of Z_i. From the from of B, it is easy to verify that $\xi_{ip} \neq 0$ for all i. Moreover, the eigenvector produced by Erdelyi's method satisfies

$$(A-\mu_i I)\hat{X}_i = a_0 Y_0 + a_1 Y_1 + \ldots + Y_p \text{ ;}$$

thus, if μ_i is not an eigenvalue, then apart from the factor ξ_{ip}, the vectors are identical.

This theorem, together with Theorem 2.1, shows that we can obtain the same results as Erdelyi by orthogonalizing the vectors $Y_0, \ldots, Y_{p-1}$ and then finding the eigenvalues and eigenvectors of the $p \times p$ matrix $B = (Y_i^T A Y_j)$. Notice that if A is symmetric, then so is B, and hence the QR method can be applied to B. Thus, the problem of finding all roots of a polynomial of degree p is replaced by the simpler problem of finding the eigenvalues of a $p \times p$ symmetric matrix. The orthogonalization also eliminates the need for solving the $p \times p$ system (4.5).

To obtain better approximations, Erdelyi recommends repeating the process, starting with a new vector Y_0 which is a combination of the approximate eigenvectors that have just been found. Our invariant subspace approach, however, indicates that a better procedure is to use, as the new subspace H, the space spanned by the vectors $A\tilde{X}_1, \ldots, A\tilde{X}_p$ where $\tilde{X}_1, \ldots, \tilde{X}_p$ are the H-approximate eigenvectors. This leads to the following method for finding the p largest eigenvalues, and corresponding eigenvectors, of an $n \times n$ symmetric matrix.

Modified Erdelyi Method:

Let Y_0 be an arbitrary vector, let $Y_k = A^k Y_0$, k=1,2,...,p-1, and let H_0 be the space spanned by $Y_0, \ldots, Y_{p-1}$. For k=1,2,... let H_{k+1} be the subspace spanned by the vectors $A\tilde{X}_1, \ldots, A\tilde{X}_p$ where $\tilde{X}_1, \ldots, \tilde{X}_p$ are the H_k-approximate eigenvectors.

Theorem 4.2. If Y_0 is not orthogonal to the subspace spanned by the eigenvectors $X_1, \ldots, X_p$, of the symmetric matrix A, which correspond to eigenvalues $\lambda_1, \ldots, \lambda_p$ where $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_p| > |\lambda_{p+1}| \geq \ldots \geq |\lambda_n|$, then the subspaces H_k produced by the Modified Erdelyi Method satisfy

$$V_A(H_k) = O\left(\left| \frac{\lambda_{p+1}}{\lambda_p} \right|^k \right) .$$

Proof: Any H_{k+1}-approximate eigenvector lies in the space H_{k+1}, hence is a linear combination of $A\tilde{X}_1, \ldots, A\tilde{X}_p$, where $\tilde{X}_1, \ldots, \tilde{X}_p$ are H_k-approximate eigenvectors. By induction, it follows that H_{k+1} is spanned by the vectors $A^{k+1}Y_i$, i = 0,1,...,p-1 where $Y_i = A^i Y_0$. That is, H_{k+1} is spanned by

$$A^{k+1}Y_0,\ A^{k+2}Y_0, \ldots, A^{k+p}Y_0 \ . \tag{4.6}$$

Now, if $Y_0 = \sum_{\ell=1}^{n} \eta_\ell X_\ell$ then

$$A^{k+i}Y_0 = \sum_{\ell=1}^{n} \eta_\ell \lambda_\ell^{k+1} X_\ell$$

$$= \lambda_p^{k+i} \{ \sum_{\ell=1}^{p} \eta_\ell (\frac{\lambda_\ell}{\lambda_p})^{k+i} X_\ell + \sum_{\ell=p+1}^{n} \eta_\ell (\frac{\lambda_\ell}{\lambda_p})^{k+i} X_\ell \}$$

$$= \lambda_p^{k+i} [\sum_{\ell=1}^{p} \alpha_{i\ell} X_\ell + O(|\frac{\lambda_{p+1}}{\lambda_p}|)^k \ .$$

Hence, H_{k+1} is spanned by the vectors Z_i, $i = 1,\ldots,p$, where

$$(4.7) \qquad Z_i = \sum_{\ell=1}^{p} \alpha_{i\ell} X_\ell + W_i \ ,$$

$$\|W_i\| = O\left(\left|\frac{\lambda_{p+1}}{\lambda_p}\right|^k \right) .$$

We may assume the vectors Z_i are linearly independent, (otherwise $V(H_{k+1}) = 0$), in which case, for large k, the matrix $(\alpha_{i\ell})$ is non-singular, and (4.7) can be inverted to obtain

$$X_\ell = \sum_{i=1}^{p} \beta_{\ell i} Z_i + V_\ell$$

where again we have $\|V_\ell\| = O\left(\left|\frac{\lambda_{p+1}}{\lambda_p}\right|^k \right)$. The vectors $\sum_{i=1}^{p} \beta_{\ell i} Z_i$ span H_{k+1}, so by Theorem 3.4 we conclude

$$V(H_{k+1}) = O\left(\left|\frac{\lambda_{p+1}}{\lambda_p}\right|^k \right)$$

which proves the theorem.

This method can be considered to be a p-dimensional power method. Closely related to the usual power method is Wielandt's inverse iteration [8], and we now discuss a p-dimensional version of this.

Let A be an $n \times n$ symmetric matrix, with eigenvalues $\lambda_1,\lambda_2,\ldots,\lambda_n$, eigenvectors $X_1,\ldots,X_n$. Suppose $Y_1,\ldots,Y_p$ are $O(\varepsilon)$ approximations to $X_1,\ldots,X_p$; i.e.,

$$\|Y_i - X_i\| = O(\varepsilon) \ .$$

Then Theorem 4.2 implies $V(H) = O(\varepsilon)$, where H is the subspace spanned by $Y_1,\ldots,Y_p$. Let $\mu_1,\ldots,\mu_p$ be the H-approximate eigenvalues, and $\tilde{X}_1,\ldots,\tilde{X}_p$ the H-approximate eigenvectors, and let

$$\tilde{Y}_i = (A-\mu_i I)^{-1}\tilde{X}_i \tag{4.8}$$

where we assume here that μ_i is not an eigenvalue. The subspace $\tilde{H}$ spanned by $\tilde{Y}_1,\ldots,\tilde{Y}_p$ will be called the <u>subspace obtained from H by inverse iteration</u>.

If $p = 1$, then we have here the inverse iteration-Rayleigh quotient method ([11], pp. 635-636). Since each iteration requires solving an $n\times n$ system, this method is not often used. On the other hand, the convergence rate is cubic [11], and hence it can be a useful method, provided good approximations are already known. In the more general case where $p > 1$, each iteration requires the solution of p linear systems of order $n\times n$. Thus, we have here the same disadvantage as in the $p = 1$ case. The next theorem shows however that the cubic convergence also holds for $p > 1$.

<u>Theorem 4.3</u>. If $\tilde{H}$ is the subspace obtained from H by inverse iteration, then $V(H) = O(\varepsilon)$ implies

$$V(\tilde{H}) = O(\varepsilon^3) .$$

<u>Proof</u>: The H-approximate eigenvectors $\tilde{X}_i$ are $O(\varepsilon)$ approximations to eigenvectors X_i, $i = 1,\ldots,p$, and for small ε,

$$|\lambda_i-\mu_i| = O(\varepsilon^2),\ i = 1,\ldots,p$$

where $\mu_1, \ldots, \mu_p$ are the H-approximate eigenvalues. But $\tilde{X}_i = X_i + Z_i$ where $Z_i = \sum_{k \neq l} \xi_{ik} X_k$, $[\sum_{k \neq l} \xi_{ik}^2]^{1/2} = O(\varepsilon)$, and $\tilde{H}$ is spanned by the vectors

$$\hat{Y}_i = (\lambda_i - \mu_i)\tilde{Y}_i = (\lambda_i - \mu_i)(A - \mu_i I)^{-1}\tilde{X}_i$$

$$= (\lambda_i - \mu_i)[(\lambda_i - \mu_i)^{-1} X_i + \sum_{k \neq i} \xi_{ik}(\lambda_k - \mu_i)^{-1} X_k]$$

$$= X_i + \sum_{k \neq i} \xi_{ik}(\lambda_i - \mu_i)(\lambda_k - \mu_i)^{-1} X_k \ .$$

If $\lambda_i \neq \lambda_j$, $j \neq 1$, $1 \leqslant j \leqslant p$, then we have $\hat{Y}_i = X_i + W_i$ where

$$\|W_i\| = \{\sum_{k \neq i} \xi_{ik}^2 (\lambda_k - \mu_i)^{-2}(\lambda_i - \mu_i)^2\}^{1/2} = O(\varepsilon^3) \ .$$

If $\lambda_i = \lambda_j$, for some $j \neq i$, then we write

$$\hat{Y}_i = X_i + \xi_{ij}(\lambda_i - \mu_i)(\lambda_j - \mu_i)^{-1} X_j + \sum_{\substack{k \neq i \\ k \neq j}} \xi_{ik}(\lambda_i - \mu_i)(\lambda_k - \mu_i)^{-1} X_k$$

$$= X_i' + W_i$$

where X_i' is an eigenvector, and

$$\|W_i\| = O(\varepsilon^3) \ .$$

Hence, by Theorem 4.2, $V(H) = O(\varepsilon^3)$.

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