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ABSTRACT

An algorithm has been developed for finding the eigenvalues of a symmetric matrix A in a given interval [a, b] and the corresponding eigenvectors using a modification of the method of simultaneous iterations with the same favorable convergence properties. The technique is most suitable for large sparse matrices and can be effectively implemented on a parallel computer such as the ILLIAC IV.

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Introduction

Consider the eigenvalue problem $Au = \lambda u$ where A is a real symmetric matrix of order n. If n is large and A is sparse, then an iterative method for finding the eigenvalues and eigenvectors which uses A only as an operator may be superior to a method which reduces A to a condensed form (e.g., tridiagonal) using orthogonal transformations resulting in a far denser matrix exceeding storage capacity. This superiority is quite demonstrable if only a few of the eigenvalues and the corresponding eigenvectors are required. Bauer's method of Simultaneous Iterations [1, 2] for finding a few of the leading eigenvalues and eigenvectors is one of such methods. In this paper we modify his method to find the eigenvalues of A in some interval [a, b]. Without loss of generality we assume that A is positive-definite. The problem is therefore to find the q eigenvalues $\lambda_p, \lambda_{p+1}, \ldots, \lambda_{p+q-1}$, where

$$c_2 \geq \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{p-1} > b > \lambda_p \geq \lambda_{p+1} \geq \cdots \geq \lambda_{p+q-1} > a > \lambda_{p+q} \geq \cdots \geq \lambda_n \geq c_1 > 0$$

and the corresponding eigenvectors.

The Algorithm

Similar to the method of "Simultaneous Iterations" [2], we propose the following iterative scheme:

(i) Choose an $n \times q$ matrix X_o such that

$$X_o^t X_o = I_q$$

(ii) $\tilde{X}_{m+k} = T_m(B)X_k \qquad k = 0, 1, 2, \ldots \qquad (1)$

where B is a polynomial of A to be defined later, and $T_m(B)$ is the Chebyshev polynomial of B of degree m.

(iii) Using Gram-Schmidt orthonormalization process we decompose $\tilde{X}_j$ as

$$\tilde{X}_j = U_j R_j, \qquad (2)$$

where $U_j^t U_j = I_q$ and R_j is an upper triangular matrix of order q.

(iv) Let

$$Z_j = AU_j. \tag{3}$$

Then form the positive-definite q×q matrix

$$G_j = Z_j^t Z_j \tag{4}$$

and solve for its eigenvectors Q_j.

(v) Thus,

$$X_{j+1} = U_j Q_j. \tag{5}$$

Go back to (ii) and so on until $X_\ell^t A X_\ell$ approaches a diagonal matrix whose elements are the eigenvalues of A in [a, b]; this occurs when Q_ℓ approaches the identity matrix.

The matrix B in (1) may be obtained as follows:

Let

$$\tilde{A} = [2A - (a+b)I]/(b-a); \tag{6}$$

then an eigenvalue of $\tilde{A}$ is given by

$$\tilde{\lambda} = [2\lambda - (a+b)]/(b-a) \tag{7}$$

and those eigenvalues of $\tilde{A}$ in [-1, 1] correspond to the eigenvalues of A in [a, b]. The interval [-c, c] that contains all the eigenvalues of $\tilde{A}$ is given by,

$$c = \max\{d_1, d_2\} \tag{8}$$

where

$$\begin{aligned} d_1 &= |2c_1 - (a+b)|/(b-a) \\ d_2 &= |2c_2 - (a+b)|/(b-a) \end{aligned} \tag{9}$$

If some mapping $y = f(x)$ can be found such that $f(\tilde{\lambda})$ is outside the interval [-1, 1] for $\tilde{\lambda}$ in [-1, 1] and $|f(\tilde{\lambda})| \leq 1$ for $\tilde{\lambda}$ outside [-1, 1], then the algorithm described above (i)-(v) will yield the eigenvalues of A in [a, b] and the corresponding eigenvectors.

Let us therefore map the interval [-1, 1] on the subintervals [-c, -1] and [1, c], one such mapping may be taken as,

$$y = \pm\sqrt{\alpha x+\beta}$$

or $$x = (y^2-\beta)/\alpha. \tag{10}$$

$x = -1$ corresponds to $y = \pm 1$, thus

$$1 = -\alpha+\beta;$$

and $x = +1$ corresponds to $y = \pm c$, thus

$$c^2 = \alpha+\beta.$$

Therefore

$$\alpha = \tfrac{1}{2}(c^2-1)$$
$$\beta = \tfrac{1}{2}(c^2+1) \tag{11}$$

Hence the matrix B is taken as

$$B = [2\tilde{A}^2 - (c^2+1)I]/(c^2-1) \tag{12}$$

and

$$\mu = \lambda(B) = [2\tilde{\lambda}^2 - (c^2+1)]/(c^2-1) \tag{13}$$

i.e., $-(\frac{\beta}{\alpha}) < \mu < -1.$

We now introduce the following theorems.

<u>Theorem 1</u>:

Let E_o be the linear space spanning the columns of X_o. In case of stable convergence (no reordering of the eigenvalues if the LR-Cholesky decomposition is applied to G_j), the angle $\phi_i^{(j)}$ between the i-th eigenvector u_i and the linear space $E_j = \{x|x=T_m(B)y,\ y\varepsilon E_{j-1}\}$, spanning the columns of X_j, is asymptotically for $j\to\infty$ of order $O(q_i^j)$ in which

$$q_i = \max_{k\notin P} \{|T_m(\mu_k)|/|T_m(\mu_i)|\} \tag{14}$$

$i\varepsilon P$, where $P = \{p, p+1, \ldots, p+q-1\}$. The proof is quite similar to that of Theorem 2 in [2] and hence will be omitted here (see Appendix I).

Theorem 2:

The columns of the matrices X_j as generated by (i)-(v) are such that

$$||u_i - x_i^{(j)}|| = O(q_i^{\,j}) \tag{15}$$

where q_i is as given by (14). The proof is again similar to that of Theorem (3) in [2] (see Appendix I).

A proper order of the Chebyshev polynomial, m, can be obtained, as in [2], by stipulating that the parallelization of the columns of $\tilde{X}_{k+m}$ should not go further than that at most one decimal digit is cancelled out when these columns are orthonormalized, i.e.,

$$|T_{m-1}\ (\mu_\ell)| < 10,$$

where

$$|\mu_\ell| = \max_{i\varepsilon P} |\mu_i|. \tag{16}$$

An approximation of μ_ℓ is obtained from (13) by replacing $\tilde{\lambda}$ by $[2\lambda_\ell^{\frac{1}{2}}(G_j) - (a+b)]/(b-a)$ where $\lambda_\ell(G_j)$ is the maximum eigenvalue of G_j. Thus,

$$\cosh\ [(m-1)\ \cosh^{-1}\ |\mu_\ell|] < 10, \text{ and}$$

$$m-1 < \frac{\cosh^{-1}\ 10}{\cosh^{-1}\ |\mu_\ell|} \simeq \frac{3}{\cosh^{-1}\ |\mu_\ell|} \tag{17}$$

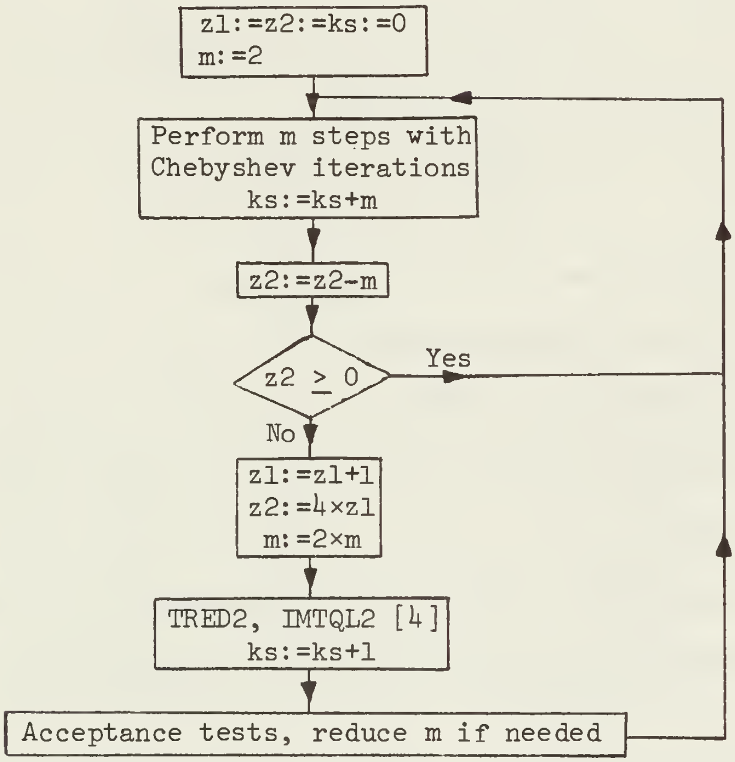
As soon as one of the eigenvalues of G_j stagnates, the corresponding eigenvalue of A can be found within computer accuracy. Once this happens we can test for acceptance of the corresponding eigenvector. The acceptance test is that of [3] except that the discounting rule is given by

$$f_i := f_i \times \frac{T_m(\sigma_{h+p})}{T_m(\sigma_i)} \tag{18}$$

where σ_i is an approximation to μ_i obtained as explained above, and h is the number of eigenvalues already accepted.

Some Numerical Results

The algorithm described above has been implemented in Fortran on UCLA's IBM 360/91 computer. The flow chart is slightly different from that of Rutishauser [3],



To demonstrate the numerical behavior of the algorithm we tested three symmetric matrices A_1, A_2, and A_3 (shown in Appendix II). In all three examples we obtained the required eigenvalues correct to 14 decimal places and the eigenvectors correct to at least 7 decimal places.

Example 1

The Gerschgorin disks of the 64×64 matrix A_1 show that we have 16 eigenvalues in the interval (1.4, 3.6), 8 eigenvalues in the interval (5.4, 6.6), and 40 eigenvalues in the interval (8.4, 16.0). We seek to obtain the 8 intermediate eigenvalues and eigenvectors. Two different intervals [a, b] have been tested [4.0, 8.0], and [5.3, 6.7] with $X_o = [e_{41}, e_{42}, \dots, e_{48}]$.

TABLE I

[a, b]	M	zl	ks
[4.0, 8.0]	16	7	114
[5.3, 6.7]	32	15	488

M: maximum degree of Chebyshev polynomials

zl: number of QL steps

ks: number of iteration steps

Table I shows that, for the same acceptance test, the number of iteration steps required (ks) is smaller when a and b are as far as possible from the eigenvalues to be evaluated ($\lambda_p, \lambda_{p+1}, \dots, \lambda_{p+q-1}$), which is clear from relation (14) and the preceeding interval transformation.

If we choose $X_o = [e_{40}, e_{41}, \dots, e_{49}]$, however, and $[a, b] \equiv [5.3, 6.7]$ the process converges to the required 8 eigenvalues and eigenvectors in only 265 iteration steps (ks = 265), zl = 10, but M = 58.

Example 2

The 6×6 positive-definite matrix A_2 has the simple roots 1, 5, 25, and a triple root at 15. If we seek the triple root 15 and take the interval [a, b] as [7, 24] we require 62 iteration steps, zl = 5, and the maximum degree M of the Chebyshev polynomials is 6. Here we only obtain an invariant subspace that corresponds to $\lambda(A_2) = 15$.

If, however, we seek the four eigenvalues in the interval [2, 24] we require only 20 iteration steps with the degree of Chebyshev polynomials not exceeding 2, and zl = 3. Again we obtain an invariant subspace corresponding to $\lambda(A_2) = 15$ and the correct eigenvector corresponding to $\lambda(A_2) = 5$.

Example 3

The positive-definite matrix A_3 has the eigenvalues $\lambda_k = 16 \sin^4[\frac{k\pi}{2(n+1)}]$, $k = 1, 2, \ldots, n$, where $n = 64$. There are 26 eigenvalues in (0, 2), 6 in (2, 4), and 32 in (4, 16). Here we would like to evaluate the eigenvalues in the interval [2, 4] and the corresponding eigenvectors. Table II shows the effect of our assumption regarding the distribution of eigenvalues on the number of iteration steps (ks) required for convergence to the eigenvalues and eigenvectors in the interval [2, 4], and degrees of the Chebyshev polynomials.

TABLE II

X_o	M	zl	ks
(i) $[e_{33}, \ldots, e_{38}]$	52	9	290
(ii) $[e_{31}, \ldots, e_{40}]$	52	8	237
(iii) $[e_{35}, \ldots, e_{37}]$	52	21	1312
(iv) $[e_{17}, \ldots, e_{28}]$	52	10	343

Experiment (iii) indicates that using fewer columns in X_o than the actual number of eigenvalues in [2, 4] led to a large number of iteration steps ks = 1312, and zl = 21 to converge to the assumed 3 eigenvalues. While experiment (iv) shows that if we use more columns in X_o than the actual number of eigenvalues, even if we completely misjudge the distribution of the eigenvalues in the intervals (0, 2), (2, 4), (4, 16), the number of iteration steps (ks) and the number of QL steps (zl) required for convergence to the 6 eigenvalues and eigenvectors in [2, 4] are only slightly more than those in experiment (i) where we used the true distribution of the eigenvalues. Since the number of iterations required appears to be largely independent of the choice of columns of the initial matrix X_o, a random number generator could be used to generate these.

We notice that the above algorithm is quite suitable for parallel computations since the major operation here is multiplying a matrix by a vector, which can be handled rather efficiently on a parallel computer such as the ILLIAC IV.

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Appendix I

Proof of Theorem 1

The iterations (i)-(v) are orthogonally invariant, i.e., replacing A by $H^tAH = \Lambda$ (where $H^tH = I$, $\Lambda = \text{diag}(\lambda_i)$) and X_o by H^tX_o has the effect that all $\tilde{X}_j$ are replaced by $H^t\tilde{X}_j$, while the G_j and X_j are not changed. Therefore we can assume, without loss of generality, that

$$A = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n).$$

In case of stable convergence E_o can be spanned by q vectors

$$\begin{bmatrix} x_{11} & x_{12} \cdots\cdots & x_{1,q} \\ \vdots & \vdots & \\ x_{p-1,1} & x_{p-1,2} \cdots & x_{p-1,q} \\ 1 & 0 & 0 \\ & 1 & \vdots \\ & & \ddots \; 1 \\ & & \\ x_{p+q,1} & x_{p+q,2} \cdots & x_{p+q,q} \\ \vdots & \vdots & \vdots \\ x_{n,1} & x_{n,2} \cdots\cdots & x_{n,q} \end{bmatrix} \begin{matrix} \\ \\ \\ \longleftarrow \text{row } p \\ \\ \longleftarrow \text{row } p+q-1 \\ \\ \\ \\ \\ \end{matrix} \qquad (A.1)$$

According to (1), E_j is spanned by

$$\begin{bmatrix}
T_m^{\,j}(\mu_1)\, x_{11} & T_m^{\,j}(\mu_1)\, x_{12} \cdots\cdots & T_m^{\,j}(\mu_1)\, x_{1,q} \\
\vdots & \vdots & \vdots \\
T_m^{\,j}(\mu_{p-1})\, x_{p-1,1} & T_m^{\,j}(\mu_{p-1})\, x_{p-1,2} & T_m^{\,j}(\mu_{p-1})\, x_{p-1,q} \\
 & & \\
T_m^{\,j}(\mu_p) & 0 \cdots\cdots & 0 \\
\vdots & T_m^{\,j}(\mu_{p+1}) & \vdots \\
\vdots & \vdots & \vdots \\
0 & 0 \cdots\cdots & T_m^{\,j}(\mu_{p+q-1}) \\
 & & \\
T_m^{\,j}(\mu_{p+q})\, x_{p+q,1} & T_m^{\,j}(\mu_{p+q})\, x_{p+q,2} \cdots\cdots & T_m^{\,j}(\mu_{p+q})\, x_{p+q,q} \\
\vdots & \vdots & \vdots \\
T_m^{\,j}(\mu_n)\, x_{n,1} & T_m^{\,j}(\mu_n)\, x_{n,2} \cdots\cdots & T_m^{\,j}(\mu_n)\, x_{n,q}
\end{bmatrix} \qquad (A.2)$$

For example, the angle between e_p and the first column of (A.2) is given by

$$\cos^2 \psi_p = \frac{T_m^{\,2j}(\mu_p)}{\sum\limits_{k \notin \tilde{P}} (T_m^{\,j}(\mu_k)\, x_{k,1})^2}, \qquad \tilde{P} = \{p+1,\ p+2,\ \ldots,\ p+q-1\}$$

hence,

$$\sin^2 \psi_p = \sum_{k \notin P}^{n} (T_m^{\,j}(\mu_k)\, x_{k,1})^2 \Big/ \sum_{k \notin \tilde{P}}^{n} (T_m^{\,j}(\mu_k)\, x_{\mu,1})^2, \qquad P = \{p,\ \tilde{P}\}$$

or

$$\psi_p \text{ is of order } O(q_p^{\,j})$$

where $\quad q_p = \max\limits_k \{|T_m(\mu_k)|/|T_m(\mu_p)|\}, \qquad k \notin P$

Therefore,

$$\phi_i^{(j)} \text{ is at most of order } O(q_i^{\,j}) \quad \blacksquare$$

Proof of Theorem 2

Taking the q vectors (A.1) each divided by $T_m^{\,j}(\mu_\ell)$, $\ell = p, p+1, \ldots, p+q-1$, as coordinate vectors $W = [w_p, w_{p+1}, \ldots, w_{p+q-1}]$ in E_j, the eigendirections of the projected operator A^{-2} are the n×q matrix $Y = WS$ where

$$Y^t A^{-2} Y = D_j^{-2} \tag{A.3}$$

in which,

$$D_j = \text{diag}(d_p^{(j)}, d_{p+1}^{(j)}, \ldots, d_{p+q-1}^{(j)}),$$

$$Y^t Y = I_q,$$

and S is a q×q orthogonal matrix. Thus

$$S^t(W^tA^{-2}W)S = D_j^{-2},$$

or

$$(W^tA^{-2}W)S = SD_j^{-2}; \tag{A.4}$$

i.e., S is the eigenvector matrix of $W^tA^{-2}W$, which can be written as

$$W^tA^{-2}W = \Lambda^{-2} + K, \tag{A.5}$$

where the elements of K are of order $O(\tau)$, i.e., $O[|T_m(\mu_i)|/|T_m(\mu_\ell)|]^{2j}$ $i \notin P$. Assume now $\lambda_i = \lambda_{i+1} = \ldots = \lambda_h$ is an h-i+1 fold eigenvalue of A; then as $j \to \infty$, h-i+1 independent eigensolutions of (A.4) with $d \to \lambda_i$ exist. Everyone of these is described by q values $s_p, s_{p+1}, \ldots, s_{p+q-1}$, and we assume that these solutions are normalized such that $s_i^2 + s_{i+1}^2 + \ldots + s_h^2 = 1$. Then the s_ℓ with $\ell \neq i, i+1, \ldots, h$ are of order $O(\tau)$. This means the angle between $\sum_i^h s_\ell w_\ell$ and $\sum_{\ell=P}^{p+q-1} s_\ell w_\ell$ is also of order $O(\tau)$, while according to Theorem 1 the angle between $\sum_i^h s_\ell w_\ell$ and the eigenspace of $\lambda_i, \lambda_{i+1}, \ldots, \lambda_h$ of A is of order $O(q_i^{\,j})$. This establishes the theorem. $\blacksquare$

Appendix II

$$A_1 = \begin{bmatrix} B_1 & & & C \\ & B_2 & & C \\ & & \ddots B_7 & \vdots \\ C & C \cdots & C & B_8 \end{bmatrix}$$

where B_k and C are matrices of order 8,

$$B_k = \begin{bmatrix} \alpha_k & 0.1 & & \\ 0.1 & \alpha_k & 0.1 & \\ & \ddots & \ddots & 0.1 \\ & 0.1 & 0.1 & \alpha_k \end{bmatrix}, \quad C = \mathrm{diag}(0.4, \ldots, 0.4)$$

and the centres of the Gerschgorin discs $\{\alpha_k\}$ are given by

(2, 3, 6, 9, 10, 11, 12, 13).

$$A_2 = \begin{bmatrix} 16.778 & -4.889 & -4.889 & -4.889 & -1.556 & -0.222 \\ -4.889 & 13.444 & -1.556 & -1.556 & 1.778 & 3.111 \\ -4.889 & -1.556 & 13.444 & -1.556 & 1.778 & 3.111 \\ -4.889 & -1.556 & -1.556 & 13.444 & 1.778 & 3.111 \\ -1.556 & 1.778 & 1.778 & 1.778 & 10.111 & 6.444 \\ -0.222 & 3.111 & 3.111 & 3.111 & 6.444 & 8.778 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 5 & -4 & 1 & & & & \\ -4 & 6 & -4 & 1 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 6 & -4 \\ & & & & 1 & -4 & 5 \end{bmatrix}, \quad n = 64$$

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15. Supplementary Notes

16. Abstracts

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