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ABSTRACT

Given a tolerance $\epsilon > 0$, we seek a criterion by which an off-diagonal element of the symmetric tri-diagonal matrix J may be deleted without changing any eigenvalue of J by more than ϵ . The criterion obtained here permits the deletion of elements of order $\sqrt{\epsilon}$ under favorable circumstances, without requiring any prior knowledge about the separation between the eigenvalues of J .

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Introduction:

The computation of the eigenvalues λ_j of the symmetric tri-diagonal matrix

$$J = \begin{pmatrix} a_1 & b_1 & & & & \\ b_1 & a_2 & b_2 & & & \\ & b_2 & \cdot & & & \\ & & \cdot & \cdot & \cdot & \\ & & & \cdot & \cdot & b_{N-1} \\ & & & & b_{N-1} & a_N \end{pmatrix}$$

can be shortened, sometimes appreciably, if any off-diagonal element b_i happens to vanish. Then the eigenvalues of the two shorter tri-diagonal matrices, of which J is the diagonal sum, can be computed separately .

This is the motive for seeking off-diagonal elements bi which are merely small. The deletion of several $b_i \neq 0$ cannot cause any eigenvalue of J to change by more than $2 \max_i |b_i|$, so the interests of economy may be well served when zero is written in place of all the b_i which satisfy, for example,

$$|b_i| < \frac{1}{2} \epsilon \quad ,$$

where ϵ is some pre-assigned tolerance compared with which any smaller error in the eigenvalues is negligible.

But experience suggests that there must be many circumstances when the deletion of a $b_i \neq 0$ causes an error much smaller than $|b_i|$; something of the order of $|b_i|^2$ would be more typical. Indeed, Wilkinson (1965, p. 312) shows that the error so induced should not much exceed ϵ if b_i is deleted whenever

$$|b_i|^2/\alpha < \epsilon \ ,$$

where

$$0 < \alpha \leq \min.|\lambda_k - \lambda_j| \text{ over } k \neq j \ .$$

Unfortunately, the constant α of minimum separation between the eigenvalues is unlikely to be known in advance of a knowledge of the eigenvalues λ_j being computed, so the last criterion for deleting a b_i could stand some improvement.

One might easily be tempted to approximate α in some sense by a difference $|a_k - a_j|$ between diagonal elements. For example, we might ask whether b_i can be deleted whenever

$$b_i^2 < \epsilon \ |a_{i+1} - a_i| \quad ?$$

The answer is definitely-no. And the condition

$$b_i^2 < \epsilon \min.|a_k - a_j| \quad \text{over } k \neq j$$

is not acceptable either. The example

$$J = \begin{pmatrix} 1 & \sqrt{2} & 0 \\ \sqrt{2} & 2 & b \\ 0 & b & 0 \end{pmatrix}$$

has eigenvalues two of which change by roughly $\sqrt{\frac{1}{3}}b$ when a tiny value of b is replaced by zero.

Evidently any criterion for deleting off-diagonal elements of the order of $\sqrt{\epsilon}$, instead of ϵ , must be more complicated. The following theorem is complicated enough to give a useful indication that b_i may be deleted whenever all three of b_{i-1}^2 , b_i^2 and b_{i+1}^2 are of the order of $\epsilon|a_{i+1} - a_i|$.

Theorem: Let J be the symmetric tri-diagonal NXN matrix shown above, and let $b_o = b_N = 0$. For any fixed i in $1 \leq i < N$ define

$$h_i = \frac{1}{2}(a_{i+1} - a_i) \qquad \text{and}$$

$$r_i^2 = (1 - \sqrt{\tfrac{1}{2}})(b_{i-1}^2 + b_{i+1}^2) \ .$$

Then the changes $\delta\lambda_3$ in the eigenvalues λ_3 of J caused by replacing b_i by zero are bounded by satisfying the inequality

$$\Sigma_j(\delta\lambda_j)^2 \leq \frac{b_i^2}{h_i^2 + r_i^2} \left\{ 2r_i^2 + \frac{h_i^2\, b_i^2}{h_i^2 + r_i^2} \right\} .$$

For example, if $b_{i+k}^2 < \frac{1}{3}|a_{i+1} - a_i|\epsilon$ for k = -1 , 0 and +1 , then the deletion of b_i will not change any eigenvalue λ_i of J by so much as ϵ .

Here is a proof of the theorem. Nothing irretrievable is lost by considering simply the 4×4 matrix

$$J = \begin{pmatrix} a_1 & b_1 & 0 & 0 \\ b_1 & a-h & b & 0 \\ 0 & b & a+h & b_3 \\ 0 & 0 & b_3 & a_4 \end{pmatrix}$$

and taking $i = 2$, $b_i = b$ and $a_{i+1} - a_i = 2h \neq 0$.

Changing J to $(J + \delta J)$ by replacing b by zero changes J's eigenvalues λ_j to $(J + \delta J)$'s eigenvalues $(\lambda_j + \delta\lambda_j)$. But another way can be found to change b to zero without changing the eigenvalues λ_j. Let us apply one step of the Jacobi iteration to liquidate b. This requires the construction of an orthogonal matrix

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & c & s & 0 \\ 0 & -s & c & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = (P^T)^{-1}$$

in which c and s are specially chosen so that $c^2 + s^2 = 1$ and $P^T JP$ has zero in place of b. The choice consists in the determination of φ in the interval

$$-\pi/4 < \varphi < \pi/4$$

such that

$$\tan 2\varphi = T = b/h \; ; \qquad (*)$$

then

$$c = \cos\varphi \quad \text{and} \quad s = \sin\varphi \; .$$

The following abbreviations will be useful in what follows:

$$C = \cos 2\varphi = 1/\sqrt{1 + T^2} \; ,$$

$$S = \sin 2\varphi = TC \; ,$$

$$c = \cos\varphi = \sqrt{\tfrac{1}{2}(1 + C)} \; ,$$

$$s = \sin\varphi = \tfrac{1}{2} S/c \quad \text{and}$$

$$\sigma = \sin \tfrac{1}{2}\varphi \; .$$

Then we define $D = J + \delta J - P^T J P$;

$$D = \begin{pmatrix} 0 & 2\sigma^2 b_1 & -sb_1 & 0 \\ 2\sigma^2 b_1 & 2s(cb-sh) & Sh-Cb & sb_3 \\ -sb_1 & Sh-Cb & 2s(sh-cb) & 2\sigma^2 b_3 \\ 0 & sb_3 & 2\sigma^2 b_3 & 0 \end{pmatrix} .$$

No use has been made yet of the relation (*) above ; on the contrary, the best value for φ might very well satisfy

$$\tan 2\varphi = T \neq b/h \; ,$$

and it could be much worth our while to leave φ unfettered for now while preserving the foregoing definitions for T, C, S, c, s, σ, and D in terms of φ.

The significance of D is revealed by the Wielandt-Hoffman theorem, which is stated and proved in an elementary way in Wilkinson's book (1965, p. 104-9):

If A and B are symmetric matrices with eigenvalues

$$\alpha_1 \le \alpha_2 \le \cdots \le \alpha_N \quad \text{and}$$

$$\beta_1 \le \beta_2 \le \cdots \le \beta_N \quad \text{respectively} ,$$

then

$$\Sigma_j(\alpha_j - \beta_j)^2 \le \text{tr.}(A - B)^2 = \Sigma_i\Sigma_j(A_{ij} - B_{ij})^2$$

Let this theorem be applied with

$$A = J + \delta J , \qquad \alpha_j = \lambda_j + \delta\lambda_3 ,$$

$$B = P^T J P , \qquad \beta_j = \lambda_j ,$$

$$\text{and} \quad A - B = D .$$

Then

$$\Sigma_j(\delta\lambda_j)^2 \le \text{tr.}\ D^2$$

$$= 8\sigma^2(b_1^2 + b_3^2) + 2b^2 - 4Sbh + 8s^2h^2$$

The right-hand side is minimized by one of the values of φ at which its derivative vanishes; i.e. when

$$\frac{1}{2} s(b_1^2 + b_3^2) - Cbh + Sh^2 = 0 \quad .$$

This equation seems too cumbersome to solve precisely, but it does show that there is a value of $|\varphi|$ between 0 and $\pi/4$ at which tr. D^2 is minimized. Over this range

$$\frac{1}{2} \le \sin \frac{1}{2}\varphi / \sin \varphi = 1/(2 \cos \frac{1}{2} \varphi) \le 1/(2 \cos \pi/8) ,$$

so the bound we seek will not be weakened much if σ^2 is increased to $s^2/(4\cos^2 \pi/8)$. Therefore, let us now choose φ to minimize the right-hand side of

$$\Sigma_j(\delta\lambda_j)^2 \le 2b^2 - 4\, Sbh + 8s^2(h^2 + r^2)$$

where

$$r^2 = (1 - \sqrt{\tfrac{1}{2}})(b_1^2 + b_3^2) \ .$$

The minimizing value of φ satisfies

$$\tan 2\varphi = T = bh/(h^2 + r^2) \ ,$$

and therefore Id lies between 0 and $\pi/4$ as is required to justify the simplifying inequality $\sigma/s \le 1/(2\cos\pi/8)$ used above.

Substituting the foregoing value for T yields

$$\Sigma_j(\delta\lambda_j)^2 \le \frac{2C}{1 + C} \frac{b^2}{h^2 + r^2} \{2r^2 + Cb^2h^2/(h^2 + r^2)\} \ .$$

This inequality is much too clumsy to be useful, so it will be weakened slightly by using the fact that $C \le 1$; in most cases of practical interest C is not much less than 1. The weakened inequality is

$$\Sigma_j(\delta\lambda_j)^2 < [2r^2 + h^2b^2/(h^2 + r^2)]b^2/(h^2 + r^2) ,$$

and is just the inequality in the theorem except for a change of notation.

The theorem's most promising application is to those compact square-root-free versions of the LL^T and QR iterations described, for example, in Wilkinson's book (1965, p. 565-7). In these schemes, each iteration overwrites J by a new tri-diagonal matrix J' with the same eigenvalues as before but with off-diagonal elements which are, hopefully, somewhat smaller than before. The element located at $b_{N\ 1}$ usually converges to zero faster than the other b_i's ; and the theorem proved here can be a convenient way to tell when that $b_{N\ 1}$ is negligible. For example, b_{N-1} can be deleted whenever

$$\frac{b_{N-1}^2}{(a_N - a_{N-1})^2 + b_{N-2}^2} \left\{ b_{N-2}^2 + (a_N - a_{N-1})^2 \frac{b_{N-1}^2}{(a_N - a_{N-1})^2 + b_{N-2}^2} \right\} < \frac{1}{4}\epsilon^2$$

without displacing any eigenvalue by more than ϵ. This simplified criterion has been used satisfactorily in a QR program written by the author and J. Varah (1966), but the program'is not much slower when the simpler criterion

$$|b_{N-1}| < \frac{1}{2}\epsilon$$

is used instead.

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