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QR Sometimes Beats Jacobi*

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ABSTRACT

This note exhibits a symmetric matrix having a small eigenvalue that is computed accurately by the QR algorithm but not by Jacobi's method.

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This note exhibits a symmetric matrix having a small eigenvalue that is computed accurately by the QR algorithm but not by Jacobi's method.

In an important paper entitled "Jacobi's Method is More Accurate than QR" Demmel and Veselić [1] show that when Jacobi's method is used to find the eigenvalues of a positive-definite matrix it computes the eigenvalues to nearly optimal *relative* accuracy. They also give a counterexample to show that the QR algorithm can fail to attain this accuracy.[1] However, positive definiteness is essential to their analysis. The purpose of this note is to show by a simple but informative example that for indefinite problems QR can beat Jacobi.

Let

$$A = \begin{pmatrix} \tau\sigma^2 & a\sigma^3 & b\sigma^2 \\ a\sigma^3 & \tau\sigma^2 & c\sigma \\ b\sigma^2 & c\sigma & 1 \end{pmatrix},$$

where σ is very large and τ, a, b, and c are of order unity. The dominant eigenvalues of this matrix are to high relative accuracy $\pm a\sigma^3$. They are insensitive to small relative changes in the elements of the matrix.

From perturbation theory for graded matrices [2], the smallest eigenvalue is given to high relative accuracy by the Schur complement of the leading 2×2 principle submatrix. This approximation is

$$\lambda_{\min} \cong 1 - \frac{(\tau b^2 - 2abc)\sigma^6 + \tau c^2\sigma^4}{\tau^2\sigma^4 - a^2\sigma^6} \tag{1}$$

Unless there is cancellation in this formula, $\lambda_{\min}$ is insensitive to perturbations in τ, a, b, and c. For definiteness, we will take $\tau = a = b = 1$, $c = -1$, and $\sigma = 10^{20}$, so that $\lambda_{\min} \cong 4$ to high accuracy. The matrix A then becomes

$$A = \begin{pmatrix} 10^{40} & 10^{60} & 10^{40} \\ 10^{60} & 10^{40} & -10^{20} \\ 10^{40} & -10^{20} & 1 \end{pmatrix}.$$

[1] Actually, the failure is in the preliminary tridiagonalization.

Now the first step in the serial Jacobi algorithm is to apply a rotation in the $(1,2)$-plane to diagonalize the leading 2×2 principle submatrix. The rotation is

$$P = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}.$$

If the transformation is carried out in standard double precision, the result will be

$$\mathrm{fl}(P^{\mathrm{T}} A P) \cong \begin{pmatrix} -10^{60} & 0 & \frac{1}{\sqrt{2}} 10^{40} \\ 0 & 10^{60} & \frac{1}{\sqrt{2}} 10^{40} \\ \frac{1}{\sqrt{2}} 10^{40} & \frac{1}{\sqrt{2}} 10^{40} & 1 \end{pmatrix}.$$

If we now repeat the calculation of the Schur complement, we find that the smallest eigenvalue has become one. It has been completely altered by the first step of the Jacobi algorithm.

Turning now to the QR algorithm, the first step is to reduce A to tridiagonal form. This is accomplished by a single rotation in the $(2,3)$-plane that annihilates the $(1,3)$ and $(3,1)$-elements. To working accuracy the rotation is

$$Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -10^{-20} \\ 0 & 10^{-20} & 1 \end{pmatrix}.$$

Then

$$\mathrm{fl}(Q^{\mathrm{T}} A Q) \cong \begin{pmatrix} 10^{40} & 10^{60} & 0 \\ 10^{60} & 10^{40} & -2 \cdot 10^{20} \\ 0 & -2 \cdot 10^{20} & 4 \end{pmatrix}.$$

The eigenvalue 4 is already present in the $(3,3)$-element, and one step of explicitly shifted QR algorithm reduces the $(3,2)$ and $(2,3)$-elements to $8 \cdot 10^{-80}$. Thus the QR algorithm finds the eigenvalue, where Jacobi fails.

There are four comments to be made about this example.

- The plane rotation used in the Jacobi algorithm is balanced — i.e., its elements are all of a size. Generally speaking, balanced rotations are the bane of computations with graded matrices, since they can combine elements of unequal size in such a way that information is lost. For example, the computed $P^{\mathrm{T}} A P$ is just the matrix that would have been obtained by exact computations on a matrix with $\tau = c = 0$. For this case the formula (1) gives $\lambda_{\min} \cong 1$ — which is what the Jacobi algorithm computes.

• The transformation Q that tridiagonalizes A is nicely graded. Not only does it preserve the information contained in the parameters defining A, but it folds the information into the $(3,3)$-element to give a highly accurate approximation to the eigenvalue.

• It should not be thought that balanced transformations are *necessarily* bad. For example, the Jacobi transformation remains balances as τ increases. When $\tau = 2\sigma^2$ (say), A is positive definite, and by the Demmel-Veselić theory the smallest eigenvalue (now $\cong 0.5$) has to be computed accurately by Jacobi's method. The computations still proceed as if c were zero; however, (1) shows that

$$\lambda_{\min} \cong 1 - \frac{b^2}{2},$$

so that the value of c is irrelevant.

• Finally, just because the QR algorithm can compute the smallest eigenvalue accurately it does not follow that a particular implementation will. When I tried to compute the eigenvalues of the original example using matlab, I got a value of 0 for $\lambda_{\min}$.

References

[1] J. Demmel and K. Veselić. Jacobi's method is more accurate than QR. *SIAM Journal on Matrix Analysis and Applications*, 13:1204–1245, 1992.

[2] G. W. Stewart and G. Zhang. Eigenvalues of graded matrices and the condition of numbers of a multiple eigenvalue. *Numerische Mathematik*, 58:703–712, 1991.