Clearly, of the direct methods approximation 4 is best both as regards simplicity of programming, the number of function evaluations, and accuracy.

There remains the comparison of approximation 4 with standard methods of solving boundary-value differential equations. The relative efficiency very much depends on the form of the function f. If f gives rise to a comparatively simple differential equation then it is best to use it. For a function like (iii), however, obtaining Euler's equation is tedious and the resulting function associated with the equation, takes more than five times as long to compute. In cases such as these, and in problems where f is defined at least partly by numerical data, these direct methods seem to have some use.

As we have said before, we could have arrived at the same recurrence relations by approximating Euler's equation in the form $\frac{d}{dx}(f_3) - f_2 = 0$ in various ways. It would not, however, have been easy to guess at an approximation which only requires four function evaluations of f. Perhaps the real use of this investigation is to stress the fundamental unity of the calculus of variations problem and the boundary value differential equation, and so complete our knowledge to some extent in this field.

This research was carried out while I was the holder of the I.C.T. Research Scholarship. Complete acknowledgements will be found in Part 2.

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Correspondence

To the Editor,

The Computer Journal.

Sir,

Recent discussion on the computation of rotational levels of rigid asymmetric top molecules (Rachmann, 1965 and Jones, 1966) calls for some comment. As Jones points out, Rachmann's approach of reducing the determinantal equation to an explicit polynomial is both unnecessary and leads to ill-conditioning. The method proposed by Jones for this problem, while stable, is, however, inefficient because it is too general and does not make use of the particular features of this problem. The asymmetric tridiagonal matrix of this problem is a quasisymmetric matrix since the diagonal elements are all real and the off-diagonal elements are both real and all positive (Wilkinson, 1965).

Denoting the diagonal elements by k_i, the lower off-diagonal elements by b_i and the upper off-diagonal elements as unity, a similarity transformation leads to a symmetric tridiagonal matrix with diagonal elements k_i and off-diagonal elements $b_i\frac{1}{2}$. Any method suitable for symmetric tridiagonal matrices can now be used. The LL^T method recently published (Fox and Johnson, 1966) is particularly efficient for this purpose. The **procedure** eigenvalue, after slight modifications to correct a few obvious misprints and to remove a **goto** instruction leading to a **label** inside a **for** statement, was used to solve the 0^+ matrix discussed by both Rachmann and Jones. Values of the energies agreeing to 8 or 9 figures with those computed by Jones were computed in 2 seconds on KDF9.

As a check and to compare the relative efficiency of several methods, the 0^+ matrix was solved by two other methods. The Sturm sequence-bisection method (Wilkinson, 1962) and a general program for the eigenvalues and eigenvectors of a real matrix using the QR Algorithm (Francis, 1961) gave results identical to 9 figures with those computed by the LL^T method in 8 and 35 seconds, respectively.

Taking advantage of the tridiagonal form of the matrices in this problem leads to a substantial improvement in efficiency.

Yours faithfully,

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