An investigation into direct numerical methods for solving some calculus of variations problems. Part 1—Second order methods

By B. T. Allen*

Several direct numerical algorithms are proposed to solve the simplest general non-linear calculus of variations problem. In this paper four new methods are described which approximate to the solution with second order accuracy in terms of the step length. Results are given when the methods are used to solve two non-linear and non-trivial problems.

1. The problem

The simplest calculus of variations problem is to find a function $y(x)$ in the range (a, b) which minimizes the integral

$$\int_a^b f(x, y(x), y'(x))dx. \tag{1.1}$$

f is a given function of three variables. Boundary conditions on $y(x)$ at $x = a$ or b may or may not be given. In general, however, in this paper we have considered them to be given. Problems arise in this form in both scientific and industrial fields.

Most analytic and numerical methods of solving this problem to date have used the fact that the problem is equivalent to solving a boundary value, second order differential equation. This equation, known as Euler's equation, is derived in many well known texts (for example Elsgolc, 1961) and is given by†

$f_{yy'}(x_1, y_1, (y_2 - y_0)/2h)$.

$$\frac{d}{dx}(f_3) - f_2 = 0, \tag{1.2}$$

or equivalently by

$$y''f_{33} + y'f_{23} + f_{13} - f_2 = 0. \tag{1.3}$$

The disadvantages of trying to solve the problem numerically in this manner are that:

(i) the differential equation often turns out to have an extremely complicated form;
(ii) the function f might be defined by numerical data; in this case the partially differentiated forms, used in Euler's equation, would have to be obtained by rather tedious numerical procedures.

We have tried, therefore, to solve the problem directly by numerically approximating the integral and not the differential equation. In this paper (Part 1) we describe those methods which have a second order error in terms of the step length h. In Part 2 (Allen, 1966) we describe more accurate methods which have only a fourth order error term. As one might expect, there is a close connection between these methods and numerical methods for solving non-linear boundary differential equations.

Very little appears to have been published on the numerical solution of this problem. Elsgolc (1961) mentions Euler's approximation as a possible method of numerical solution, but gives no details. Bellman (1957) provides a method of maximization when in effect Euler's approximation is used. This method was examined, but in comparison to our own methods for the reasonably smooth functions we were working with it seemed to be fairly slow computationally. Some work has been done using series, mainly by Ritz and Galerkin at the beginning of this century, but their methods carry out the integration analytically.

2. The general numerical procedure

In this paper we have considered five different approximations for solving this problem. However, the general numerical procedure we have used is very similar in each case; it is in fact similar to that commonly used in solving non-linear boundary value differential equations. The complete range is divided into short intervals and a relationship is shown to hold over each of these subintervals. These relationships are then used to solve the problem over the complete range. We describe this general procedure now.

We divide the range (a, b) into n equal intervals such that the step length $h = (x_i - x_{i-1}) = (a - b)/n$. We consider the value of $y(x)$ only at points x_i. Let the numerical approximation we get for $y(x_i)$ be called y_i. $y(x_0) = y_0 = A$ and $y(x_n) = y_n = B$ are given.

We now consider the problem over short ranges of length $2h$, and to simplify our notation we consider the range (x_0, x_2). We now have to maximize the integral,

$$\int_{x_0}^{x_2} f(x, y(x), y'(x))dx. \tag{2.1}$$

One of the five methods we describe later approximates

† Throughout this paper (Part 1 and Part 2) we use the notation that a subscript on f means partial differentiation with respect to that variable whose position is specified by the subscript. Thus f_{23} represents the function obtained when f has been partially differentiated with respect to its second and third variables. This is in preference to a more standard notation of the form $f_{yy'}$. The latter would have led to confusion over the meaning of an expression of the form.

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$y(x)$ and $y'(x)$ in terms of y_0, y_1, y_2 and the integral (2.1) by a function $\phi(y_0, y_1, y_2)$. We now consider y_0 and y_2 fixed and choose y_1 so as to maximize this function.

In the methods we have devised we have assumed that we can evaluate only the function f. Thus if a partial derivative of f is wanted, then it must be obtained numerically. Therefore, to maximize with respect to y_1, we must carry out the partial differentiation of the function numerically and equate the partial derivative equal to zero. This we do by writing either

$$\{\phi(y_0, y_1 + \epsilon, y_2) - \phi(y_0, y_1, y_2)\}/\epsilon = 0 + O(\epsilon), \quad (2.2)$$

or

$$\{\phi(y_0, y_1 + \epsilon, y_2) - \phi(y_0, y_1 - \epsilon, y_2)\}/\epsilon = 0 + O(\epsilon^2). \quad (2.3)$$

We chose to use (2.3) since this is more accurate. We now have to choose a value of ϵ so as to compromise between the loss of accuracy due to round-off error in the subtraction and the truncation error in the form $O(\epsilon^2)$. We chose $\epsilon = 10^{-4}$ since the number of significant figures we were working with was 12 and the values of f and its derivatives were of the order of unity. This would mean that the loss in significant figures due to the truncation error $O(\epsilon^2)$ would be about four, and the loss due to round-off error in the subtraction would similarly be about four. We might expect that our accuracy would be reduced to about eight significant figures.

If we had used (2.2) a more suitable value of ϵ would have been 10^{-6} and we would have expected our accuracy to have been reduced to six significant figures.

Similar relations can be obtained over other ranges giving us $n - 1$ relations for the $n - 1$ unknowns $y_1, \ldots, y_{n-1}$. Thus the problem can be solved.

We now have the numerical problem of solving a set of non-linear recurrence relations of the form

$$\psi_i(y_{i-1}, y_i, y_{i+1}) = 0, \quad \text{for} \quad i = 1, \ldots, n-1,$$

with $y_0 = A$ and $y_n = B$ given. To solve this the following standard technique of using trial runs was used.

A value of y_1 is guessed. y_2 must then obey the relation $\psi_1(y_0, y_1, y_2) = 0$. A regula-falsi method was used to solve the non-linear equation in terms of y_2. Continuing this we find values for $y_3, \ldots, y_n$. The value of y_n will presumably be incorrect but now a regula-falsi method is used over the whole problem to find the correct value of y_1 which gives a true value for y_n. The non-linear equations for y_{i+1} are not difficult to solve as good first approximations can be found by extrapolating on previous values of y_i.

3. Approximation 1

We first try the simplest possible approximation

$$\int_{x_0}^{x_2} f(x, y, y')dx = hf(x_0, y_0, (y_1 - y_0)/h) + hf(x_1, y_1, (y_2 - y_1)/h) + O(h^2). \quad (3.1)$$

This approximation was used originally by Euler to obtain Euler's equation. We have approximated both the integral and the derivatives so that they give rise to errors $O(h)$. Numerical partial differentiation with respect to y_1 gives the recurrence relation

$$f(x_0, y_0, (y_1 + \epsilon - y_0)/h) - f(x_0, y_0, (y_1 - \epsilon - y_0)/h) + f(x_1, y_1 + \epsilon, (y_2 - y_1 - \epsilon)/h) - f(x_1, y_1 - \epsilon, (y_2 - y_1 + \epsilon)/h) = 0, \quad (3.2)$$

which is then used to solve numerically the problem as described in the previous section.

To investigate the error in this recurrence relation, however, we must use the recurrence relation obtained analytically. Partial differentiation of (3.1) with respect to y_1 gives

$$\begin{aligned}
&\frac{\partial}{\partial y_1}\{f(x_0, y_0, (y_1 - y_0)/h) + f(x_1, y_1, (y_2 - y_1)/h)\} \\
&= \{f_3(x_0, y_0, (y_1 - y_0)/h) - f_3(x_1, y_1, (y_2 - y_1)/h)\}/h + f_2(x_1, y_1, (y_2 - y_1)/h), \\
&= \left\{f_2(x_1, y_1, (y_2 - y_1)/h) - \frac{d}{dx} f_3(x_1, y_1, (y_2 - y_1)/h)\right\} + \tfrac{1}{2}h \frac{d^2}{dx^2}(f_3(x_1, y_1, (y_2 - y_1)/h)) + O(h^2), \\
&= \left\{f_2(x_1, y_1, y_1') - \frac{d}{dx} f_3(x_1, y_1, y_1')\right\} + \tfrac{1}{2}hy_1''f_{23} - \tfrac{1}{2}hy_1''\frac{d}{dx}f_{33} - \tfrac{1}{6}hy_1'''f_{33} + \tfrac{1}{2}h\frac{d^2}{dx^2}f_3 + O(h^2). \quad (3.3)
\end{aligned}$$

The first and dominant term is Euler's equation. We have assumed this to exist and to give rise to the unique solution of the problem. The first term will therefore be zero for a correct value of y_1 and thus the other terms represent the error in the approximation which in general is $O(h)$.

However, when

$$\tfrac{1}{2}hy_1''\left(f_{23} - \frac{d}{dx}f_{33}\right) - \tfrac{1}{6}hy_1'''f_{33} + \tfrac{1}{2}h\frac{d^2}{dx^2}f_3$$

is zero (which it will be when f has no terms in y and y' higher than second order, there is no yy' term, the coefficient of y'^2 is constant and the coefficient of y' is linear) then we will have an error of only $O(h^2)$. This was the case for our test functions (i) and (ii), explaining our unexpectedly good results for these problems. These are not really very useful results because Euler's equation could be solved still more easily in these cases.

4. Approximation 2

Here we use the approximation

$$\int_{x_0}^{x_2} f(x, y, y')dx = \frac{h}{3}f(x_0, y_0, (-3y_0 + 4y_1 - y_2)/2h) + \frac{4h}{3}f(x_1, y_1, (y_2 - y_0)/2h) + \frac{h}{3}f(x_2, y_2, (y_0 - 4y_1 + 3y_2)/2h) + O(h^5). \quad (4.1)$$

We have used Simpson's rule as the integration formula and approximated y_0', y_1' and y_2' as well as possible in terms of y_0, y_1 and y_2. The numerically partially differentiated form is again used to obtain the numerical results. Analytic partial differentiation gives

$$\frac{3}{4h}\frac{\partial}{\partial y_1}\text{ (approx. in (4.1))}$$

$$\begin{aligned}
&= -\{f_3(x_2, y_2, (y_0 - 4y_1 + 3y_2)/2h) \\
&\quad - f_3(x_0, y_0, (-3y_0 + 4y_1 - y_2)/2h)\}/2h \\
&\quad + f_2(x_1, y_1, (y_2 - y_0)/2h), \qquad (4.2)\\
&= f_2(x_1, y_1, y_1') - \{f_3(x_2, y_2, y_2') - f_3(x_0, y_0, y_0')\}/2h \\
&\quad + \tfrac{1}{6}h^2 y_1''' f_{23} + (\tfrac{1}{6}hy_1''' + \tfrac{1}{24}h^2 y_1^{\text{iv}}) f_{33}(x_2, y_2, y_2') \\
&\quad - (\tfrac{1}{6}hy_1''' - \tfrac{1}{24}y_1^{\text{iv}}) f_{33}(y_0, y_0, y_0') + O(h^4), \\
&= \left\{f_2(x_1, y_1, y_1') - \frac{d}{dx}f_3(x_1, y_1, y_1')\right\} - \tfrac{1}{6}h^2\frac{d^3}{dx^3}f_3 \\
&\quad + \tfrac{1}{6}h^2 y_1''' f_{23} + \tfrac{1}{3}h^2 y_1'''\frac{d}{dx}f_{33} + \tfrac{1}{12}h^2 y_1^{\text{iv}} f_{33} + O(h^4). \qquad (4.3)
\end{aligned}$$

The first term is again Euler's equation, but this time our error term is in general of order h^2. Experience with second order boundary differential equations then leads us to expect an overall error of $O(h^2)$ which our results on our test problems confirm.

From (4.2) we see that our approximation is the same as would be obtained by approximating Euler's equation by a central difference approximation to the total derivative, using the values of f_3 at $x = 0$ and $2h$ and using the usual approximations to y_0', y_1' and y_2'. It might now appear that Euler's equation would in general prove a better starting point. In fact, however, it would have been difficult to have foreseen some of the computing procedures which we shall later obtain direct from the integral.

5. Approximation 3

This method is very similar to the previous method except that we now use a Gaussian fourth order integration formula instead of Simpson's rule. Thus

$$\begin{aligned}
\int_{x_0}^{x_2} f(x, y, y')dx &= hf(x_1 - h/\sqrt{3}, \\
&\quad (y_0(1 + \sqrt{3}) + 4y_1 + y_2(1 - \sqrt{3}))/6, \\
&\quad (-y_0(2 + \sqrt{3}) + 4y_1 - y_2(2 - \sqrt{3}))/2\sqrt{3}h) \\
&\quad + hf(x_1 + h/\sqrt{3}, \\
&\quad (y_0(1 - \sqrt{3}) + 4y_1 + y_2(1 + \sqrt{3}))/6, \\
&\quad (y_0(2 - \sqrt{3}) - 4y_1 + y_2(2 + \sqrt{3}))/2\sqrt{3}h) \\
&\quad + O(h^5) \qquad (5.1)
\end{aligned}$$

Using this Gaussian integration formula in effect reduces the total number of function evaluations by a third. The integration still has an error of only $O(h^5)$. $y(x_1 - h/\sqrt{3})$, $y(x_1 + h/\sqrt{3})$, $y'(x_1 - h/\sqrt{3})$ and $y'(x + h/\sqrt{3})$ are approximated as well as possible using Lagrangian formulae in terms of y_0, y_1 and y_2.

Our numerical results are again obtained by solving the recurrence relation derived from (5.1) by numerical partial differentiation.

We can again show that the recurrence relation obtained by analytic partial differentation has an error of $O(h^2)$ but we will not give the somewhat lengthy details here. Our method this time corresponds to an approximation to Euler's equation

$$\frac{d}{dx}f_3 - f_2 = 0$$

where the total derivative is derived by evaluating f_3 at $x_1 - h/\sqrt{3}$ and $x_1 + h/\sqrt{3}$. f_2 is this time taken as the mean sum of the values at $x_1 - h/\sqrt{3}$ and $x_1 + h/\sqrt{3}$.

6. Approximation 4

This approximation is fundamentally different from the previous types. Here we divide the range in two and approximate the integral over each section. This gives

$$\begin{aligned}
\int_{x_0}^{x_2} f(x, y, y')dx &= hf((x_0 + x_1)/2, (y_0 + y_2)/2, (y_1 - y_0)/h) \\
&\quad + hf((x_1 + x_2)/2, (y_1 + y_2)/2, (y_2 - y_1)/h) + O(h^3), \qquad (6.1)
\end{aligned}$$

using the midpoint rule over (x_0, x_1) and (x_1, x_2). In contrast to the previous two methods we can extend this approximation to the complete range (a, b). Thus

$$\begin{aligned}
\int_a^b f(x, y, y')dx &= hf(a + h/2, (y_0 + y_1)/2, (y_1 - y_0)/h) \\
&\quad + hf\left(a + \frac{3h}{2}, (y_1 + y_2)/2, (y_2 - y_1)/h\right) \\
&\quad + \ldots + hf(b - h/2, (y_{n-1} + y_n)/2, \\
&\quad (y_n - y_{n-1})/h) + O(h^2). \qquad (6.2)
\end{aligned}$$

We could not have done this in the previous two methods as the intervals then overlapped. This could give us the chance of carrying out our maximization by a different process. For instance we could use a general n-dimensional maximization procedure or use dynamic programming. Such methods appear to be inefficient for the functions we have considered but there may be less regular functions for which they would be useful. In fact our numerical results are still obtained by solving the recurrence relation derived from (6.1) by numerical partial differentiation.

As this is a somewhat different type of approximation we give the details when the analytic partial differentiation is carried out. Thus $\frac{1}{h}\frac{\partial}{\partial y_1}$ (approx. in (6.1))

$$\begin{aligned}
&= \{f_2((x_0 + x_1)/2, (y_0 + y_1)/2, (y_1 - y_0)/h) \\
&\quad + f_2((x_1 + x_2)/2, (y_1 + y_2)/2, (y_2 - y_1)/h)\}/2 \\
&\quad - \{f_3((x_1 + x_2)/2, (y_1 + y_2)/2, (y_2 - y_1)/h) \\
&\quad - f_3((x_0 + x_1)/2, (y_0 + y_1)/2, (y_1 - y_0)/h)\}/h, \qquad (6.3)
\end{aligned}$$

$$= \left(1 + \tfrac{1}{8} h^2 \frac{d^2}{dx^2}\right) f_2(x_1, y_1 + \tfrac{1}{8} h^2 y_1'', y_1' + \tfrac{1}{12} h^2 y_1''')$$
$$- \left(\frac{d}{dx} + \tfrac{1}{12} h^2 \frac{d^3}{dx^3}\right) f_3(x_1, y_1 + \tfrac{1}{8} h^2 y_1'',$$
$$y_1' + \tfrac{1}{12} h^2 y_1''') + O(h^4),$$
$$= \left(1 + \tfrac{1}{8} h^2 \frac{d^2}{dx^2}\right)\left(f_2 - \frac{d}{dx} f_3\right) + \tfrac{1}{24} h^2 \frac{d^3}{dx^3} f_3$$
$$+ \tfrac{1}{8} h^2 y_1'' f_{22} + \tfrac{1}{12} h^2 y_1''' f_{23} - \tfrac{1}{8} h^2 y_1'' f_{32}$$
$$- \tfrac{1}{12} h^2 y_1^{\text{iv}} f_{33} - \tfrac{1}{8} h^2 y_1'' \frac{d}{dx} f_{32}$$
$$- \tfrac{1}{12} h^2 y_1''' \frac{d}{dx} f_{33} + O(h^4). \tag{6.4}$$

In general the error is $O(h^2)$ and our results on our test problems again confirm this. The approximation to Euler's equation, which corresponds to this method, evaluates the total derivative in Euler's equation at $\frac{1}{2}h$ and $\frac{3}{2}h$. It differs from the two previous approximations in that $y(\frac{1}{2}h)$ and $y(\frac{3}{2}h)$ are approximated only in terms of the two nearest co-ordinates and not all three.

7. Approximation 5

As in approximation 4 we divide the range in two but this time we evaluate the integrals using the trapezoidal rule instead of the midpoint rule. This gives

$$2\int_{x_0}^{x_2} f(x, y, y')dx = hf(x_0, y_0, (y_1 - y_0)/h)$$
$$+ hf(x_1, y_1, (y_1 - y_0)/h) + hf(x_1, y_1, (y_2 - y_1)/h)$$
$$+ hf(x_2, y_2, (y_2 - y_1)/h) + O(h^3). \tag{7.1}$$

Using the trapezoidal rule instead of the midpoint rule, however, means that we have doubled the number of function evaluations required to solve the problem. Similar comparisons can be made with Euler's equation but we shall not give the details here. The method can again be used directly over the complete range (a, b).

8. Numerical results

These methods were programmed in ALGOL and then compiled and run on an English Electric KDF 9. This machine represents the mantissa of a real number by 40 bits and the exponent by 8 bits. All the methods call on the user to supply the boundary conditions and an ALGOL procedure for the function f, and to specify the step length h. As a first investigation into these methods the programs were not written to be quite as economical in the number of evaluations of f as they might have been.

All the methods were tried on the four following problems with the stated boundary conditions.

(i) $f = (y')^2 + 12xy, \quad y(0)=0, y(1)=1,$

(ii) $f = (y')^2 - y^2 - 2xy, y(0)=0, y(1)=\sin(1)-1,$

(iii) $$f = (1\cdot 05 - \exp(1 - 4y'))\frac{(1-y)}{(1+y^2)} \times\left(\frac{1}{1 + x\exp(-6(x - 0\cdot 4)^2)}\right) \times\left(2 - \frac{1}{2(1-y)(1 + x\exp(-6(x-0\cdot 4)^2))}\right)$$
$$y(0) = 0\cdot 5, \quad y(1) = 0,$$

(iv) $$f = 4(3 + \sin\pi(\tfrac{1}{2} - x))(-\tfrac{1}{2}y'^2 - 3y') - (\tfrac{4}{3}y)^4,$$
$$y(0) = 1, \qquad y(1) = 0.$$

In addition Euler's equation for problem (iv) was solved using a standard central difference approximation.

Problems (i) and (ii) give rise to linear differential equations with solutions x^3 and $\sin x - x$, respectively, and were used, therefore, more to test the methods for programming errors than for comparing their efficiency. In particular they belong to the special case for which approximation gives an error $O(h^2)$ as will be seen from (3.3). Methods 2 to 5 gave predicted results. As the solution to (ii) is x^3 all the methods gave exact results (within round-off error) for any value of h. This gave us a chance to look at the round-off error by itself. As we expected, it appeared to be negligible, being only a little larger than the last place of decimals.

Problem (iii) arises from the question of how a ship should use its fuel in order to cross an ocean in a minimum time. The way the problem arises assures us of a well-behaved solution. The analytic solution is not known, but when the various methods are plotted for various values of h the true solution is taken to be a very obvious limit as h becomes smaller. Euler's equation for this function is so large and complicated that its numerical solution would be very difficult. In **Table 1** are shown the errors at $x = 0\cdot 5$ for the various methods and for different values of h. The errors are only approximate. The error for $h = 0\cdot 1$ with approximation 1 was not calculated. Errors at other points were similar, although approximations 2 and 5 showed up in a slightly better light. Clearly approximations 2 to 5 have an overall error of $O(h^2)$ and approximation 1 an overall error of $O(h)$. Richardson's extrapolation could have been used to obtain yet moıe accurate results.

Problem (iv) represents an inventory problem. This again assures us of a well-behaved solution. In this case Euler's equation is comparatively simple, and our methods were compared with a standard method of solving the differential equation using the central difference formulae $y_i'' = (y_{i-1} - 2y_i + y_{i+1})/h^2$ and $y_i' = (y_{i+1} - y_{i-1})/2h$. In **Table 2** are shown the errors at $x = 0\cdot 5$ for three values of h. Again the error for larger values of h with approximation 1 was not calculated. Errors at other points were quite similar although the error in Euler's equation was less in some places.

Several values of ϵ were tried and it was found that

Table 1

Errors at midpoint for problem (iii)

	$h = 0{\cdot}1$	$h = 0{\cdot}05$	$h = 0{\cdot}025$	$h = 0{\cdot}0125$
Approximation 1		−0·000900	−0·000400	−0·000200
Approximation 2	−0·000245	−0·000061	−0·000014	−0·000004
Approximation 3	0·000072	0·000021	0·000007	0·000001
Approximation 4	0·000078	0·000022	0·000007	0·000002
Approximation 5	−0·000295	−0·000072	−0·000016	−0·000004

values in the range $10^{-5} \leqslant |\epsilon| \leqslant 10^{-4}$ gave nearly identical results for each method and function. At each stage the recurrence relation was solved to 10 decimal accuracy, more than adequate for the final accuracy we wished to achieve. For these functions five or six trial runs were necessary before the correct value of y_1 could be found to give the correct boundary condition on y_n. The number of trial runs was naturally independent of the method.

Table 2

Errors at midpoint for problem 4

	$h = 0{\cdot}05$	$h = 0{\cdot}025$	$h = 0{\cdot}0125$
Approximation 1			0·001000
Approximation 2	0·000644	0·000157	0·000038
Approximation 3	−0·000240	−0·000073	−0·000019
Approximation 4	−0·000293	−0·000083	−0·000023
Approximation 5	0·000574	0·000142	0·000032
Euler's equation	−0·000369	−0·000093	−0·000025

9. Comparison of methods

In comparing accuracy we see that approximation 1 (Euler's) would be much too inaccurate for most problems. There is little difference between approximations 2 to 5 although 3 and 4 seem slightly better.

To compare the efficiency, however, we must also compare the amount of computing done in each method.

As we said before the number of trial runs with different values of y_1 is independent of the method so we merely compare the amount of work done at each stage. The bulk of the computing work is done in evaluating the function, and we will only in fact consider this. Suppose we must do q times as much work to solve the associated function in Euler's equation. The first column in **Table 3** then shows the number of function evaluations (or the equivalent) necessary to evaluate the recurrence relation. It usually took three evaluations of the recurrence relations to solve them, so

Table 3

No. of function evaluations

Approximation 1	4	12	8	5
Approximation 2	6	18	18	12
Approximation 3	4	12	12	8
Approximation 4	4	12	8	5
Approximation 5	8	24	16	10
Euler's equation	q	$3q$	$3q$	$3q$

the second column, being three times the first, is the number of function evaluations used per step. However, the methods were not programmed quite as efficiently as they might have been as sometimes the evaluation of a function was duplicated in evaluating the recurrence relation again. The third column shows the number if this saving had been made. The fourth column shows the number of function evaluations necessary if we had approximated our partial differentiation by (2.2). Such a method might, however, have led to significant round-off error.

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.

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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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