

A Multistep Generalization of the Fourth Order

Runge Kutta Method *

by

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Abstract. To obtain high order integration methods for ordinary differential equations which combine to some extent the advantages of Runge-Kutta methods on one hand and linear multistep methods on the other, the use of "modified multistep" or "hybrid" methods has been proposed [1], [2], [3]. In this paper formulae are derived for methods which use one extra intermediate point than in the previously published methods so that they are analogues of the fourth order Runge-Kutta method.

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Introduction

In papers by Gragg and Stetter [1], by the present author [2], and by Gear [3], integration processes were considered which combine features of both Runge-Kutta methods and multi-step methods. In fact these new methods were multi-step analogues to third order Runge-Kutta methods in that one additional derivative calculation was made at some point between steps. There is no reason in principle why more than one of these additional evaluations should not be made and in the present paper the case of two evaluations is considered. It is found that an order of accuracy $2k + 2$ is possible and examples of processes where this order is achieved and which are stable exist for $k = 1, 2, \dots, 15$. Detailed formulae for some of these cases are given for $k = 2, 3, 4$.

The initial value problem whose numerical solution is sought will be written as

$$\frac{dy}{dx} = f(x,y) , \quad y(x_0) = y_0 \quad (1)$$

where y, f are vectors with N components. For some purposes it is more convenient to consider the autonomous system

$$\frac{dy}{dx} = \underline{f}(y) , \quad \underline{y}(x_0) = \underline{y}_0 \quad (2)$$

where \underline{y} is the vector (x, y) with $N + 1$ components, $\underline{f} = (1, f(x, y))$ and $\underline{y}_0 = (x_0, y_0)$.

The Corrector Formula.

Postponing for the present considerations as to how y_{n-u}, y_{n-v} are to be computed, we write

$$y_n = \sum_{j=1}^k A_j y_{n-j} + h \left(b_1 f_{n-u} + b_2 f_{n-v} + \sum_{j=0}^k B_j f_{n-j} \right) \quad (3)$$

for the formula with which $y_n = y(x_0 + nh)$ is to be computed. f_j for any subscript j denotes $f(x_0 + jh, y_j)$. If u, v are given constants, there are $2k + 3$ coefficients $A_1, A_2, \dots, A_k, b_1, b_2, B_0, B_1, \dots, B_k$ to be chosen so we shall seek values of these coefficients so that

$$0 = -p(0) + \sum_{j=1}^k A_j p(-hX_j) + h(b_1 p'(-hx_1) + b_2 p'(-hx_2) + \sum_{j=0}^k B_j p'(-hX_j)) \quad (4)$$

for all polynomials p of degree $\leq 2k + 2$ where $x_1, x_2, X_0 = 0, X_1, \dots, X_k$ are distinct real numbers and h is a constant. We will recover the coefficients in (3) by writing $x_1 = u, x_2 = v, X_j = j$ ($j = 1, 2, \dots, k$).

Consider the function

$$\varphi(z) = -\frac{1}{z} + \sum_{j=1}^k \frac{A_j}{z+hX_j} + h \left\{ \frac{b_1}{(z+hx_1)^2} + \frac{b_2}{(z+hx_2)^2} + \sum_{j=0}^k \frac{B_j}{(z+hX_j)^2} \right\} \quad (5)$$

so that the integral $L(p)$ given by

$$L(p) = \frac{1}{2\pi i} \int_C p(z) \varphi(z) dz \quad (6)$$

where C is a counterclockwise circle with centre 0 and radius $R > \max(|hx_1|, |hx_2|, |hX_1|, \dots, |hX_k|)$, expresses the error in (4) for a polynomial p . For $L(p)$ to vanish for $p(z)$ any polynomial of degree $\leq 2k + 2$ it is clearly necessary and sufficient that

$$|\varphi(z)| = O(|z|^{-2k-4}) \quad (7)$$

as $|z| \rightarrow \infty$.

If we write

$$\varphi(z) = \frac{K \prod_{j=1}^k X_j^2 h^{2k+2}}{z^2 \prod_{j=1}^k (z+hX_j)^2} \left(\frac{1}{z+hX_1} + \frac{hU}{2(z+hX_1)^2} - \frac{1}{z+hX_2} - \frac{hV}{2(z+hX_2)^2} \right) \quad (8)$$

we see that (7) is satisfied and that (8) is of the form of (5) if the constant U, V, K are chosen so that the residues of $\varphi(z)$ (given by (8)) at $z = -hx_1$ and at $z = -hx_2$ are zero and so that the residue at $z = 0$ is -1 . Assuming that $x_1, x_2, X_1, X_2, \dots, X_k$ do not have values such that one of the right hand sides of (9), (10), or (11) vanishes we find

$$\frac{1}{U} = \sum_{j=0}^k \frac{1}{X_j - x_1} \quad (9)$$

$$\frac{1}{V} = \sum_{j=0}^k \frac{1}{X_j - x_2} \quad (10)$$

$$\frac{1}{K} = \sum_{j=1}^k \frac{1}{X_j} \cdot \left(\frac{2}{x_1} + \frac{U}{x_1^2} - \frac{2}{x_2} - \frac{V}{x_2^2} \right) + \frac{1}{x_1^2} + \frac{U}{x_1^3} - \frac{1}{x_2^2} - \frac{V}{x_2^3} \quad (11)$$

Writing (8) in partial fractions and comparing with (5) we find

$$b_1 = \frac{KU}{2x_1^2} \prod_{j=1}^k \left(\frac{X_j}{X_j - x_1} \right)^2 \quad (12)$$

$$b_2 = -\frac{KV}{2x_2^2} \prod_{j=1}^k \left(\frac{X_j}{X_j - x_2} \right)^2 \quad (13)$$

$$B_j = K \prod_{i=1}^k \left(\frac{X_i}{X_i - X_j} \right)^2 \left(-\frac{1}{X_j - x_1} + \frac{U}{2(X_j - x_1)^2} + \frac{1}{X_j - x_2} - \frac{V}{2(X_j - x_2)^2} \right) \quad (14)$$

$$A_j = K \prod_{i=1}^k \left(\frac{X_i}{X_i - X_j} \right)^2 \left(-\frac{1}{(X_j - x_1)^2} + \frac{U}{(X_j - x_1)^3} + \frac{1}{(X_j - x_2)^2} - \frac{V}{(X_j - x_2)^3} \right) \\ - 2B_j \sum_{i=0}^k \frac{1}{X_i - X_j} \quad (15)$$

where the prime on $\prod_{i=1}^k$, and $\sum_{i=0}^k$ indicates that the subscript $i=j$

is to be excluded from the product or sum.

At this stage it is convenient to examine the error in (4) when $p(x)$ is not a polynomial of degree $2k+2$. We will suppose that $p(x) \in C^{2k+4} [a, b]$ where $[a, b]$ contains $0, -hx_1, -hx_2, -hX_1, \dots, -hX_k$. We can expand $p(-hX_1), p(-hX_2), \dots, p(-hX_k), hp'(-hX_1), hp'(-hX_2), \dots, hp'(-hX_k), hp'(-hx_1), hp'(-hx_2)$ in Taylor series about 0 up to terms in $p^{(2k+3)}(0)$ with remainder terms $O(h^{2k+4})$ as $h \rightarrow 0$.

Substitute into the right hand side of (4) and we obtain, since $A_1, A_2, \dots, A_k, b_1, b_2, B_0, B_1, \dots, B_k$ were chosen to make this expression zero for a polynomial of degree $2k+2$, only an expression $\epsilon p^{(2k+3)}(0)h^{2k+3} + O(h^{2k+4})$, where ϵ is a constant. To determine ϵ we write

$$p(z) = z^3 \prod_{j=1}^k (z + hX_j)^2, \text{ for which } p^{(2k+3)}(0) = (2k+3)!. \text{ We now}$$

have

$$h^{2k+3}(2k+3)! \epsilon = \frac{1}{2\pi i} \int_C K \prod_{j=1}^k X_j^2 h^{2k+2} z \left(\frac{1}{z+hx_1} + \frac{hU}{2(z+hx_1)^2} \right. \\ \left. - \frac{1}{z+hx_2} - \frac{hV}{2(z+hx_2)^2} \right) dz \quad (16)$$

from which

$$\epsilon = \frac{K \prod_{j=1}^k X_j^2}{(2k+3)!} (x_2 - x_1 + \frac{1}{2} (U - V)) \quad (17)$$

By applying this argument to every component of y in turn we find the error in (3) to be $\epsilon y^{(2k+3)}(x_n) h^{2k+3} + o(h^{2k+4})$.

To find the coefficients in (3) we now write $x_1 = u$, $x_2 = v$, $X_j = j$ ($j = 1, 2, \dots, k$). We find

$$1/U = \sum_{j=0}^k \frac{1}{j-u} \quad (18)$$

$$1/V = \sum_{j=0}^k \frac{1}{j-v} \quad (19)$$

$$1/K = H_k \left(\frac{2}{u} + \frac{U}{u^2} - \frac{2}{v} - \frac{V}{v^2} \right) + \frac{1}{u^2} + \frac{U}{u^3} - \frac{1}{v^2} - \frac{V}{v^3} \quad (20)$$

where $H_k = 1 + \frac{1}{2} + \dots + \frac{1}{k}$, $k > 0$, $H_0 = 0$.

We have

$$b_1 = \frac{KU}{2u^2} \frac{k!^2}{\prod_{j=1}^k (j-u)^2} \quad (21)$$

$$b_2 = -\frac{KV}{2v^2} \frac{k!^2}{\prod_{j=1}^k (j-v)^2} \quad (22)$$

$$B_j = K \binom{k}{j}^2 \left(-\frac{1}{(j-u)} + \frac{U}{2(j-u)^2} + \frac{1}{(j-v)} - \frac{V}{2(j-v)^2} \right) \quad (23)$$

$$A_j = K \binom{k}{j}^2 \left(-\frac{1}{(j-u)^2} + \frac{U}{(j-u)^3} + \frac{1}{(j-v)^2} - \frac{V}{(j-v)^3} \right) + 2B_j (H_j - H_{k-j}) \quad , \quad (24)$$

and the "error constant" ϵ is given by

$$\epsilon = \frac{K(k!)^2}{(2k+3)!} \left(v - u + \frac{U-V}{2} \right) .$$

Stability Considerations

So far the only restrictions that are imposed on the parameter u, v are that they are not equal, that each differs from each of the integers $0, 1, 2, \dots, k$ and that the right hand sides of (18), (19), (20) do not vanish. However, for a given k , it may happen that some combinations of u, v do not yield a formula (3) which is stable when used as a final "corrector". Excluding the "principal root" at 1, let R be the greatest magnitude for a root of the equation,

$$z^k - A_1 z^{k-1} - A_2 z^{k-2} - \dots - A_k = 0 \quad (26)$$

R is a convenient measure of the stability of the formula: if $R < 1$ the method is (asymptotically) stable and if $R > 1$ it is unstable.

For $k = 1$ only the principal root is present. For $k = 2$ it is found that $R = |(15uv - 7(u+v) + 4)/(15uv - 23(u+v) + 36)|$.

For higher k it has seemed most convenient to study R as a function of u, v numerically. For $k = 2$ it happens that $R < 1$ whenever

$u, v \in (0,1)$. Figure 1 shows the contour lines $R = 1$ for $k = 3, 4, 5, 6, 7, 8$ and $u, v \in (0,1)$. For each curve, the value of the corresponding k is written beside it. Here a convention is adopted in that the side of the curve where k is written corresponds to the region to which $R < 1$. We see from this figure, that the region for which u, v give stability tends to decrease in area as k increases. The same pattern continues up to $k = 15$ but there does not appear to be any region where $R < 1$ for $k = 16$. To illustrate the behaviour of R for $k = 6, 7, \dots, 15$ figures 2 and 3 are presented. As u varies from .51 to .64 the values of v which minimize R and the values of the minimum R have been computed. Since the v which minimizes R is approximately $.3u$ it was found convenient to plot $v - .3u$ as a function of u (figure 2). The minimum value of R is plotted in figure 3.

The Predictor Formulae

We now consider a method for computing the values of y_{n-u}, y_{n-v} and the "predicted" value of y_n . The formulae proposed are

$$y_{n-u} = \sum_{j=1}^k A_{1j} y_{n-j} + h \sum_{j=1}^k B_{1j} f_{n-j} \quad (27)$$

$$y_{n-v} = \sum_{j=1}^k A_{2j} y_{n-j} + h \left(b_{21} f_{n-u} + \sum_{j=1}^k B_{2j} f_{n-j} \right) \quad (28)$$

$$y_n = \sum_{j=1}^k A_{3j} y_{n-j} + h \left(b_{31} f_{n-u} + b_{32} f_{n-v} + \sum_{j=1}^k B_{3j} f_{n-j} \right) \quad (29)$$

Before we consider the choice of the coefficients occurring in (27), (28),

(29) we generalize the problem to that of unequally spaced points in the same way as for the "corrector formula". We shall thus consider the overall procedure for finding $\tilde{y}(0)$ from $\tilde{y}(-hX_1), \tilde{y}(-hX_2), \dots, \tilde{y}(-hX_k)$ using the formulae

$$\tilde{y}(-hx_1) = \sum_{j=1}^k A_{1j} \tilde{y}(-hX_j) + h \sum_{j=1}^k B_{1j} f(\tilde{y}(-hX_j)) \quad , \quad (30)$$

$$\tilde{y}(-hx_2) = \sum_{j=1}^k A_{2j} \tilde{y}(-hX_j) + h \left(b_{21} f(\tilde{y}(-hx_1)) + \sum_{j=1}^k B_{2j} f(\tilde{y}(-hX_j)) \right) \quad , \quad (31)$$

$$\hat{\tilde{y}}(0) = \sum_{j=1}^k A_{3j} \tilde{y}(-hX_j) + h \left(b_{31} f(\tilde{y}(-hx_1)) + b_{32} f(\tilde{y}(-hx_2)) + \sum_{j=1}^k B_{3j} f(\tilde{y}(-hX_j)) \right) \quad , \quad (32)$$

$$\tilde{\tilde{y}}(0) = \sum_{j=1}^k A_j \tilde{y}(-hX_j) + h \left(b_1 f(\tilde{y}(-hx_1)) + b_2 f(\tilde{y}(-hx_2)) + b_3 f(\hat{\tilde{y}}(0)) + \sum_{j=1}^k B_j f(\tilde{y}(-X_j)) \right) \quad . \quad (33)$$

where we have written b_3 in place of B_0 .

We can choose the coefficients in (30) so that $\tilde{y}(-hx_1)$ is given exactly when the components of $\tilde{y}(x)$ are polynomials of degree $2k-1$. When this is done, suppose the error can be written in the form

$$\epsilon_1 \tilde{y}^{(2k)}(0) h^{2k} + \epsilon_1 \tilde{y}^{(2k+1)}(0) h^{2k+1} + \epsilon_1 \tilde{y}^{(2k+2)}(0) h^{2k+2} + o(h^{2k+3}).$$

The same is true for (31), (32), and we suppose that the error for these formulae can be written in the same form (with subscripts 2, 3, respectively

on the ϵ 's) where it is supposed that exact values are used for all quantities on the right hand sides. If exact quantities are used on the right hand side of (33) the error in this quantity is $\epsilon \tilde{y}^{(2k+3)}(0)$ $h^{2k+3} + o(h^{2k+4})$ where ϵ is given by (17). Using the same type of calculation as in [2] we now find the total error in $\tilde{y}(0)$, the approximation to $y(0)$ due to all sources. It is given by

$$\begin{aligned}
\tilde{y}(0) - y(0) = & h^{2k+1} \left\{ b_1 \epsilon_1^{(2k)} + b_2 \epsilon_2^{(2k)} + b_3 \epsilon_3^{(2k)} \right\} \frac{\partial f}{\partial y} \tilde{y}^{(2k)} \\
& + h^{2k+2} \left\{ \left[b_1 \epsilon_1^{(2k+1)} + b_2 \epsilon_2^{(2k+1)} + b_3 \epsilon_3^{(2k+1)} \right] \frac{\partial f}{\partial y} \tilde{y}^{(2k+1)} \right. \\
& \quad + \left[b_2 b_{21} \epsilon_1^{(2k)} + b_3 b_{31} \epsilon_1^{(2k)} + b_3 b_{32} \epsilon_2^{(2k)} \right] \left(\frac{\partial f}{\partial y} \right)^2 \tilde{y}^{(2k)} \\
& \quad \left. - \left[b_1 x_1 \epsilon_1^{(2k)} + b_2 x_2 \epsilon_2^{(2k)} \right] \frac{\partial^2 f}{\partial y^2} \tilde{y}^{(2k)} \right\} \\
& + h^{2k+3} \left\{ \left[b_1 \epsilon_1^{(2k+2)} + b_2 \epsilon_2^{(2k+2)} + b_3 \epsilon_3^{(2k+2)} \right] \frac{\partial f}{\partial y} \tilde{y}^{(2k+2)} \right. \\
& \quad \left. + \epsilon y^{(2k+3)} \right\} \\
& + h^{2k+3} \left\{ \left[b_2 b_{21} \epsilon_1^{(2k+1)} + b_3 b_{31} \epsilon_1^{(2k+1)} + b_3 b_{32} \epsilon_2^{(2k+1)} \right] \left(\frac{\partial f}{\partial y} \right)^2 \tilde{y}^{(2k+1)} \right. \\
& \quad \left. - \left[b_1 x_1 \epsilon_1^{(2k+1)} + b_2 x_2 \epsilon_2^{(2k+1)} \right] \frac{\partial^2 f}{\partial y^2} \tilde{y}^{(2k+1)} \right\} \\
& + h^{2k+3} \left\{ b_3 b_{32} b_{21} \epsilon_1^{(2k)} \left(\frac{\partial f}{\partial y} \right)^3 \tilde{y}^{(2k)} \right. \\
& \quad \left. - b_2 x_2 b_{21} \epsilon_1^{(2k)} \frac{\partial^2 f}{\partial y^2} \tilde{y} \frac{\partial f}{\partial y} \tilde{y}^{(2k)} \right\}
\end{aligned}$$

$$\begin{aligned}
& + h^{2k+3} \left\{ \frac{1}{2} \left(b_1 x_1^2 \epsilon_1^{(2k)} + b_2 x_2^2 \epsilon_2^{(2k)} \right) \left(\frac{\partial^3 f}{\partial y^3} f_y^2(2k) + \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f_y(2k) \right) \right. \\
& \quad - \left[\left(b_2 b_{21} + b_3 b_{31} \right) x_1 \epsilon_1^{(2k)} \right. \\
& \quad \left. \left. + b_3 b_{32} x_2 \epsilon_2^{(2k)} \right] \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f_y(2k) \right\} \\
& + \frac{1}{2} h^{4k+1} \left\{ b_1 \left(\epsilon_1^{(2k)} \right)^2 + b_2 \left(\epsilon_2^{(2k)} \right)^2 + b_3 \left(\epsilon_3^{(2k)} \right)^2 \frac{\partial^2 f}{\partial y^2} \left(y^{(2k)} \right)^2 \right. \\
& \left. + o \left(h^{2k+4} \right) \right\} \tag{34}
\end{aligned}$$

In this expression, the various factors involving derivatives of y and f are supposed to be evaluated at $y = y(0)$. As in [2], the various products of such factors are to be interpreted in a conventional way. Thus one would associate with $y^{(n)}$, f , $\frac{\partial f}{\partial y}$, $\frac{\partial^2 f}{\partial y^2}$, ..., the tensors $y^{(n)i}$, f^i , $f_j^i (= \frac{\partial f^i}{\partial y^j})$, f_{jk}^i , Two tensors in juxtaposition are supposed contracted over subscripts in the first member and superscripts in the second in such a way that the terms actually occurring above have only one non-contracted superscript. Note that a term of order h^{4k+1} is present in (34). When $k > 1$ this term could be absorbed into $o(h^{2k+4})$.

If the method is to be accurate to terms in h^{2k+2} then we see from (34) that

$$b_1 \epsilon_1^{(2k)} + b_2 \epsilon_2^{(2k)} + b_3 \epsilon_3^{(2k)} = 0 \tag{35}$$

$$b_1 \epsilon_1^{(2k+1)} + b_2 \epsilon_2^{(2k+1)} + b_3 \epsilon_3^{(2k+1)} = 0 \tag{36}$$

$$b_2 b_{21} \epsilon_1^{(2k)} + b_3 b_{31} \epsilon_1^{(2k)} + b_3 b_{32} \epsilon_2^{(2k)} = 0 \quad (37)$$

$$b_1 x_1 \epsilon_1^{(2k)} + b_2 x_2 \epsilon_2^{(2k)} = 0 \quad (38)$$

We now derive formulae for the coefficients in (30) and (31) so that these are accurate for polynomials of degree $2k-1$ and so that (35) is satisfied. We then find formulae for the coefficients in (32) so that this is also accurate for polynomials of degree $2k-1$ and so that (36), (37) and (38) are satisfied.

By analogy with (5) we write

$$\varphi_1(z) = -\frac{1}{z+hx_1} + \sum_{j=1}^k \frac{A_{1j}}{z+hX_j} + h \sum_{j=1}^k \frac{B_{1j}}{(z+hX_j)^2} \quad (39)$$

$$\varphi_2(z) = -\frac{1}{z+hx_2} + \sum_{j=1}^k \frac{A_{2j}}{z+hX_j} + h \left(\frac{b_{21}}{(z+hx_1)^2} + \sum_{j=1}^k \frac{B_{2j}}{(z+hX_j)^2} \right) \quad (40)$$

$$\varphi_3(z) = -\frac{1}{z} + \sum_{j=1}^k \frac{A_{3j}}{z+hX_j} + h \left(\frac{b_{31}}{(z+hx_1)^2} + \frac{b_{32}}{(z+hx_2)^2} + \sum_{j=1}^k \frac{B_{3j}}{(z+hX_j)^2} \right) \quad (41)$$

and

$$L_j(p) = \frac{1}{2\pi i} \int_C p(z) \varphi_j(z) dz, \quad j = 1, 2, 3 \quad (42)$$

so that $L_1(p)$, $L_2(p)$, $L_3(p)$ is the error in (39), (40), (41) respectively for a polynomial $p(z)$. $L_j(p)$ is to vanish identically for $j = 1, 2, 3$ when $p(z)$ is of degree $2k-1$. Hence,

$$|\varphi_j(z)| = O(|z|^{-2k-1}), \quad j = 1, 2, 3. \quad (43)$$

It is clear that $\varphi_1(z)$ must be given by

$$\varphi_1(z) = - \frac{h^{2k} \prod_{j=1}^k (x_1 - X_j)^2}{z + hx_1 \prod_{j=1}^k (z + hX_j)^2} \quad (44)$$

where the numerator has been chosen so that the residue at $z = -hx_1$ equals -1 .

Thus

$$B_{1j} = \frac{\prod_{\ell=1}^k (x_1 - X_\ell)^2}{(X_j - x_1) \prod_{\ell=1}^k (X_j - X_\ell)^2} \quad (45)$$

$$A_{1j} = B_{1j} \left(\frac{1}{X_j - x_1} + 2 \sum_{\ell=1}^k \frac{1}{X_j - X_\ell} \right) \quad (46)$$

We write $\varphi_2(z)$ in the form

$$\varphi_2(z) = - \frac{h^{2k} \prod_{j=1}^k (x_2 - X_j)^2}{(z + hx_2) \prod_{j=1}^k (z + hX_j)^2} \left(P + hQ \left(\frac{1}{z + hx_1} + \frac{hR}{(z + hx_1)^2} \right) \right) \quad (47)$$

so that

$$B_{2j} = \frac{\prod_{\ell=1}^k (x_2 - X_\ell)^2}{(X_j - x_2) \prod_{\ell=1}^k (X_j - X_\ell)^2} \left(P + Q \left(\frac{1}{x_1 - X_j} + \frac{R}{(x_1 - X_j)^2} \right) \right) \quad (48)$$

$$A_{2j} = \frac{\prod_{\ell=1}^k (x_2 - X_\ell)^2}{(X_j - x_2) \prod_{\ell=1}^k (X_j - X_\ell)^2} \left(- \frac{Q}{(X_j - x_1)^2} + \frac{2QR}{(X_j - x_1)^3} \right) + B_{2j} \left(2 \sum_{\ell=1}^k \frac{1}{X_j - X_\ell} + \frac{1}{X_j - x_2} \right) \quad (49)$$

$$b_{21} = \frac{QR \prod_{j=1}^k (x_2 - X_j)^2}{(x_1 - x_2) \prod_{j=1}^k (x_1 - X_j)^2} \quad (50)$$

The form for $\varphi_2(z)$ given by (47) has the correct behavior at infinity and at $-hX_1, -hX_2, \dots, -hX_k, -hx_1, -hx_2$. However, P, Q, R must be fixed so that the residue at $-hx_1$ is 0 and the residue at $-hx_2$ is -1 .

We thus have

$$\frac{1}{R} = \frac{1}{x_2 - x_1} + 2 \sum_{j=1}^k \frac{1}{X_j - x_1} = \frac{2}{U} + \frac{2}{x_1} + \frac{1}{x_2 - x_1} \quad (51)$$

$$P + Q \left(\frac{1}{x_1 - x_2} + \frac{R}{(x_1 - x_2)^2} \right) = 1 \quad (52)$$

To obtain a third equation for P, Q, R we use (38). In the same way as for ϵ we obtain for $\epsilon_j^{(2k)}$, $j=1, 2$ the expression

$$\epsilon_j^{(2k)} = \frac{h^{-2k}}{2\pi i (2k)!} \int_C \prod_{j=1}^k (z + hX_j)^2 \cdot \varphi_j(z) dz \quad (53)$$

so that

$$\epsilon_1^{(2k)} = - \frac{1}{(2k)!} \prod_{j=1}^k (x_1 - X_j)^2 \quad (54)$$

$$\epsilon_2^{(2k)} = - \frac{P}{(2k)!} \prod_{j=1}^k (x_2 - X_j)^2 \quad (55)$$

Using the expressions (21), (22) for b_1, b_2 and substituting in (38)

we find

$$P = \frac{x_2 U}{x_1 V} \quad (56)$$

$\varphi_2(z)$ is now determined. We must now choose $\varphi_3(z)$ of such a form that (35), (36), (37) are satisfied. This can be done by defining $\varphi_3(z)$ by the equation

$$b_1\varphi_1(z) + b_2\varphi_2(z) + b_3\varphi_3(z) + \frac{z}{h}\varphi(z) = 0 \quad (57)$$

To see this, we observe that $\varphi_3(z)$ defined thus has the correct behavior at $-hx_1$, $-hx_2$, 0 , $-hX_1$, $-hX_2$, \dots , $-hX_k$ and at infinity. To see that (35) and (36) are satisfied we see that

$$\epsilon_j^{(2k+m)} = \frac{h^{-2k-m}}{2\pi i (2k+m)!} \int_C z^{2k+m} \varphi_j(z) dz \quad (58)$$

for $m = 0, 1$ and $j = 1, 2, 3$. Making use of (57) we see that

$$\sum_{j=1}^k b_j \epsilon_j^{(2k+m)} = - \frac{h^{-2k-m-1}}{2\pi i (2k+m)!} \int_C z^{2k+m+1} \varphi(z) dz = 0 \quad (59)$$

since $|\varphi(z)| = O(|z|^{-2k-4})$ as $|z| \rightarrow \infty$. To see that (37) is satisfied, we multiply (57) by $(z+hx_1)^2/h$ and by $(z+hx_2)^2/h$ and take the limits as $z \rightarrow -hx_1$ and $z \rightarrow -hx_2$ respectively. We find

$$b_2 b_{21} + b_3 b_{31} - x_1 b_1 = 0 \quad , \quad (60)$$

$$b_3 b_{32} - x_2 b_2 = 0 \quad , \quad (61)$$

so that (37) follows immediately from (38). Using (57) we now list expressions for all the coefficients in (32).

$$A_{3j} = \frac{1}{b_3} (x_j A_j - b_1 A_{1j} - b_2 A_{2j} - B_j) \quad , \quad (62)$$

$$B_{3j} = \frac{1}{b_3} (x_j B_j - b_1 B_{1j} - b_2 B_{2j}) \quad , \quad (63)$$

$$b_{31} = \frac{1}{b_3} (x_1 b_1 - b_2 b_{21}) \quad , \quad (64)$$

$$b_{32} = \frac{1}{b_3} x_2 b_2 \quad . \quad (65)$$

The Truncation Error

In this section we shall find expressions for the coefficients in the asymptotic error term which we see from (34) to have the form h^{2k+3}

$$\left\{ c_1 y^{(2k+3)} + c_1' \frac{\partial f}{\partial y} y^{(2k+2)} + c_2 \left(\frac{\partial f}{\partial y} \right)^2 y^{(2k+1)} - c_2' \frac{\partial^2 f}{\partial y^2} y^{(2k+1)} \right. \\ \left. + c_3 \left(\frac{\partial f}{\partial y} \right)^3 y^{(2k)} - c_3' \frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(2k)} + \frac{1}{2} c_4 \left(\frac{\partial^3 f}{\partial y^3} f^2 y^{(2k)} + \frac{\partial^2 f}{\partial y^2} f y^{(2k)} \right) \right. \\ \left. - c_4' \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f y^{(2k)} \right\}$$

where we have supposed $k > 1$ and the c 's are

given by (34). From (57) we immediately find $c_1' = - (2k+3) c_1 = - (2k+3) \epsilon$.

From (60), (61), we find that $c_2 = c_2'$, $c_3 = c_3'$, $c_4 = c_4'$. c_2 is given by

$$c_2 = b_1 x_1 \epsilon_1^{(2k+1)} + b_2 x_2 \epsilon_2^{(2k+1)} \\ = \frac{h^{-2k-1}}{2\pi i (2k+1)!} \oint_C [b_1 x_1 \phi_1(z) + b_2 x_2 \phi_2(z)] z^{2k+1} dz \quad (66)$$

Since $\oint_C (b_1 x_1 \phi_1(z) + b_2 x_2 \phi_2(z)) p(z) dz = 0$ when $p(z)$ is any polynomial

of degree $2k$, we may replace z^{2k+1} in (66) by any polynomial with the same leading term. We choose the polynomial $(z+hx_1) \prod_{j=1}^k (z+hX_j)^2$

so that

$$c_2 = - \frac{b_2 x_2 \prod_{j=1}^k (x_2 - X_j)^2}{(2k+1)!} [P(x_1 - x_2) + Q] \quad (67)$$

To find $c_3 = b_2 x_2 b_{21} \epsilon_1^{(2k)}$ we evaluate $\epsilon_1^{(2k)} = (h^{-2k}/2\pi i(2k)!)$

$\int_C \phi_1(z) \prod_{j=1}^k (z+hX_j)^2$ to find

$$c_3 = - \frac{b_2 x_2 b_{21}}{(2k)!} \prod_{j=1}^k (x_1 - X_j)^2 \quad (68)$$

Finally we find $c_4 = b_1 x_1^2 \epsilon_1^{(2k)}$ by making use of (38) and the value of $\epsilon_1^{(2k)}$ to give

$$c_4 = - \frac{b_1 x_1 (x_1 - x_2)}{(2k)!} \prod_{j=1}^k (x_1 - X_j)^2 \quad (69)$$

Particular Methods

By writing $X_1 = 1, X_2 = 2, \dots, X_k = k$ we obtain expressions for coefficients in (27), (28), (29), so that practical methods may be devised. However, other values of X_1, X_2, \dots, X_k would be used for such special needs as changing the step size in the middle of the solution to a problem. For the methods about to be given explicitly, we shall restrict ourselves to the simple case. Since the complexity of the coefficients increases

rapidly with k , we restrict ourselves to $k = 2, 3, 4$. For each such value of k we have selected two methods: with $(u, v) = (\frac{2}{3}, \frac{1}{3})$ and $(u, v) = (\frac{1}{2}, \frac{1}{4})$. For $k = 2$ the two methods are

$$y_{n-2/3} = (16y_{n-1} + 11y_{n-2})/27 + h(16f_{n-1} + 4f_{n-2})/27 \quad (70)$$

$$y_{n-1/3} = (47y_{n-1} - 20y_{n-2})/27 + h(27f_{n-2/3} - 22f_{n-1} - 7f_{n-2})/27 \quad (71)$$

$$\hat{y}_n = (-13y_{n-1} + 23y_{n-2})/10 + h(108f_{n-1/3} - 189f_{n-2/3} + 284f_{n-1} + 61f_{n-2})/80 \quad (72)$$

$$\begin{aligned} \tilde{y}_n = (48y_{n-1} + y_{n-2})/49 + h(160\hat{f}_n + 648f_{n-1/3} + 405f_{n-2/3} + 280f_{n-1} \\ + 7f_{n-2})/1470 \end{aligned} \quad (73)$$

with truncation error

$$\begin{aligned} \tilde{y}_n - y(x_n) = h^7 \left\{ \frac{4}{416745} \left(\tilde{y}^{(7)} - 7 \frac{\partial f}{\partial y} \tilde{y}^{(6)} \right) + \frac{26}{99225} \left(\frac{\partial^2 f}{\partial x^2} \tilde{y}^{(5)} - \left(\frac{\partial f}{\partial y} \right)^2 \tilde{y}^{(5)} \right) \right. \\ \left. + \frac{8}{6615} \left(\frac{\partial^2 f}{\partial x^2} f \frac{\partial f}{\partial y} \tilde{y}^{(4)} - \left(\frac{\partial f}{\partial y} \right)^3 \tilde{y}^{(4)} \right) \right. \\ \left. + \frac{1}{3969} \left(2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial x^2} \tilde{y}^{(4)} - \frac{\partial^3 f}{\partial x^3} \tilde{y}^{(4)} - \frac{\partial^2 f}{\partial x^2} \frac{\partial f}{\partial y} \tilde{y}^{(4)} \right) \right\} + o(h^8) \quad (74) \end{aligned}$$

and

$$y_{n-1/2} = y_{n-2} + h(9f_{n-1} + 3f_{n-2})/8 \quad (75)$$

$$y_{n-1/4} = (1309y_{n-1} - 1053y_{n-2})/256 + h(756f_{n-1/2} - 1659f_{n-1} - 819f_{n-2})/512 \quad (76)$$

$$\hat{y}_n = (-140y_{n-1} + 193y_{n-2})/53 + h(512f_{n-1/4} - 560f_{n-1/2} + 3640f_{n-1} + 1574f_{n-2})/1113 \quad (77)$$

$$\tilde{y}_n = (32y_{n-1} + y_{n-2})/33 + h(1113\hat{f}_n + 2048f_{n-1/4} + 4928f_{n-1/2} + 2548f_{n-1} + 73f_{n-2})/10395 \quad (78)$$

with truncation error

$$\begin{aligned} \tilde{y}_n - y(x_n) = h^7 & \left\{ \frac{13}{997920} \left(y^{(7)} - 7 \frac{\partial f}{\partial y} y^{(6)} \right) + \frac{13}{79200} \left(\left(\frac{\partial f}{\partial y} \right)^2 y^{(5)} - \frac{\partial^2 f}{\partial y^2} f y^{(5)} \right) \right. \\ & + \frac{3}{1760} \left(\frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(4)} - \left(\frac{\partial f}{\partial y} \right)^3 y^{(4)} \right) + \frac{1}{1440} \left(2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f y^{(4)} \right. \\ & \left. \left. - \frac{\partial^3 f}{\partial y^3} f^2 y^{(4)} - \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f y^{(4)} \right) \right\} \\ & + o(h^8) \end{aligned} \quad (79)$$

For $k = 3$ the two methods are

$$y_{n-2/3} = (49y_{n-2} + 32y_{n-3})/81 + h(196f_{n-1} + 196f_{n-2} + 28f_{n-3})/243 \quad (80)$$

$$\begin{aligned} y_{n-1/3} = & (14992y_{n-1} - 6784y_{n-2} - 2943y_{n-3})/5265 \\ & + h(118584f_{n-2/3} - 148400f_{n-1} - 145208f_{n-2} - 17336f_{n-3})/110565 \end{aligned} \quad (81)$$

$$\begin{aligned} \hat{y}_n = & (-164007y_{n-1} + 139716y_{n-2} + 47015y_{n-3})/22724 \\ & + h(995085f_{n-1/3} - 2405700f_{n-2/3} + 4819248f_{n-1} + 3412836f_{n-2}) \end{aligned}$$

$$\begin{aligned}\tilde{y}_n &= (9369y_{n-1} + 837y_{n-2} + 71y_{n-3})/10277 \\ &+ h(20976\hat{f}_n + 98415f_{n-1/3} + 39366f_{n-2/3} + 58536f_{n-1} \\ &+ 7506f_{n-2} + 321f_{n-3})/205540\end{aligned}\quad (83)$$

with truncation error

$$\begin{aligned}\tilde{y}_n - y(x_n) &= h^9 \left\{ \frac{47}{43163400} \left(y^{(9)} - 9 \frac{\partial f}{\partial y} y^{(8)} \right) + \frac{3938}{70140525} \left(\frac{\partial^2 f}{\partial y^2} f y^{(7)} - \left(\frac{\partial f}{\partial y} \right)^2 y^{(7)} \right) \right. \\ &+ \frac{854}{3340025} \left(\frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(6)} - \left(\frac{\partial f}{\partial y} \right)^3 y^{(6)} \right) \\ &+ \left. \frac{49}{1541550} \left(2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f y^{(6)} - \frac{\partial^3 f}{\partial y^3} f^2 y^{(6)} - \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f y^{(6)} \right) \right\} \\ &+ o(h^{10})\end{aligned}\quad (84)$$

and

$$\begin{aligned}y_{n-1/2} &= (-225y_{n-1} + 200y_{n-2} + 153y_{n-3})/128 \\ &+ h(225f_{n-1} + 300f_{n-2} + 45f_{n-3})/128\end{aligned}\quad (85)$$

$$\begin{aligned}y_{n-1/4} &= (6339487y_{n-1} - 2981088y_{n-2} - 2604735y_{n-3})/753664 \\ &+ h(4124736f_{n-1/2} - 13604745f_{n-1} - 24795540f_{n-2} - 3851001f_{n-3})/3768320\end{aligned}\quad (86)$$

$$\begin{aligned}\hat{y}_n &= (-206118y_{n-1} + 125037y_{n-2} + 101758y_{n-3})/20677 \\ &+ h(5652480f_{n-1/4} - 7746816f_{n-1/2} + 49298865f_{n-1} + 75689130f_{n-2} \\ &+ 11559891f_{n-3})/7960645\end{aligned}\quad (87)$$

$$\begin{aligned}
\tilde{y}_n &= (5319y_{n-1} + 513y_{n-2} + 41y_{n-3})/5873 \\
&+ h(207669\hat{f}_n + 589824f_{n-1/4} + 887040f_{n-1/2} \\
&+ 715869f_{n-1} + 86229f_{n-2} + 3549f_{n-3})/2261105
\end{aligned} \tag{88}$$

with truncation error

$$\begin{aligned}
\tilde{y}_n - y(x_n) &= h^9 \left\{ \frac{29}{28190400} \left(y^{(9)} - 9 \frac{\partial f}{\partial y} y^{(8)} \right) + \frac{5787}{756442400} \left(\left(\frac{\partial f}{\partial y} \right)^2 y^{(7)} \right. \right. \\
&\quad \left. \left. - \frac{\partial^2 f}{\partial y^2} f_y^{(7)} \right) \right. \\
&+ \frac{7533}{21612640} \left(\frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(6)} - \left(\frac{\partial f}{\partial y} \right)^3 y^{(6)} \right) \\
&+ \frac{45}{375872} \left(2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f_y^{(6)} - \frac{\partial^3 f}{\partial y^3} f^2 y^{(6)} - \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f_y^{(6)} \right) \left. \right\} \\
&+ o(h^{10})
\end{aligned} \tag{89}$$

Finally, for $k = 4$ the two methods are

$$\begin{aligned}
y_{n-2/3} &= (-39200y_{n-1} - 33075y_{n-2} + 108000y_{n-3} + 23324y_{n-4})/59049 \\
&+ h(19600f_{n-1} + 44100f_{n-2} + 25200f_{n-3} + 1960f_{n-4})/19683
\end{aligned} \tag{90}$$

$$y_{n-1/3} = (653682800y_{n-1} - 54440316y_{n-2} - 381259575y_{n-3} - 62034500y_{n-4})/$$

$$\begin{aligned}
& + h(418263750f_{n-2/3} - 691608400f_{n-1} - 1248768990f_{n-2} \\
& \quad - 540581400f_{n-3} - 35198600f_{n-4})/363879621 \quad (91)
\end{aligned}$$

$$\begin{aligned}
\hat{y}_n & = (-17463266y_{n-1} + 4428891y_{n-2} + 12250002y_{n-3} + 1782557y_{n-4})/998184 \\
& + h(40431069f_{n-1/3} - 122509179f_{n-2/3} + 304934560f_{n-1} + 425424951f_{n-2} \\
& \quad + 164835435f_{n-3} + 9960664f_{n-4})/23290960 \quad (92)
\end{aligned}$$

$$\begin{aligned}
\tilde{y}_n & = (301456y_{n-1} + 65448y_{n-2} + 22640y_{n-3} + 1457y_{n-4})/391001 \\
& + h(14710080\hat{f}_n + 76606236f_{n-1/3} + 16021962f_{n-2/3} + 62942880f_{n-1} \\
& \quad + 20844054f_{n-2} + 3604260f_{n-3} + 119028f_{n-4})/150535385 \quad (93)
\end{aligned}$$

with truncation error

$$\begin{aligned}
\tilde{y}_n - y(x_n) & = h^{11} \left\{ \frac{28027}{182900492775} \left(y^{(11)} - 11 \frac{\partial f}{\partial y} y^{(10)} \right) \right. \\
& + \frac{1663988}{139004374509} \left(\frac{\partial^2 f}{\partial y^2} f y^{(9)} - \left(\frac{\partial f}{\partial y} \right)^2 y^{(9)} \right) \\
& + \frac{42500}{735472881} \left(\frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(8)} - \left(\frac{\partial f}{\partial y} \right)^3 y^{(8)} \right) \\
& + \frac{37}{10557027} \left(2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f y^{(8)} - \frac{\partial^3 f}{\partial y^3} f^2 y^{(8)} - \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f y^{(8)} \right) \\
& \left. + o(h^{12}) \right\} \quad (94)
\end{aligned}$$

and

$$y_{n-1/2} = (-6125y_{n-1} - 3675y_{n-2} + 9261y_{n-3} + 2075y_{n-4})/1536$$

$$+ h(1225f_{n-1} + 3675f_{n-2} + 2205f_{n-3} + 175f_{n-4})/512 \quad (95)$$

$$y_{n-1/4} = (884331175y_{n-1} + 449223975y_{n-2} - 1027077975y_{n-3} - 232028279y_{n-4})$$

$$/74448896$$

$$+ h(72817920f_{n-1/2} - 314524875f_{n-1} - 1207478475f_{n-2}$$

$$- 737261595f_{n-3} - 58733115f_{n-4})/74448896 \quad (96)$$

$$\hat{y}_n = (-99742024y_{n-1} - 45909828y_{n-2} + 123367176y_{n-3} + 27180523y_{n-4})/4895847$$

$$+ h(148897792f_{n-1/4} - 239486976f_{n-1/2} + 1662170440f_{n-1} + 5185974240f_{n-2}$$

$$+ 3056346216f_{n-3} + 240266188f_{n-4})/171354645 \quad (97)$$

$$\tilde{y}_n = (8494880y_{n-1} + 1482624y_{n-2} + 477408y_{n-3} + 30127y_{n-4})/10485039$$

$$+ h(342709290\hat{f}_n + 1191182336f_{n-1/4} + 1372225536f_{n-1/2} + 1575099680f_{n-1}$$

$$+ 450881640f_{n-2} + 75396384f_{n-3} + 2456234f_{n-4})/4036740015 \quad (98)$$

with truncation error

$$\begin{aligned}
\tilde{y}_n - y(x_n) = & h^{11} \left\{ \frac{36923}{322939201200} \left[y^{(11)} - 11 \frac{\partial f}{\partial y} y^{(10)} \right] \right. \\
& + \frac{2759}{3690733728} \left[\frac{\partial^2 f}{\partial y^2} f_y(9) - \left(\frac{\partial f}{\partial y} \right)^2 y^{(9)} \right] \\
& + \frac{94815}{1230244576} \left[\frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(8)} - \left(\frac{\partial f}{\partial y} \right)^3 y^{(8)} \right] \\
& + \frac{1269}{55920208} \left[2 \frac{\partial f}{\partial y} \frac{\partial^2 f}{\partial y^2} f_y(8) - \frac{\partial^3 f}{\partial y^3} f^2 y^{(8)} - \frac{\partial^2 f}{\partial y^2} \frac{\partial f}{\partial y} f_y(8) \right] \left. \right\} \\
& + o(h^{12})
\end{aligned} \tag{99}$$

Numerical Examples

As an illustration of the use of the method given by (70), (71), (72), (73) five equations have been integrated from $x_0 = 0$ to $x = 40$ by this method and by the fourth order Runge-Kutta method. Using step sizes $h = 1/2, 1/4, 1/8, 1/16, 1/32, 1/64, 1/128$ each equation was integrated by the two methods and the greatest of the errors produced at $x = 1, 2, \dots, 40$ for each method were compared. For a given equation and step size let E denote the maximum error for the new method divided by the maximum error for the Runge-Kutta method. In figure 4, E is plotted as a function of h for each of the equations. The five equations used were given by

$$\text{I: } \dot{y} = y, \quad y_0 = 1, \quad , \quad (100)$$

$$\text{II: } \dot{y} = -\frac{xy}{x+2}, \quad y_0 = 4, \quad , \quad (101)$$

$$\text{III: } \dot{y} = y \cos x, \quad y_0 = 1, \quad , \quad (102)$$

$$\text{IV: } \dot{y} = -y + 2 \sin x, \quad y_0 = -1, \quad , \quad (103)$$

$$\text{V: } \dot{y} = -y + 10 \sin 3x, \quad y_0 = -3, \quad . \quad (104)$$

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LIST OF FIGURES

1. $R = 1$ contours for $k = 3, 4, 5, 6, 7, 8$.
2. $v = .3u$ where v minimizes R for given u . $k = 6, 7, 8, \dots, 15$.
3. Minimum R for given u . $k = 6, 7, 8, \dots, 15$.
4. Error of a $k = 2$ method compared with Runge-Kutta for five equations and for various step sizes.

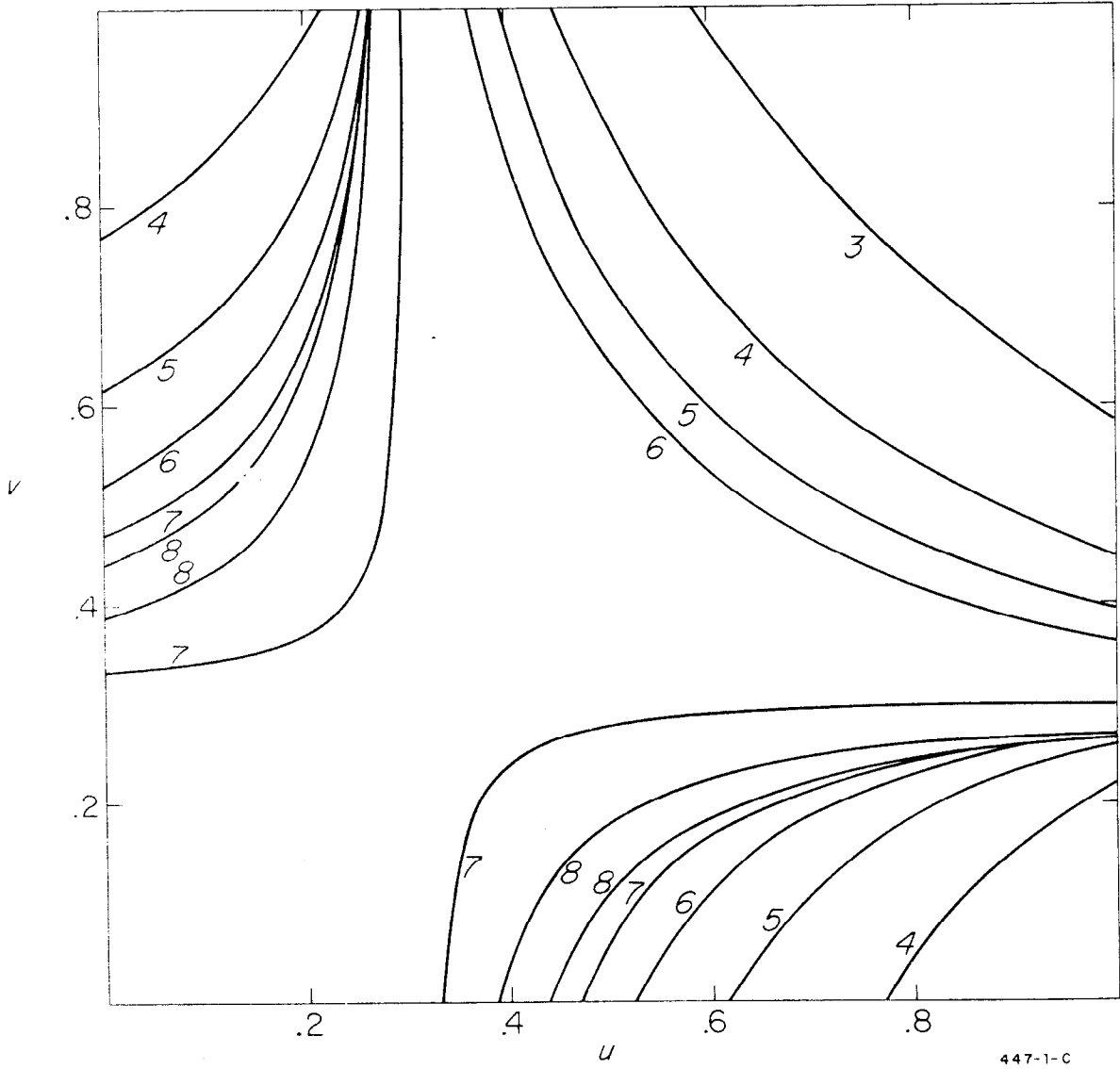
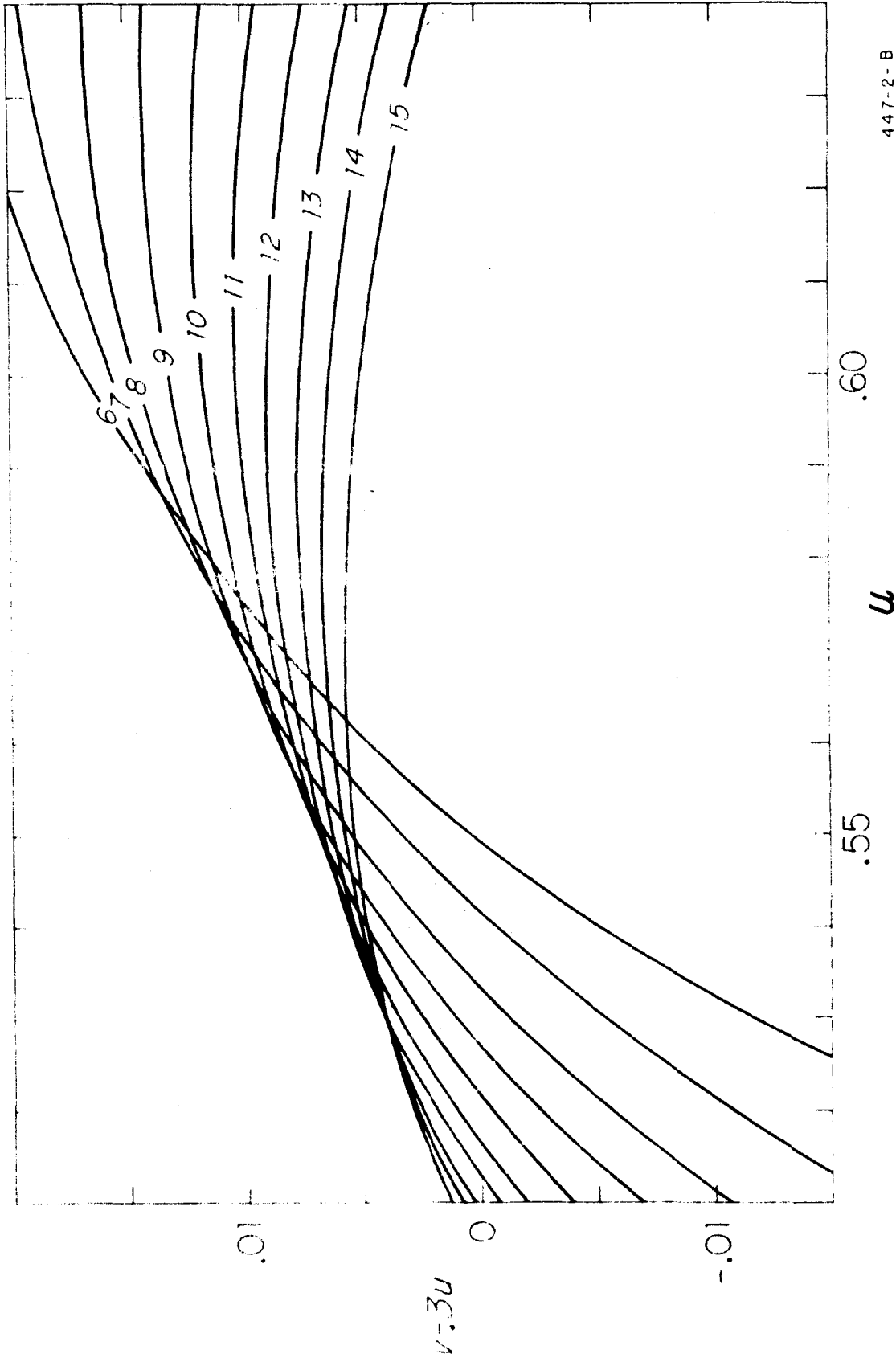


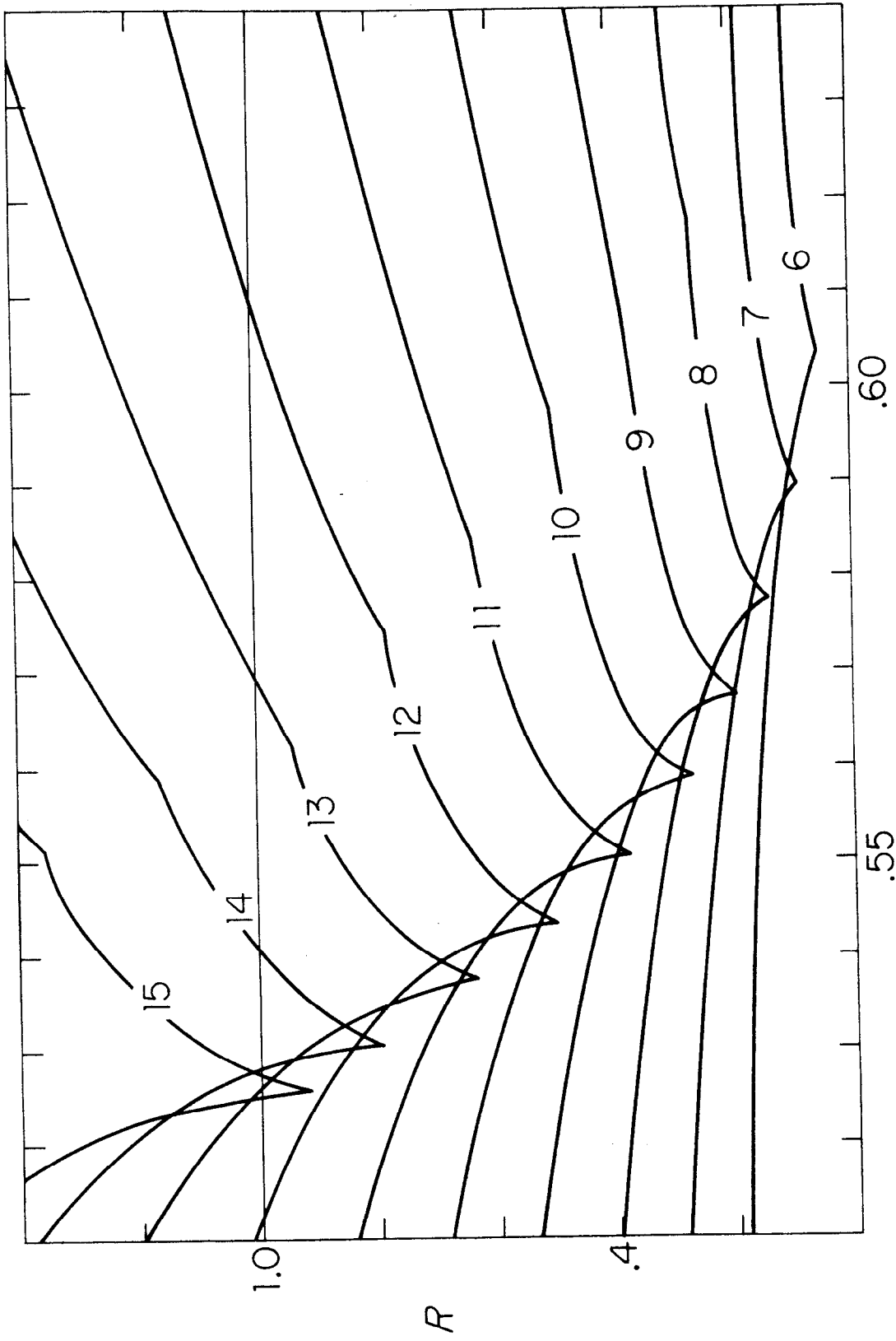
Fig. 1

447-1-C



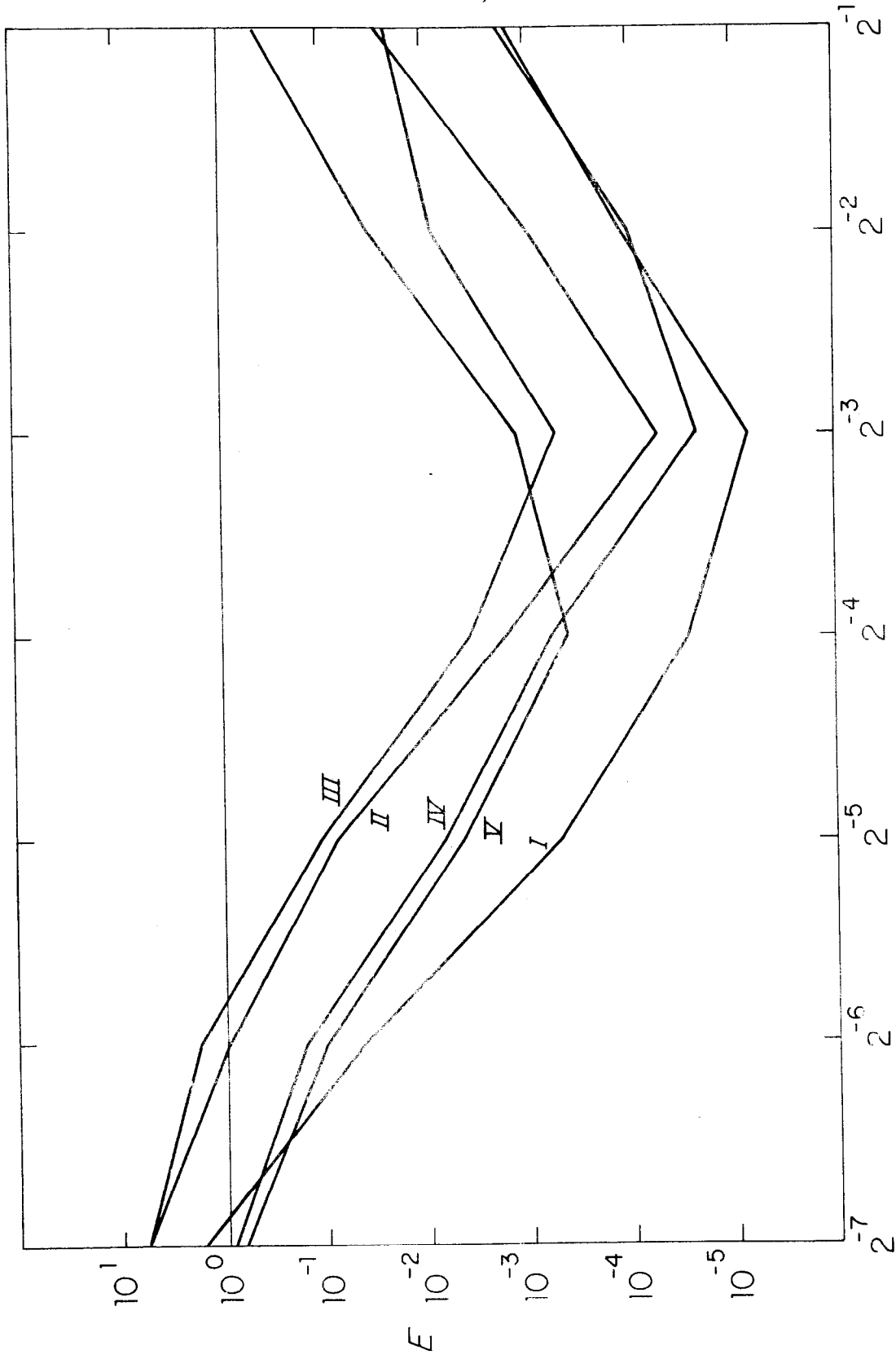
447-2-B

Fig. 2



447-3-B

Fig. 3



h
Fig. 4

447-4-B