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A MULTISTEP GENERALIZATION OF RUNGE-KUTTA METHODS WITH 4 OR 5 STAGES*

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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. A five stage method of order 7 is also given.

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1. 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 the present paper is mainly concerned with the case of two evaluations. 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 $k = 1, 2, \ldots, 15$. Detailed formulae for some of these cases are given for $k = 2, 3, 4$.

For a stable k step method requiring r intermediate calculations per step (that is a total of $r + 2$ derivative calculations per step) it seems worthwhile to aim for an order $2k + r$. For $r = 0$ this has been shown by Dahlquist [4] to be possible only for $k < 3$. For $r = 1$ it appears to be possible up to $k = 7$ [2] and, as just noted, it appears to be possible when $r = 2$ up to $k = 15$. $r = 3$ is a particularly interesting case as the Runge-Kutta case, $k = 1$, does not exist.

However, using a construction that could in principle be used for cases of higher k, we have found that there exists a two parameter family of methods of order 7 with $k = 2$, $r = 3$. One example of such a method is given here.

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

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

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

$$\frac{dy}{dx} = f(y) \ , \ y(x_o) = y_o \tag{2}$$

where y is the vector (x,y) with N + 1 components, $f = \big(1, f(x,y)\big)$ and $y_o = (x_o, y_o)$.

2. The Corrector Formula for the Four Stage Methods

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

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

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

$$0 = -p(0) + \sum_{j=1}^{k} A_j p(-hj) + h\left(b_1 p'(-hu) + b_2 p'(-hv) + \sum_{j=0}^{k} B_j p'(-hj)\right) \tag{4}$$

for all polynomials p of degree $\leqq 2k + 2$. We shall suppose that $u \neq v$ and that neither equals one of 0, 1, 2, ..., k .

Consider the function

$$\phi(z) = -\frac{1}{z} + \sum_{j=1}^{k} \frac{A_j}{z+hj} + h\left\{\frac{b_1}{(z+hu)^2} + \frac{b_2}{(z+hv)^2} + \sum_{j=0}^{k} \frac{B_j}{(z+hj)^2}\right\} \tag{5}$$

so that the integral L(p) given by

$$L(p) = \frac{1}{2\pi i} \int_C p(z)\, \phi(z)\, dz \tag{6}$$

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

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

as $|z| \to \infty$.

If we write

$$\phi(z) = \frac{K(k!)^2 h^{2k+2}}{\prod_{j=0}^{k} (z + hj)^2} \left(\frac{1}{z + hu} + \frac{hU}{2(z + hu)^2} - \frac{1}{z + hv} - \frac{hV}{2(z + hv)^2} \right) \tag{8}$$

we see that (7) is satisfied and that (8) is of the form of (5) if the constants U, V, K are chosen so that the residues of $\phi(z)$ (given by (8)) at $z = -hu$ and at $z = -hv$ are zero and so that the residue at $z = 0$ is -1. Assuming that u, v do not have values such that one of the right hand sides of (9), (10), or (11) vanishes we find

$$1/U = \sum_{j=0}^{k} \frac{1}{j-u} \tag{9}$$

$$1/V = \sum_{j=0}^{k} \frac{1}{j-v} \tag{10}$$

$$1/K = H_k \left(\frac{2}{u} + \frac{U}{u^2} - \frac{2}{v} - \frac{V}{v^2} \right) + \frac{1}{u^2} + \frac{U}{u^3} - \frac{1}{v^2} - \frac{V}{v^3} \tag{11}$$

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

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

$$b_1 = \frac{KU}{2u^2} \frac{k!^2}{\prod_{j=1}^{k} (j-u)^2} \tag{12}$$

$$b_2 = -\frac{KV}{2v^2} \frac{k!^2}{\prod_{j=1}^{k} (j-v)^2} \tag{13}$$

$$B_j = K\binom{k}{j}^2 \left(-\frac{1}{(j-u)} + \frac{U}{2(j-u)^2} + \frac{1}{(j-v)} - \frac{V}{2(j-v)^2} \right), \tag{14}$$

$$A_j = K\binom{k}{j}^2 \left(-\frac{1}{(j-u)^2} + \frac{U}{(j-u)^3} + \frac{1}{(j-v)^2} - \frac{V}{(j-v)^3} \right) + 2B_j(H_j - H_{k-j}) \tag{15}$$

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 $0, -hu, -hv, -hk$. We can expand $p(-h), p(-2h), \ldots, p(-kh)$, $hp'(-h), hp'(-2h), \ldots, hp'(-kh), hp'(-uh), hp'(-vh)$ in Taylor series about 0 up to terms in $p^{(2k+3)}(0)$ with remainder terms $O(h^{2k+4})$ as $h \to 0$. Substitute into the right hand side of (4) and we obtain, since $A_1, A_2, \ldots, A_k, b_1, b_2$, $B_0, B_1, \ldots, B_k$ 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 $p(z) = z^3 \prod_{j=1}^{k} (z+hj)^2$, for which $p^{(2k+3)}(0) = (2k+3)!$. We now have

$$h^{2k+3}(2k+3)!\,\epsilon = \frac{1}{2\pi i} \int_C K(k!)^2 h^{2k+2} z \left(\frac{1}{z+hu} + \frac{hU}{2(z+hu)^2} - \frac{1}{z+hv} - \frac{hV}{2(2+hv)^2} \right) dz \tag{16}$$

from which

$$\epsilon = \frac{K(k!)^2}{(2k+3)!} \left(v - u + \frac{U-V}{2} \right) \tag{17}$$

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

3. Stability Considerations

So far the only restrictions that are imposed on the parameters u, v are that they are not equal, that each differs from each of the integers $0, 1, 2, \ldots, k$ and that the right hand sides of (9), (10), (11) 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,

$$z^k - A_1 z^{k-1} - A_2 z^{k-2} - \ldots - A_k = 0 \tag{18}$$

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 $R = \left| (15uv - 7(u+v) + 4)/(15uv - 23(u+v) + 36) \right|$.

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 for 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, ..., 15, Figs. 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 u (Fig. 2). The minimum value of R is plotted in Fig. 3.

4. 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

$$y_{n-u} = \sum_{j=1}^{k} A_{1j} y_{n-j} + h \sum_{j=1}^{k} B_{1j} f_{n-j} \tag{19}$$

$$y_{n-v} = \sum_{j=1}^{k} A_{2j} y_{n-j} + h \left(b_{21} f_{n-u} + \sum_{j=1}^{k} B_{2j} f_{n-j} \right) \tag{20}$$

$$y_{n} = \sum_{j=1}^{k} A_{3j} y_{n-j} + h \left(b_{31} f_{n-u} + b_{32} f_{n-v} + \sum_{j=1}^{k} B_{3j} f_{n-j} \right) \tag{21}$$

The value of y_n given by (21) we will write as $\hat{y}_n$ and the final "corrected" value as $\tilde{y}_n$. For simplicity we will suppose that $x_n = 0$ and for compactness of notation we will consider the autonomous form (2) of (1). Thus we consider the overall procedure for finding y(0) from y(-h), y(-2h), ..., y(-kh) using the formulae

$$y(-hu) = \sum_{j=1}^{k} A_{1j} y(-hj) + h \sum_{j=1}^{k} B_{1j} f\left(y(-hj)\right), \tag{22}$$

$$y(-hv) = \sum_{j=1}^{k} A_{2j} y(-hj) + h\left[b_{21} f\left(y(-hu)\right) + \sum_{j=1}^{k} B_{2j} f\left(y(-hj)\right)\right] , \qquad (23)$$

$$\hat{y}(0) = \sum_{j=1}^{k} A_{3j} y(-hj) + h\left[b_{31} f\left(y(-hu)\right) + b_{32} f\left(y(-hv)\right) + \sum_{j=1}^{k} B_{3j} f\left(y(-hj)\right)\right] , \qquad (24)$$

$$\tilde{y}(0) = \sum_{j=1}^{k} A_j y(-hj) + h\left[b_1 f\left(y(-hu)\right) + b_2 f\left(y(-hv)\right) + b_3 f\left(\hat{y}(0)\right) + \sum_{j=1}^{k} B_j f\left(y(-hj)\right)\right], \qquad (25)$$

where we have written b_3 in place of B_0 .

We can choose the coefficients in (22) so that $y(-hu)$ is given exactly when the components of $y(x)$ are polynomials of degree $2k-1$. When this is done, suppose the error can be written in the form

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

The same is true for (23), (24), 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 (25) the error in this quantity is $\epsilon\, y^{(2k+3)}(0)\, h^{2k+3} + O(h^{2k+4})$ 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

$$\tilde{y}(0) - y(0) = h^{2k+1}\left(b_1 \epsilon_1^{(2k)} + b_2 \epsilon_2^{(2k)} + b_3 \epsilon_3^{(2k)}\right) \frac{\partial f}{\partial y}\, y^{(2k)}$$

$$+ h^{2k+2}\left\{\left(b_1 \epsilon_1^{(2k+1)} + b_2 \epsilon_2^{(2k+1)} + b_3 \epsilon_3^{(2k+1)}\right) \frac{\partial f}{\partial y}\, y^{(2k+1)}\right.$$

$$
\begin{aligned}
&+ \left(b_2 b_{21} \epsilon_1^{(2k)} + b_3 b_{31} \epsilon_1^{(2k)} + b_3 b_{32} \epsilon_2^{(2k)}\right) \left(\frac{\partial f}{\partial y}\right)^2 y^{(2k)} \\
&- \left.\left(b_1 u \epsilon_1^{(2k)} + b_2 v \epsilon_2^{(2k)}\right) \frac{\partial^2 f}{\partial y^2} f y^{(2k)}\right\} \\
&+ h^{2k+3} \left\{\left(b_1 \epsilon_1^{(2k+2)} + b_2 \epsilon_2^{(2k+2)} + b_3 \epsilon_3^{(2k+2)}\right) \frac{\partial f}{\partial y} y^{(2k+2)} + \epsilon\, y^{(2k+3)}\right\} \\
&+ h^{2k+3} \left\{\left(b_2 b_{21} \epsilon_1^{(2k+1)} + b_3 b_{31} \epsilon_1^{(2k+1)} + b_3 b_{32} \epsilon_2^{(2k+1)}\right) \left(\frac{\partial f}{\partial y}\right)^2 y^{(2k+1)}\right. \\
&- \left.\left(b_1 u \epsilon_1^{(2k+1)} + b_2 v \epsilon_2^{(2k+1)}\right) \frac{\partial^2 f}{\partial y^2} f y^{(2k+1)}\right\} \\
&+ h^{2k+3} \left\{ b_3 b_{32} b_{21} \epsilon_1^{(2k)} \left(\frac{\partial f}{\partial y}\right)^3 y^{(2k)} - b_2 v b_{21} \epsilon_1^{(2k)} \frac{\partial^2 f}{\partial y^2} f \frac{\partial f}{\partial y} y^{(2k)}\right\} \\
&+ h^{2k+3} \left\{ \frac{1}{2}\left(b_1 u^2 \epsilon_1^{(2k)} + b_2 v^2 \epsilon_2^{(2k)}\right)\left(\frac{\partial^3 f}{\partial y^3} f^2 y^{(2k)} + \frac{\partial^2 f}{\partial y^2}\frac{\partial f}{\partial y} f y^{(2k)}\right)\right. \\
&- \left.\left[\left(b_2 b_{21} + b_3 b_{31}\right) u \epsilon_1^{(2k)} + b_3 b_{32} v \epsilon_2^{(2k)}\right] \frac{\partial f}{\partial y}\frac{\partial^2 f}{\partial y^2} f y^{(2k)}\right\} \\
&+ \frac{1}{2} h^{4k+1} \left\{ b_1 \left(\epsilon_1^{(2k)}\right)^2 + b_2 \left(\epsilon_2^{(2k)}\right)^2 + b_3 \left(\epsilon_3^{(2k)}\right)^2\right\} \frac{\partial^2 f}{\partial y^2} \left(y^{(2k)}\right)^2 + O\left(h^{2k+4}\right)
\end{aligned}
\tag{26}
$$

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, $f^i_j \left(=\frac{\partial f^i}{\partial y^j}\right)$, f^i_{jk}, ... 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 (26). 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 (26) that

$$b_1 \epsilon_1^{(2k)} + b_2 \epsilon_2^{(2k)} + b_3 \epsilon_3^{(2k)} = 0 \tag{27}$$

$$b_1 \epsilon_1^{(2k+1)} + b_2 \epsilon_2^{(2k+1)} + b_3 \epsilon_3^{(2k+1)} = 0 \tag{28}$$

$$b_2 b_{21} \epsilon_1^{(2k)} + b_3 b_{31} \epsilon_1^{(2k)} + b_3 b_{32} \epsilon_2^{(2k)} = 0 \tag{29}$$

$$b_1 u \epsilon_1^{(2k)} + b_2 v \epsilon_2^{(2k)} = 0 \tag{30}$$

We now derive formulae for the coefficients in (22) and (23) so that these are accurate for polynomials of degree $2k-1$ and so that (27) is satisfied. We then find formulae for the coefficients in (24) so that this is also accurate for polynomials of degree $2k-1$ and so that (28), (29) and (30) are satisfied.

By analogy with (5) we write

$$\varphi_1(z) = -\frac{1}{z+hu} + \sum_{j=1}^{k} \frac{A_{1j}}{z+hj} + h \sum_{j=1}^{k} \frac{B_{1j}}{(z+hj)^2} \tag{31}$$

$$\varphi_2(z) = -\frac{1}{z+hv} + \sum_{j=1}^{k} \frac{A_{2j}}{z+hj} + h\left(\frac{b_{21}}{(z+u)^2} + \sum_{j=1}^{k} \frac{B_{2j}}{(z+hj)^2} \right) \tag{32}$$

$$\varphi_3(z) = -\frac{1}{z} + \sum_{j=1}^{k} \frac{A_{3j}}{z+hj} + h \left(\frac{b_{31}}{(z+hu)^2} + \frac{b_{32}}{(z+hv)^2} + \sum_{j=1}^{k} \frac{B_{3j}}{(z+hj)^2} \right) \tag{33}$$

and

$$L_j(p) = \frac{1}{2\pi i} \int_C p(z) \ \varphi_j(z) \, dz \ , \quad j = 1,\ 2,\ 3 \tag{34}$$

so that $L_1(p)$, $L_2(p)$, $L_3(p)$ is the error in (31), (32), (33) 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,

$$|\varphi_j(z)| = O(|z|^{-2k-1}) \ , \quad j = 1,\ 2,\ 3 \ . \tag{35}$$

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

$$\varphi_1(z) = - \frac{h^{2k}}{z+hu} \frac{\prod_{j=1}^{k} (u-j)^2}{\prod_{j=1}^{k} (z+hj)^2} \tag{36}$$

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

Thus

$$B_{1j} = \frac{\prod_{\ell=1}^{k} (u-\ell)^2}{(j-u) \left[(k-j)! \ (j-1)! \right]^2} \tag{37}$$

$$A_{1j} = B_{1j} \left(\frac{1}{j-u} + 2 \left[H_{j-1} - H_{k-j} \right] \right) \tag{38}$$

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

$$\varphi_2(z) = - \frac{h^{2k} \prod_{j=1}^{k} (v-j)^2}{(z+hv) \prod_{j=1}^{k} (z+hj)^2} \left[P + hQ \left(\frac{1}{z+hu} + \frac{hR}{(z+hu)^2} \right) \right] \tag{39}$$

so that

$$B_{2j} = \frac{\prod_{\ell=1}^{k} (v-\ell)^2}{(j-v)\ \left[(k-j)!\ (j-1)!\right]^2} \left[P + Q\left(\frac{1}{u-j} + \frac{R}{(u-j)^2}\right)\right] \tag{40}$$

$$A_{2j} = \frac{\prod_{\ell=1}^{k} (v-\ell)^2}{(j-v)\ \left[(k-j)!\ (j-1)!\right]^2} \left(- \frac{Q}{(j-u)^2} + \frac{2QR}{(j-u)^3}\right) + B_{2j}\left(2\left[H_{j-1} - H_{k-j}\right] + \frac{1}{j-v}\right) \tag{41}$$

$$b_{21} = \frac{QR \prod_{j=1}^{k} (v-j)^2}{(u-v) \prod_{j=1}^{k} (u-j)^2} \tag{42}$$

The form for $\varphi_2(z)$ given by (39) has the correct behavior at infinity and at $-h, -2h, \ldots, -kh, -uh, -vh$. However, P, Q, R must be fixed so that the residue at $-hu$ is 0 and the residue at $-hv$ is -1.

We thus have

$$\frac{1}{R} = \frac{1}{v-u} + 2\sum_{j=1}^{k} \frac{1}{j-u} = \frac{2}{U} + \frac{2}{u} + \frac{1}{v-u} \quad , \tag{43}$$

$$P + Q\left(\frac{1}{u-v} + \frac{R}{(u-v)^2}\right) = 1 \quad . \tag{44}$$

To obtain a third equation for P, Q, R we use (30). In the same way as for ϵ we obtain for $\epsilon_j^{(2k)}$, $j = 1, 2$ the expression

$$\epsilon_j^{(2k)} = \frac{h^{-2k}}{2\pi i\ (2k)!} \int_C \prod_{j=1}^{k} (z+hj)^2 \cdot \varphi_j(z)\ dz \tag{45}$$

so that

$$\epsilon_1^{(2k)} = -\frac{1}{(2k)!} \prod_{j=1}^{k} (u-j)^2 \tag{46}$$

$$\epsilon_2^{(2k)} = -\frac{P}{(2k)!} \prod_{j=1}^{k} (v-j)^2 \quad . \tag{47}$$

Using the expressions (12), (13) for b_1, b_2 and substituting in (30) we find

$$P = \frac{vU}{uV} \tag{48}$$

$\varphi_2(z)$ is now determined. We must now choose $\varphi_3(z)$ of such a form that (27), (28), (29) are satisfied. This can be done by defining $\varphi_3(z)$ by the equation

$$b_1\varphi_1(z) + b_2\varphi_2(z) + b_3\varphi_3(z) + \frac{z}{h}\varphi(z) = 0 \quad . \tag{49}$$

To see this, we observe that $\varphi_3(z)$ defined thus has the correct behavior at $-hu$, $-hv$, 0, $-h$, $-2h$, ..., $-kh$ and at infinity. To see that (27) and (28) are satisfied we see that

$$\epsilon_j^{(2k+m)} = \frac{h^{-2k-m}}{2\pi i\ (2k+m)!} \int_C z^{2k+m} \varphi_j(z)\ dz \tag{50}$$

for $m = 0, 1$ and $j = 1, 2, 3$. Making use of (49) we see that

$$\sum_{j=1}^{k} b_j \epsilon_j^{(2k+m)} = -\frac{h^{-2k-m-1}}{2\pi i\ (2k+m)!} \int_C z^{2k+m+1} \varphi(z)\ dz = 0 \tag{51}$$

since $|\varphi(z)| = O(|z|^{-2k-4})$ as $|z| \to \infty$. To see that (29) is satisfied, we multiply (49) by $(z+hu)^2/h$ and by $(z+hv)^2/h$ and take the limits as $z \to -hu$

and $z \to -hv$ respectively. We find

$$b_2 b_{21} + b_3 b_{31} - u b_1 = 0 \quad , \tag{52}$$

$$b_3 b_{32} - v b_2 = 0 \quad , \tag{53}$$

so that (29) follows immediately from (30). Using (49) we now list expressions for all the coefficients in (24).

$$A_{3j} = \frac{1}{b_3} \left(j A_j - b_1 A_{1j} - b_2 A_{2j} - B_j \right) \quad , \tag{54}$$

$$B_{3j} = \frac{1}{b_3} \left(j B_j - b_1 B_{1j} - b_2 B_{2j} \right) \quad , \tag{55}$$

$$b_{31} = \frac{1}{b_3} \left(u b_1 - b_2 b_{21} \right) \quad , \tag{56}$$

$$b_{32} = \frac{1}{b_3} v b_2 \quad . \tag{57}$$

5. The Truncation Error

In this section we shall find expressions for the coefficients in the asymptotic error term which we see from (26) to have the form

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

where we have supposed $k > 1$ and the c's are given by (26). From (49) we immediately find $c_1' = -(2k+3) \quad c_1 = -(2k+3)\,\epsilon$. From (52), (53), we find that $c_2 = c'_2$, $c_3 = c'_3$, $c_4 = c'_4$. c_2 is given by

$$c_2 = b_1 u \epsilon_1^{(2k+1)} + b_2 v \epsilon_2^{(2k+1)} = \frac{h^{-2k-1}}{2\pi i\,(2k+1)!} \int_C \left[b_1 u \varphi_1(z) + b_2 v \varphi_2(z)\right] z^{2k+1}\, dz \tag{58}$$

Since $\int_C \left(b_1 u \varphi_1(z) + b_2 v \varphi_x(z)\right) p(z)\, dz = 0$ when $p(z)$ is any polynomial of degree $2k$, we may replace z^{2k+1} in (58) by any polynomial with the same leading term. We choose the polynomial $(z+hu)\prod_{j=1}^{k}(z+hj)^2$ so that

$$c_2 = -\frac{b_2 v \prod_{j=1}^{k}(v-j)^2}{(2k+1)!}\left[P(u-v) + Q\right] . \tag{59}$$

To find $c_3 = b_2 v b_{21} \epsilon_1^{(2k)}$ we evaluate $\epsilon_1^{(2k)} = \left(h^{-2k}/2\pi i(2k)!\right)\int_C \varphi_1(z) \prod_{j=1}^{k}(z+hj)^2\, dz$ to find

$$c_3 = -\frac{b_2 v b_{21}}{(2k)!}\prod_{j=1}^{k}(u-j)^2 \tag{60}$$

Finally we find $c_4 = b_1 u^2 \epsilon_1^{(2k)}$ by making use of (30) and the value of $\epsilon_1^{(2k)}$ to give

$$c_4 = -\frac{b_1 u(u-v)}{(2k)!}\prod_{j=1}^{k}(u-j)^2 \tag{61}$$

6. Particular Methods

In this section we list some special methods. 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 $(u, v) = \left(\frac{2}{3}, \frac{1}{3}\right)$ and

$(u, v) = \left(\frac{1}{2}, \frac{1}{4}\right)$. For $k = 2$ the two methods are

$$y_{n-2/3} = (16y_{n-1} + 11y_{n-2})/27 + h(16f_{n-1} + 4f_{n-2})/27 \tag{62}$$

$$y_{n-1/3} = (47y_{n-1} - 20y_{n-2})/27 + h(27f_{n-2/3} - 22f_{n-1} - 7f_{n-2})/27 \tag{63}$$

$$\hat{y}_n = (-13y_{n-1} + 23y_{n-2})/10 + h(108f_{n-1/3} - 189f_{n-2/3} + 284f_{n-1} + 61f_{n-2})/80 \tag{64}$$

$$\tilde{y}_n = (48y_{n-1} + y_{n-2})/49 + h(160f_n + 648f_{n-1/3} + 405f_{n-2/3} + 280f_{n-1} + 7f_{n-2})/1470 \tag{65}$$

and

$$y_{n-1/2} = y_{n-2} + h(9f_{n-1} + 3f_{n-2})/8 \tag{66}$$

$$y_{n-1/4} = (1309y_{n-1} - 1053y_{n-2})/256 + h(756f_{n-1/2} - 1659f_{n-1} - 819f_{n-2})/512 \tag{67}$$

$$\hat{y}_n = (-140y_{n-1} + 193y_{n-2})/53 + h(512f_{n-1/4} - 560f_{n-1/2} + 3640f_{n-1} + 1574f_{n-2})/1113 \tag{68}$$

$$\tilde{y}_n = (32y_{n-1} + y_{n-2})/33 + h(1113\hat{f}_n + 2048f_{n-1/4} + 4928f_{n-1/2} + 2548f_{n-1} + 73f_{n-2})/10395 \; . \tag{69}$$

For $k = 3$ the two methods are

$$y_{n-2/3} = (49y_{n-2} + 32y_{n-3})/81 + h(196f_{n-1} + 196f_{n-2} + 28f_{n-3})/243 \tag{70}$$

$$y_{n-1/3} = (14992y_{n-1} - 6784y_{n-2} - 2943y_{n-3})/5265$$

$$+ h(118584f_{n-2/3} - 148400f_{n-1} - 145208f_{n-2} - 17336f_{n-3})/110565 \quad (71)$$

$$\hat{y}_n = (-164007y_{n-1} + 139716y_{n-2} + 47015y_{n-3})/22724$$

$$+ h(995085f_{n-1/3} - 2405700f_{n-2/3} + 4819248f_{n-1} + 3412836f_{n-2} + 359691f_{n-3})$$

(72)

$$\tilde{y}_n = (9369y_{n-1} + 837y_{n-2} + 71y_{n-3})/10277$$

$$+ h(20976\hat{f}_n + 98415f_{n-1/3} + 39366f_{n-2/3} + 58536f_{n-1}$$

$$+ 7506f_{n-2} + 321f_{n-3})/205540 \quad (73)$$

and

$$y_{n-1/2} = (-225y_{n-1} + 200y_{n-2} + 153y_{n-3})/128 + h(225f_{n-1} + 300f_{n-2} + 45f_{n-3})/128$$

(74)

$$y_{n-1/4} = (6339487y_{n-1} - 2981088y_{n-2} - 2604735y_{n-3})/753664$$

$$+ h(4124736f_{n-1/2} - 13604745f_{n-1} - 24795540f_{n-2} - 3851001f_{n-3})/3768320$$

(75)

$$\hat{y}_n = (-206118y_{n-1} + 125037y_{n-2} + 101758y_{n-3})/20677$$

$$+ h(5652480f_{n-1/4} - 7746816f_{n-1/2} + 49298865f_{n-1} + 75689130f_{n-2}$$

$$+ 11559891f_{n-3})/7960645 \quad (76)$$

$$\tilde{y}_n = (5319y_{n-1} + 513y_{n-2} + 41y_{n-3})/5873$$

$$+ h(207669\hat{f}_n + 589824f_{n-1/4} + 887040f_{n-1/2}$$

$$+ 715869f_{n-1} + 86229f_{n-2} + 3549f_{n-3})/2261105 \quad . \tag{77}$$

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

$$y_{n-2/3} = (-39200y_{n-1} - 33075y_{n-2} + 108000y_{n-3} + 23324y_{n-4})/59049$$

$$+ h(19600f_{n-1} + 44100f_{n-2} + 25200f_{n-3} + 1960f_{n-4})/19683 \tag{78}$$

$$y_{n-1/3} = (653682800y_{n-1} - 54440316y_{n-2} - 381259575y_{n-3} - 62034500y_{n-4})/ 155948409$$

$$+ h(418263750f_{n-2/3} - 691608400f_{n-1} - 1248768990f_{n-2}$$

$$- 540581400f_{n-3} - 35198800f_{n-4})/363879621 \tag{79}$$

$$\hat{y}_n = (-17463266y_{n-1} + 4428891y_{n-2} + 12250002y_{n-3} + 1782557y_{n-4})/998184$$

$$+ h(40431069f_{n-1/3} - 122509179f_{n-2/3} + 304934560f_{n-1} + 425424951f_{n-2}$$

$$+ 164835435f_{n-3} + 9960664f_{n-4})/23290960 \tag{80}$$

$$\tilde{y}_n = (301456y_{n-1} + 65448y_{n-2} + 22640y_{n-3} + 1457y_{n-4})/391001$$

$$+ h(14710080\hat{f}_n + 76606236f_{n-1/3} + 16021962f_{n-2/3} + 62942880f_{n-1}$$

$$+ 20844054f_{n-2} + 3604260f_{n-3} + 119028f_{n-4})/15053585 \tag{81}$$

and

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

$$+ h(1225f_{n-1} + 3675f_{n-2} + 2205f_{n-3} + 175f_{n-4})/512 \qquad (82)$$

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

$$/74448896$$

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

$$- 737261595f_{n-3} - 58733115f_{n-4})/74448896 \qquad (83)$$

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

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

$$+ 3056346216f_{n-3} + 240266188f_{n-4})/171354645 \qquad (84)$$

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

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

$$+ 450881640f_{n-2} + 75396384f_{n-3} + 2456234f_{n-4})/4036740015 \; . \qquad (85)$$

The coeffieicnts c_1, c_2, c_3, c_4 in the expressions for the asymptotic truncation errors of these methods are tabulated in Table I.

7. A Seventh Order Method

In this section we consider a method in which three intermediate calculations are performed within a step. We consider only the case $k = 2$ although the method of derivation would be the same for higher k. The method we seek then, will be defined by the equations

$$y_{n-u} = A_{11}\, y_{n-1} + A_{12}\, y_{n-2} + h(B_{11} f_{n-1} + B_{12}\, f_{n-2}) \tag{86}$$

$$y_{n-v} = A_{21}\, y_{n-1} + A_{22}\, y_{n-2} + h(b_{21}\, f_{n-u} + B_{21}\, f_{n-1} + B_{22}\, f_{n-2}) \tag{87}$$

$$y_{n-w} = A_{31}\, y_{n-1} + A_{32}\, y_{n-2} + h(b_{31}\, f_{n-u} + b_{32}\, f_{n-v} + B_{31}\, f_{n-1} + B_{32}\, f_{n-2}) \tag{88}$$

$$\hat{y}_n = A_{41}\, y_{n-1} + A_{42}\, y_{n-2} + h(b_{41}\, f_{n-u} + b_{42}\, f_{n-v} + b_{43}\, f_{n-w} + B_{41}\, f_{n-1} + B_{42}\, f_{n-2}) \tag{89}$$

$$\tilde{y}_n = A_1\, y_{n-1} + A_2\, y_{n-2} + h(b_1\, f_{n-u} + b_2\, f_{n-v} + b_3\, f_{n-w} + b_4\, \hat{f}_n + B_1\, f_{n-1} + B_2\, f_{n-2}) \tag{90}$$

where u, v, w are distinct from each other and from 0, 1, 2 and $A_{11}, A_{12}, \ldots, B_2$ are the coefficients for the method.

It is now our purpose to choose the various parameters so that $y_{n-u}, y_{n-v}, y_{n-w}, \hat{y}_n$ agree with their exact values with error $O(h^4)$ and so that $\tilde{y}_n$ agrees with y_n with error $O(h^8)$. As for the previous methods we shall identify the various coefficients in (86) - (90) as the numerators in the partial fraction expansions of certain rational functions

$$\varphi_1(z),\ \varphi_2(z),\ \varphi_3(z),\ \varphi_4(z),\ \varphi(z).$$

Setting $h = 1$ for simplicity we shall suppose that these functions are related by

$$b_1 \varphi_1(z) + b_2 \varphi_2(z) + b_3 \varphi_3(z) + b_4 \varphi_4(z) + z\varphi(z) = 0 \tag{91}$$

and that $\varphi_1, \varphi_2, \varphi_3, \varphi$ take the forms

$$\varphi_1(z) = - \frac{K_1}{(z+u)(z+1)^2(z+2)^2} \tag{92}$$

$$\varphi_2(z) = - \frac{K_2}{(z+v)(z+1)^2(z+2)^2} \left\{ 1 + \frac{L_{21}}{z+u} \left(1 + \frac{M_{21}}{z+u} \right) \right\} \tag{93}$$

$$\varphi_3(z) = - \frac{K_3}{(z+w)(z+1)^2(z+2)^2} \left\{ 1 + \frac{L_{31}}{z+u} \left(1 + \frac{M_{31}}{z+u} \right) + \frac{L_{32}}{z+v} \left(1 + \frac{M_{32}}{z+v} \right) \right\} \tag{94}$$

$$\varphi(z) = - \frac{1}{z^2(z+1)^2(z+2)^2} \left\{ \frac{L_1}{z+u} \left(1 + \frac{M_1}{z+u} \right) + \frac{L_2}{z+v} \left(1 + \frac{M_2}{z+v} \right) + \frac{L_3}{z+w} \left(1 + \frac{M_3}{z+w} \right) \right\} \tag{95}$$

For a rational function $\psi(z)$ let $\rho(\psi, z_o)$ denote the residue at $z = z_o$. Also denote by B the set of functions bounded in $\{ z: |z| \geqq R \}$ where R is some real constant satisfying $R > \max \{ 2, |u|, |v|, |w| \}$. Then using the type of analysis in the previous sections we see that $K_1, K_2, \ldots, M_3$ must be chosen so that the following conditions are satisfied.

$$\rho(\varphi_1, u) = -1 \quad , \tag{96}$$

$$\rho(\varphi_2, u) = 0 \quad , \tag{97}$$

$$\rho(\varphi_2, v) = -1 \quad , \tag{98}$$

$$\rho(\varphi_3,\ u) = 0 \quad , \tag{99}$$

$$\rho(\varphi_3,\ v) = 0 \quad , \tag{100}$$

$$\rho(\varphi_3,\ w) = -1 \quad , \tag{101}$$

$$\rho(\varphi,\ u) = 0 \quad , \tag{102}$$

$$\rho(\varphi,\ v) = 0 \quad , \tag{103}$$

$$\rho(\varphi,\ w) = 0 \quad , \tag{104}$$

$$\rho(\varphi,\ 0) = -1 \quad , \tag{105}$$

$$z^8\varphi(z) \in B \quad , \tag{106}$$

$$z^9\varphi(z) \in B \quad , \tag{107}$$

$$z^6\left\{b_1u\varphi_1(z) + b_2v\varphi_2(z) + b_3w\varphi_3(z)\right\} \in B \quad , \tag{108}$$

$$z^7\left\{b_1u\varphi_1(z) + b_2v\varphi_2(z) + b_3w\varphi_3(z)\right\} \in B \quad , \tag{109}$$

$$z^6\left\{b_1u^2\varphi_1(z) + b_2v^2\varphi_2(z) + b_3w^2\varphi_3(z)\right\} \in B \quad , \tag{110}$$

$$z^6\left\{(b_2vb_{21} + b_3wb_{31})\varphi_1(z) + b_3wb_{32}\varphi_2(z)\right\} \in B \ . \tag{111}$$

These constitute 16 independent conditions on u, v, w and the 15 constants $K_1, K_2, \ldots, M_3$. Hence u, v, w cannot be chosen independently. A tedious calculation yields the following relationship between these numbers

$$(6\pm12\sqrt{22}) - (6\pm8\sqrt{22})(u+v+w) + (8\pm6\sqrt{22})(uv+vw+wu) - (15\pm6\sqrt{22})\ uvw = 0 \tag{112}$$

where either value of the surd may be chosen. We select the values $v = \frac{2}{3}$, $w = \frac{1}{3}$, resulting in $u = (1312 - 4\sqrt{22})/819$ or its conjugate. As it happens, the conjugate value leads to an unstable method, so only the one value of u need be considered.

We are now in a position to compute $K_1, K_2, \ldots, M_3$ and hence, the coefficients $A_{11}, A_{12}, \ldots, B_2$. First we use (102), (103), (104) to compute M_1, M_2, M_3

and (105), (106), (107) to find L_1, L_2, L_3. We now determine $b_1\left(= \lim_{z \to -u} (z+u)^2 \varphi(z)\right)$, b_2, b_3. M_{21}, M_{31}, M_{32} are now found from (97), (99), (100); K_1 is found from (96) and then K_2 and K_3 from the simultaneous equations (108), (110). L_{21} is now given from (98) and L_{31}, L_{32} from the system (109) and (101). We are now in a position to compute the remaining coefficients and to substitute into (111) as a check. For the calculations performed by the author, this check was indeed satisfied.

Values of the coefficients are given in Table II in algebraic and in decimal form. For the number $(\alpha + \beta\sqrt{22})/\gamma$ the integers α, β, γ are given as is the decimal value rounded to 20D. That a method of the form we are considering should be (asymptotically) stable it is necessary and sufficient that $-1 < A_2 \leqq 1$. In our case, it is found that $A_2 = -751 + 160\sqrt{22} \approx -0.53$ so the method is stable.

8. Numerical Comparisons

In this section we present the results of numerical tests made using five different methods to solve the initial value problem

$$\frac{dy}{dx} = 3y/(2+x) - 1/y \quad , \qquad y(0) = 1 \tag{113}$$

and to give the result at $x = 10$. For each method, stepsizes $h = .4, .2, .1, .05$ were used and the results are shown in Fig. 4 as plots of the error E against the number N of derivative calculations performed. Attached to each curve is the order of the corresponding method. The methods used were

the 4th order Runge-Kutta method,

the 5th order method given by (17), (18), (19) of [2],

the 6th order method given by (62), (63), (64), (65) in this paper,

the 7th order method with coefficients in Table II,

the 8th order method given by (74), (75), (76), (77).

It should be emphasized that for many problems it would be unrealistic to measure the effort expended in obtaining a solution in terms of only the number of derivative evaluations. For the problem (113), for example, it would certainly be appropriate to take into account also the number of other multiplications performed. As far as Fig. 4 is concerned, this would have the effect of decreasing the relative advantage of a high order over a low order method. However, apart from the seventh order method which shows up rather badly, it appears that even for quite large stepsizes, the higher order methods are preferable for this problem.

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LIST OF FIGURES

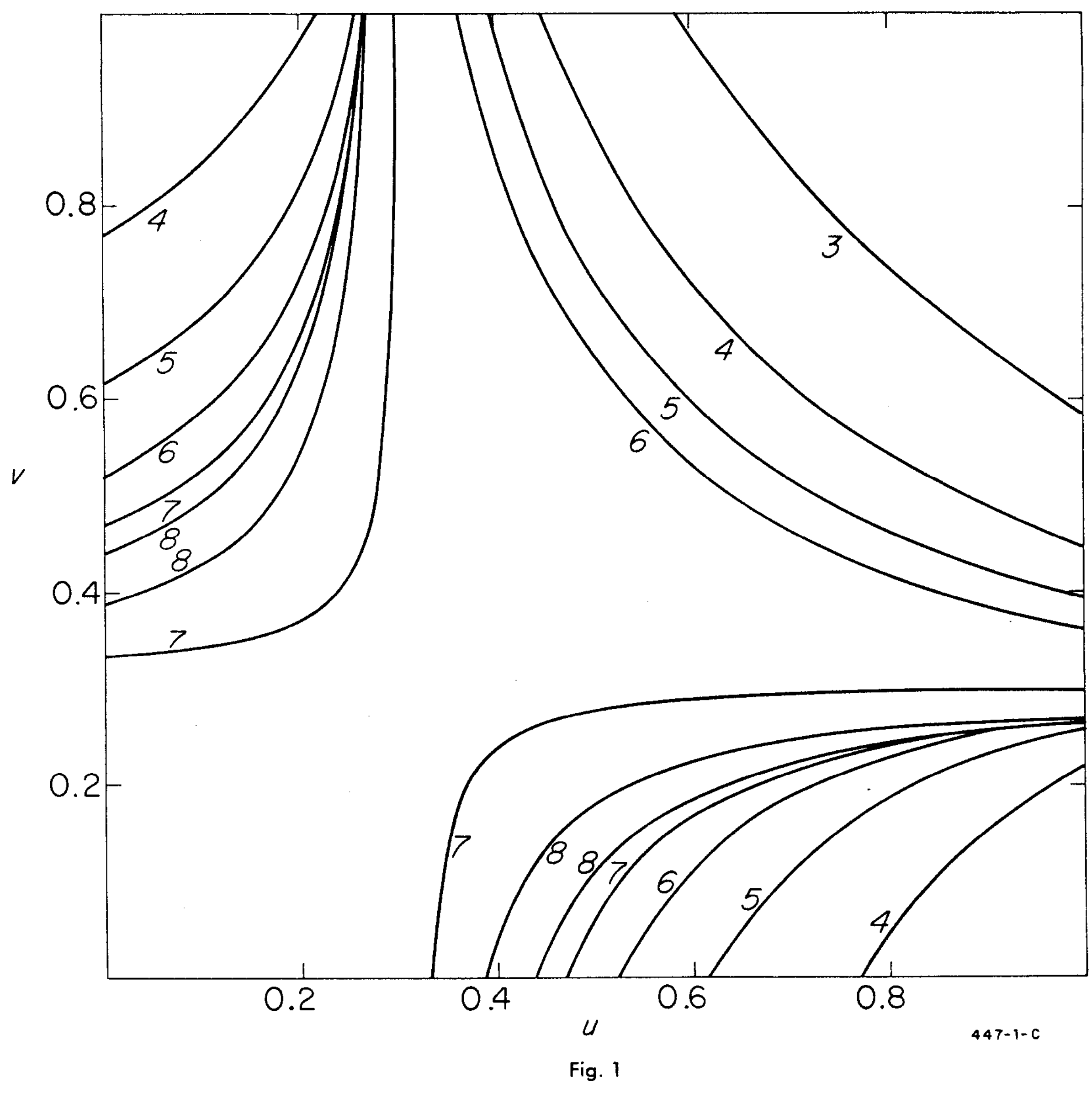

Fig. 1

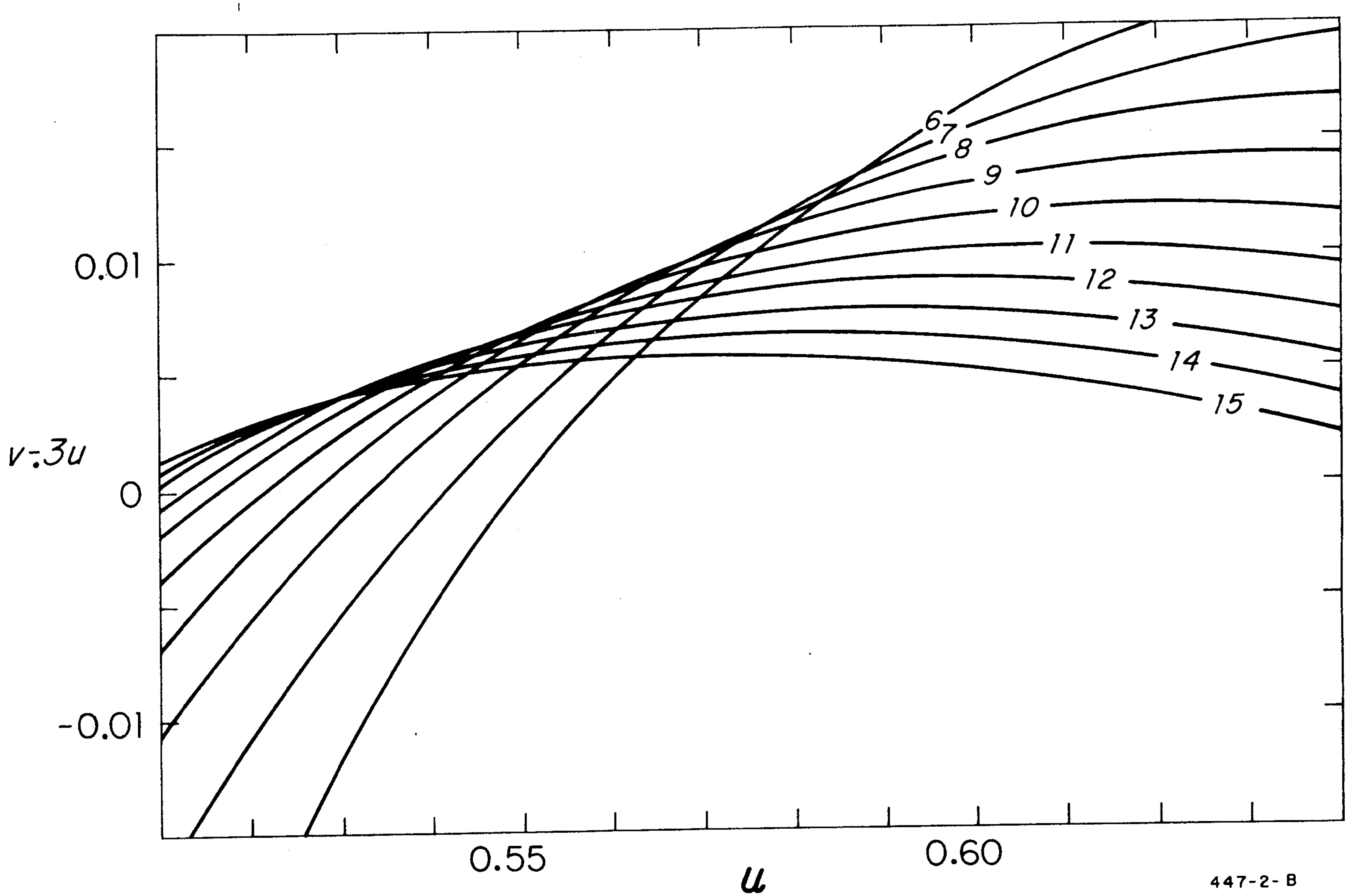

Fig. 2

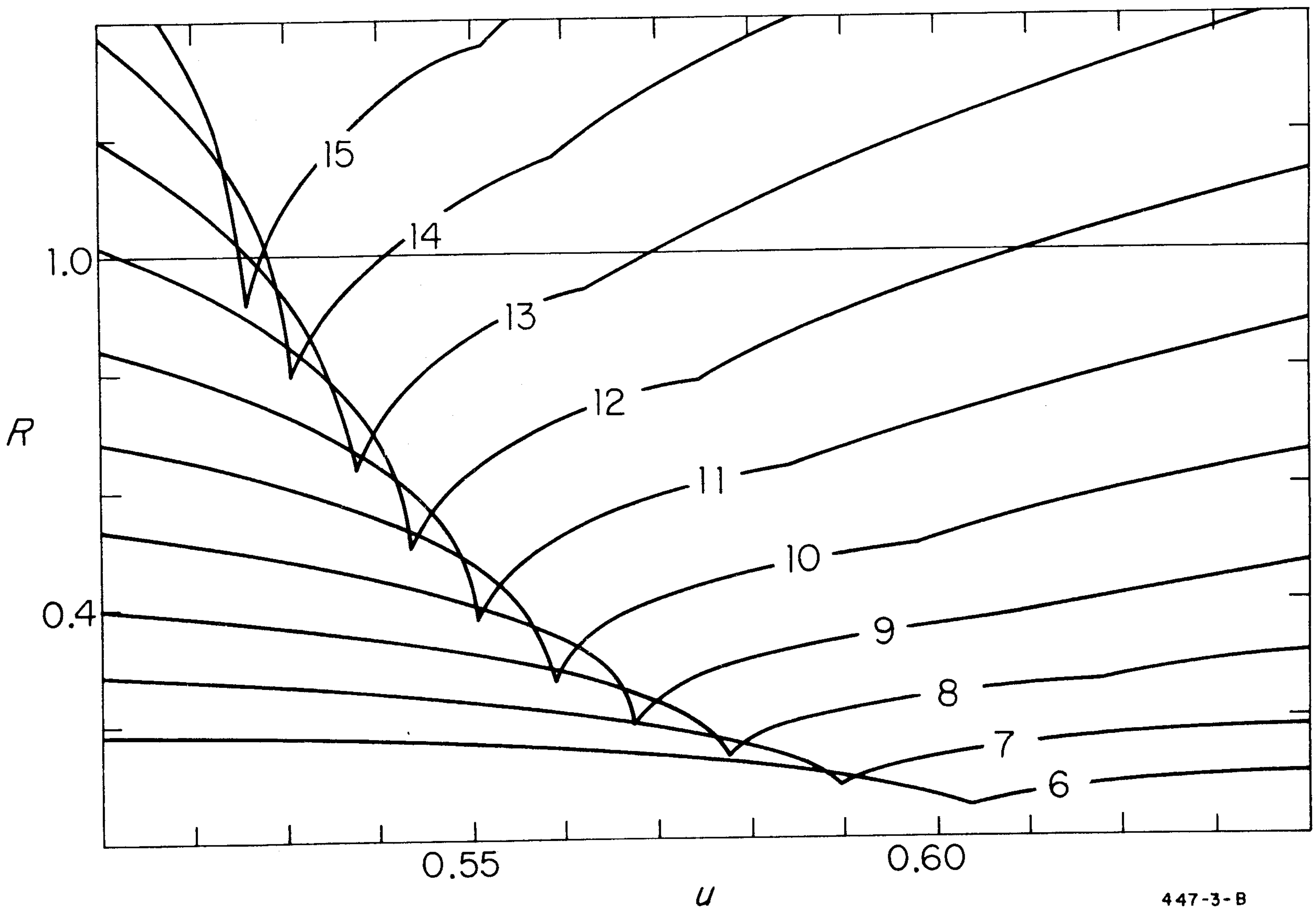

Fig. 3

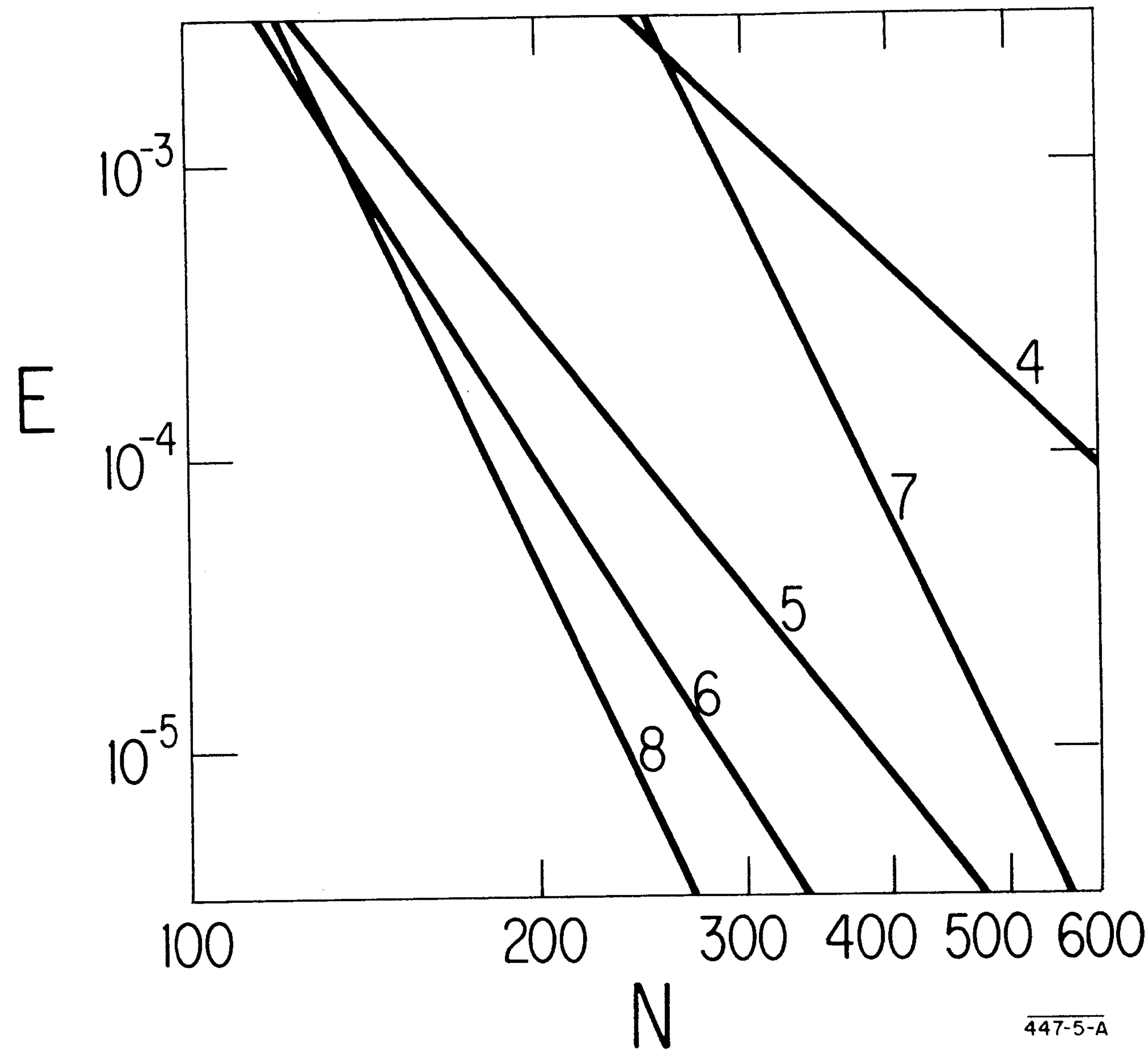

Fig. 4

TABLE I

k	u	v	c_1	c_2	c_3	c_4
2	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{4}{416745}$	$\frac{-26}{99225}$	$\frac{-8}{6615}$	$\frac{-2}{3969}$
2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{13}{997920}$	$\frac{13}{79200}$	$\frac{-3}{1760}$	$\frac{-1}{720}$
3	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{47}{43163400}$	$\frac{-3938}{70140525}$	$\frac{-854}{3340025}$	$\frac{-49}{770775}$
3	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{29}{28190400}$	$\frac{5787}{756442400}$	$\frac{-7533}{21612640}$	$\frac{-45}{187936}$
4	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{28027}{182900492775}$	$\frac{-1663988}{139004374509}$	$\frac{-42500}{735472881}$	$\frac{-74}{10557027}$
4	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{36923}{322939201200}$	$\frac{-2759}{3690733728}$	$\frac{-94815}{1230244576}$	$\frac{-1269}{27960104}$

TABLE II

	α	β	γ	
A_{11}	1920 04532	38 54416	5493 53259	0.38241 94033 79411 97879
A_{12}	3573 48727	-38 54416	5493 53259	0.61758 05966 20588 02121
B_{11}	-523 38100	-8 59232	5493 53259	-0.10260 83933 98362 64633
B_{12}	790 01654	-3 12140	5493 53259	0.14114 34015 44339 82287
A_{21}	78 37472	-6 59016	5 31657	8.92758 48293 62169 12157
A_{22}	-73 05815	6 59016	5 31657	-7.92758 48293 62169 12157
B_{21}	-1769 07184	207 90000	675 20439	-1.17584 30710 62836 24075
B_{22}	-4 47520	13878	5 31657	-0.71931 04014 15142 55364
b_{21}	-248 73684	22 64538	25 00757	-5.69909 80235 50856 99385
A_{31}	2356 68275	-248 08500	49 68243	24.01373 99926 73556 40526
A_{32}	-2307 00032	248 08500	49 68243	-23.01373 99926 73556 40526
B_{31}	-4 37253 79630	22536 17550	44167 68027	-7.50661 48265 39844 05295
B_{32}	-539 51980	-22 81995	198 72972	-3.25343 81526 74812 15826
b_{31}	-588 30744 33970	74 77481 18375	17 56892 17074	-13.52288 38441 74063 47633
b_{32}	13 53320	13 93235	40 74756	1.93586 34973 81829 94895
A_{41}	3659 24924	-1943 56296	49 58737	-110.04554 38107 13772 93095
A_{42}	-3609 66187	1943 56296	49 58737	111.04554 38107 13772 93095
B_{41}	-6 31513 79588	4 62481 58232	44083 17193	34.88217 92792 85014 55736
B_{42}	210 94684	741 45132	247 93685	14.87742 46203 01035 56676
b_{41}	-2 71216 34824 37940	1 24595 63159 44878	4655 62378 75273	67.27110 69634 10131 18380
b_{42}	41 87502	-133 65846	91 50659	-6.39340 54062 96196 43986
b_{43}	-11 22984	8 86248	21 54385	1.40823 83540 13788 06289
A_1	752	-160	1	1.53347 84282 51271 26950
A_2	-751	160	1	-0.53347 84282 51271 26950
B_1	-8 63124	1 84040	2667	0.03753 89718 42510 39455
B_2	-2 42355	51629	2910	-0.06650 33457 30637 63826
b_1	-10 42768 14958 67067	2 22142 25284 35759	2404 08358 09774	-0.34467 43420 54428 78832
b_2	43371	-9225	358	0.28467 76972 87325 02551
b_3	-6 99300	1 50984	19765	0.44916 43349 95228 32616
b_4	5787	-1207	1182	0.10631 82554 08731 41086