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On One-step Methods for Ordinary Differential Equations

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1. Introduction

Let us consider the initial value problem

$$y' = f(x, y), \quad y(x_0) = y_0, \tag{1.1}$$

where the function $f(x, y)$ is assumed to be sufficiently smooth and $y(x)$ denotes the solution to this problem. We are concerned with the case where this problem is solved numerically by explicit one-step methods. Various methods have been devised to obtain two approximations of different orders of accuracy after one or several steps of integration [1–6]. The discrepancy of these two approximations is often used for step-size control.

In Section 3 we raise the question: How many steps of integration by the r-stage method of order r with step-size h are required to obtain approximations of order $r+1$ without any extra evaluation of f? It is shown that two steps are necessary in the case $r=1, 2$ and that three steps are required in the case $r=3, 4$.

In Section 4 we are concerned with $2p$-stage block methods ($p=2, 3$) which produce approximations to $y(x_0+h)$ and $y(x_0+2h)$ simultaneously.

In Section 5 it is shown that each 4-stage method of order 4 makes it possible to construct methods of order 3 by incorporating the first value of f in the next step of integration.

2. Preliminaries

Let

$$x_j = x_0 + jh \qquad (j = 1, 2, \ldots), \tag{2.1}$$

$$z = y_0 + h\sum_{i=1}^{s} p_i k_i, \tag{2.2}$$

where

$$k_i = f(x_0 + a_i h,\ y_0 + h\sum_{j=1}^{i-1} b_{ij} k_j) \qquad (i = 1, 2, \ldots, s), \tag{2.3}$$

$$a_1 = 0,\ \sum_{j=1}^{i-1} b_{ij} = a_i \quad (i = 2, 3, \ldots, s), \qquad a_2 \neq 0. \tag{2.4}$$

Put

(2.5) $c_i = \sum_{j=2}^{i-1} a_j b_{ij},\ d_i = \sum_{j=2}^{i-1} a_j^2 b_{ij},\ e_i = \sum_{j=2}^{i-1} a_j^3 b_{ij} \qquad (i = 3, 4,\dots, s),$

(2.6) $l_i = \sum_{j=3}^{i-1} c_j b_{ij},\ m_i = \sum_{j=3}^{i-1} d_j b_{ij},\ g_i = \sum_{j=3}^{i-1} a_j c_j b_{ij} \qquad (i = 4, 5,\dots, s).$

Let D be the differential operator defined by

$$D = \frac{\partial}{\partial x} + k_1 \frac{\partial}{\partial y} \tag{2.7}$$

and put

(2.8) $$D^j f(x_0, y_0) = T^j,\ D^j f_y(x_0, y_0) = S^j \qquad (j = 1, 2,\dots),$$
$$(Df)^2(x_0, y_0) = P,\ (Df_y)^2(x_0, y_0) = Q,\ Df_{yy}(x_0, y_0) = R,$$
$$f_y(x_0, y_0) = f_y,\ f_{yy}(x_0, y_0) = f_{yy}.$$

Then z can be expanded into power series in h as follows:

(2.9) $$z = y_0 + hA_1k_1 + h^2A_2T + (h^3/2!)(A_3T^2 + 2A_4f_yT) + (h^4/3!)(B_1T^3$$
$$+ 6B_2TS + 3B_3f_yT^2 + 6B_4f_y^2T) + (h^5/4!)(C_1T^4 + 12C_2TS^2$$
$$+ 12C_3T^2S + 12C_4f_{yy}P + 4C_5f_yT^3 + 12C_6f_y^2T^2 + 24C_7f_y^3T$$
$$+ 24C_8f_yTS) + (h^6/5!)(D_1T^5 + 20D_2TS^3 + 30D_3T^2S^2$$
$$+ 20D_4T^3S + 60D_5f_{yy}TT^2 + 60D_6PR + 120D_7TQ + 60D_8f_yf_{yy}P$$
$$+ 60D_9f_yTS^2 + 60D_{10}f_yT^2S + 120D_{11}f_y^2TS + 5D_{12}f_yT^4$$
$$+ 20D_{13}f_y^2T^3 + 60D_{14}f_y^3T^2 + 120D_{15}f_y^4T) + O(h^7),$$

where

(2.10) $A_1 = \sum_{i=1}^{s} p_i,\ A_2 = \sum_{i=2}^{s} a_i p_i,$

(2.11) $A_3 = \sum_{i=2}^{s} a_i^2 p_i,\ B_1 = \sum_{i=2}^{s} a_i^3 p_i,\ C_1 = \sum_{i=2}^{s} a_i^4 p_i,\ D_1 = \sum_{i=2}^{s} a_i^5 p_i,$

(2.12) $A_4 = \sum_{i=3}^{s} c_i p_i,\ B_2 = \sum_{i=3}^{s} a_i c_i p_i,\ B_3 = \sum_{i=3}^{s} d_i p_i,\ C_2 = \sum_{i=3}^{s} a_i^2 c_i p_i,$
$C_3 = \sum_{i=3}^{s} a_i d_i p_i,\ C_4 = \sum_{i=3}^{s} c_i^2 p_i,\ C_5 = \sum_{i=3}^{s} e_i p_i,\ D_2 = \sum_{i=3}^{s} a_i^3 c_i p_i,$
$D_3 = \sum_{i=3}^{s} a_i^2 d_i p_i,\ D_4 = \sum_{i=3}^{s} a_i e_i p_i,\ D_5 = \sum_{i=3}^{s} c_i d_i p_i,\ D_6 = \sum_{i=3}^{s} a_i c_i^2 p_i,$

(2.13) $B_4 = \sum_{i=4}^{s} l_i p_i,\ C_6 = \sum_{i=4}^{s} m_i p_i,\ C_7 = \sum_{i=5}^{s} (\sum_{j=4}^{i-1} l_j b_{ij}) p_i,$
$C_8 = \sum_{i=4}^{s} (a_i l_i + g_i) p_i,\ D_7 = \sum_{i=4}^{s} a_i g_i p_i,$

(2.14) $D_8 = \sum_{i=4}^{s}(2c_il_i + \sum_{j=3}^{i-1}c_j^2b_{ij})p_i,\ D_9 = \sum_{i=4}^{s}(a_i^2l_i + \sum_{j=3}^{i-1}a_j^2c_jb_{ij})p_i,$

$D_{10} = \sum_{i=4}^{s}(a_im_i + \sum_{j=3}^{i-1}a_jd_jb_{ij})p_i,$

$D_{11} = \sum_{i=5}^{s}[\sum_{j=4}^{i-1}(a_il_j + a_jl_j + g_j)b_{ij}]p_i,$

$D_{12} = \sum_{i=3}^{s}(\sum_{j=2}^{i-1}a_j^4b_{ij})p_i,\ D_{13} = \sum_{i=4}^{s}(\sum_{j=3}^{i-1}e_jb_{ij})p_i,$

$D_{14} = \sum_{i=5}^{s}(\sum_{j=4}^{i-1}m_jb_{ij})p_i,\ D_{15} = \sum_{i=6}^{s}[\sum_{j=5}^{i-1}(\sum_{k=4}^{j-1}l_kb_{jk})b_{ij}]p_i.$

If it is required that $z-y(x_t)=O(h^7)$ $(t=1, 2,\dots)$, then the following conditions must be satisfied:

(2.15) $A_1 = t,\ A_2 = t^2/2,\ A_3 = 2A_4 = t^3/3,$

(2.16) $B_1 = 2B_2 = 3B_3 = 6B_4 = t^4/4,$

(2.17) $C_1 = 2C_2 = 3C_3 = 4C_4 = 4C_5 = 12C_6 = 24C_7 = 24C_8/7 = t^5/5,$

(2.18) $D_1 = 2D_2 = 3D_3 = 4D_4 = 6D_5 = 4D_6 = 8D_7 = 60D_8/13$

$= 15D_9/4 = 20D_{10}/3 = 10D_{11} = 5D_{12} = 20D_{13} = 60D_{14}$

$= 120D_{15} = t^6/6.$

If we impose the condition

(2.19) $$p_2 = 0,\ c_i = a_i^2/2,\ d_i = a_i^3/3 \qquad (i = 3, 4,\dots, s),$$

then it follows that

(2.20) $$2A_4 = A_3,\ 2B_2 = 3B_3 = B_1,\ 2C_2 = 3C_3 = 4C_4 = C_1,$$

$$2D_2 = 3D_3 = 6D_5 = 4D_6 = D_1,$$

(2.21) $$3a_2 = 2a_3,$$

(2.22) $$a_3^2b_{i3} + 3\sum_{j=4}^{i-1}a_j(a_j - a_2)b_{ij} = a_i^2(a_i - a_3) \qquad (i = 4, 5,\dots, s).$$

Suppose that

(2.23) $$y_1 = y_0 + h\sum_{i=1}^{r}q_ik_i$$

is a method of order r $(r\leq 4)$. Then after $n+1$ steps of integration with step-size h we have

(2.24) $$y_{n+1} = y_n + h\sum_{i=1}^{r}q_ik_{nr+i} \qquad (n = 0, 1,\dots),$$

where

$$k_{nr+i} = f(x_n + a_i h,\ y_n + h\textstyle\sum_{j=1}^{i-1} b_{ij} k_j) \qquad (i = 1, 2,\dots, r).$$

Since

$$y_n = y_0 + h\textstyle\sum_{m=0}^{n-1} \sum_{i=1}^{r} q_i k_{mr+i} \qquad (n = 1, 2,\dots),$$

we have

$$(2.25)\quad a_{nr+i} = n + a_i \qquad (i = 1, 2,\dots, r;\ n = 0, 1,\dots),$$

$$(2.26)\quad b_{nr+i\,mr+j} = q_j \qquad (j = 1, 2,\dots, r;\ m = 0, 1,\dots, n-1;\ n = 1, 2,\dots),$$

$$(2.27)\quad b_{nr+i\,nr+j} = b_{ij} \qquad (i > j;\ i = 1, 2,\dots, r;\ n = 0, 1,\dots).$$

Making use of the conditions

$$\textstyle\sum_{i=1}^{r} a_i^j q_i = 1/(j+1) \qquad (j = 0, 1,\dots, r-1),$$

$$\textstyle\sum_{i=1}^{r} c_i q_i = 1/6 \quad (r \geqq 3), \quad \sum_{i=1}^{r} d_i q_i = 1/12 \quad (r = 4),$$

from (2.5), (2.6) and (2.25)–(2.27) we have

$$(2.28)\quad \begin{aligned} c_{nr+i} &= n^2/2 + na_i + c_i \qquad (r \geqq 2), \\ d_{nr+i} &= n^3/3 + n^2 a_i + 2nc_i + d_i \qquad (r \geqq 3), \\ e_{nr+i} &= n^4/4 + n^3 a_i + 3n^2 c_i + 3nd_i + e_i \qquad (r = 4), \\ l_{nr+i} &= n^3/6 + n^2 a_i/2 + nc_i + l_i \qquad (r = 4), \\ m_{nr+i} &= n^4/12 + n^3 a_i/3 + n^2 c_i + 2nl_i + m_i \qquad (r = 4) \\ &\qquad (i = 1, 2,\dots, r;\ n = 0, 1,\dots), \end{aligned}$$

where

$$c_j = d_j = e_j = 0 \quad (j = 1, 2), \quad l_k = m_k = 0 \quad (k = 1, 2, 3).$$

3. Methods with a few steps of integration

For each one-step method (2.23) of order r we seek the formulas

$$(3.1)\quad z_t = y_0 + h\textstyle\sum_{j=1}^{pr} p_{tj} k_j \qquad (t = 1, 2,\dots, p)$$

such that

$$(3.2)\quad z_t - y(x_t) = O(h^{r+2})$$

and the formulas

(3.3) $$w_t = y_0 + h\sum_{j=1}^{qr+1} p_{tj}k_j \qquad (t = 1, 2,\dots, q)$$

such that

(3.4) $$w_t - y(x_t) = O(h^{r+2}).$$

Comparison of Euler's method with the modified Euler method shows that such formulas exist only for $p \geqq 2$ and $q \geqq 1$ in the case $r=1$. Hence we have only to consider the cases $r \geqq 2$.

3.1. Case r=2

The method of order 2 is given by

$$y_1 = y_0 + h[k_1 + (k_2 - k_1)/(2a_2)].$$

By (2.25) and (2.28) the condition (3.2) with $p=2$ yields the equations:

$$p_1 + p_2 + p_3 + p_4 = t,$$

$$a_2p_2 + p_3 + (1 + a_2)p_4 = t^2/2,$$

$$a_2^2p_2 + p_3 + (1 + a_2)^2p_4 = t^3/3,$$

$$p_3 + (1 + 2a_2)p_4 = t^3/3 \qquad (t = 1, 2),$$

which can be reduced to

$$p_1 + p_3 = t,\ p_2 + p_4 = 0,\ p_3 + p_4 = t^2/2,\ a_2p_4 = t^2(2t - 3)/12.$$

Hence the choice $p_4 = 0$ is impossible and we have the formulas

(3.5) $$z_1 = y_0 + h(k_1 + k_3 - m)/2,\ z_2 = y_0 + 2h(k_3 + m),$$

where

$$m = (k_1 - k_2 - k_3 + k_4)/(6a_2),$$

$$z_1 - y(x_1) = -(h^4/4!)[a_2T^3 + 2a_2TS + (2 - 3a_2)f_yT^2 + 2f_y^2T] + O(h^5),$$

$$z_2 - y(x_2) = (h^4/3!)[(a_2 - 1)(T^3 + 3f_yT^2) + (2a_2 - 3)TS - 3f_y^2T] + O(h^5).$$

Thus we have the following

THEOREM 1. *For each one-step method of order* 2 *the formulas* (3.1) *satisfying* (3.2) *exist only for* $p \geqq 2$ *and are given by* (3.5) *when* $p=2$. *The formulas* (3.3) *satisfying* (3.4) *do not exist for* $q=1$.

EXAMPLE 1. For the improved Euler method we have $a_2=1$,

$$z_1 = y_0 + h(5k_1 + k_2 + 7k_3 - k_4)/12, \quad z_2 = y_0 + h(k_1 - k_2 + 5k_3 + k_4)/3,$$

where

$$z_2 - y(x_2) = -(h^4/3!)(TS + 3f_y^2T) + O(h^5).$$

EXAMPLE 2. For the modified Euler method we have $a_2=1/2$,

$$z_1 = y_0 + h(2k_1 + k_2 + 4k_3 - k_4)/6, \ z_2 = y_0 + 2h(k_1 - k_2 + 2k_3 + k_4)/3,$$

where

$$z_2 - y(x_2) = -(h^4/3!)[(T^3 + 3f_yT^2)/2 + 2TS + 3f_y^2T] + O(h^5).$$

3.2. Case r=3

For the method of order 3 the following equations must be satisfied:

$$a_3(a_3 - a_2) = (2 - 3a_2)c_3, \ \textstyle\sum_{i=1}^3 q_i = 1, \ \sum_{i=2}^3 a_iq_i = 1/2, \ 6c_3q_3 = 1.$$

From these it follows that $c_3 \neq 0$, and the condition (3.2) with $p=3$ yields the equations:

$$p_1 + p_4 + p_7 = t, \ p_2 + p_5 + p_8 = 0, \ p_3 + p_6 + p_9 = 0,$$

$$p_4 + p_5 + p_6 + 2p_7 + 2p_8 + 2p_9 = t^2/2,$$

$$a_2p_5 + a_3p_6 + p_7 + (1 + 2a_2)p_8 + (1 + 2a_3)p_9 = t^2(2t - 3)/12,$$

$$c_3p_6 - 2a_2p_8 + 2(c_3 - a_3)p_9 = -t^2(t - 2)^2/12,$$

$$p_7 + (1 + 6a_2)p_8 + (1 + 6a_3)p_9 = t^2(3t^2 - 10t + 9)/12.$$

From these p_j $(j=1, 2,\dots, 7)$ are determined uniquely for any given p_8 and p_9.

The choice $p_{t8}=p_{t9}=0$ $(t=1, 2)$ leads to the formulas

(3.6) $$w_1 = y_0 + h(4k_1 + k_4 + k_7)/6 - hp_2(k_1 - k_2 - k_4 + k_5) - hp_3(k_1 - k_3 - k_4 + k_6),$$

(3.7) $$w_2 = y_0 + h(k_1 + 4k_4 + k_7)/3,$$

where

$$a_2p_2 + a_3p_3 = 1/4, \ 12c_3p_3 = 1,$$

$$w_2 - y(x_2) = (h^5/5!)(2/3)[2(T^4 + 6TS^2 + 4T^2S + 3f_{yy}P) + (20a_2 + 20a_3$$

$$- 30a_2a_3 - 13)f_yT^3 + (30a_2 - 13)f_y^2T^2 - 13f_y^3T$$

$$+ (60a_3 - 31)f_yTS] + O(h^6).$$

The choice $p_{tk}=0$ $(k=7, 8, 9;\ t=1, 2)$ is impossible because $t^2(3t^2-10t+9)\neq 0$ for $t>0$. Thus we have the following

THEOREM 2. *For each one-step method of order* 3 *the formulas* (3.1) *satisfying* (3.2) *exist only for* $p\geqq 3$. *The formulas* (3.3) *satisfying* (3.4) *with* $q=2$ *exist and are given by* (3.6) *and* (3.7).

EXAMPLE 3. For Kutta's method we have

$$z_1 = y_0 + h(636k_1 + 599k_2 + 88k_3 + 1658k_4 - 734k_5 - 60k_6$$

$$+ 46k_7 + 135k_8 - 28k_9)/2340,$$

$$z_2 = y_0 + h(229k_1 + 374k_2 + 93k_3 + 1142k_4 - 300k_5 - 74k_6$$

$$+ 789k_7 - 74k_8 - 19k_9)/1080,$$

$$z_3 = y_0 + 3h(27k_1 + 286k_2 + 97k_3 + 381k_4 - 432k_5 - 159k_6$$

$$+ 812k_7 + 146k_8 + 62k_9)/1220,$$

where

$$z_3 - y(x_3) = (h^5/5!)(3/122)(-121T^4 - 798TS^2 - 223T^2S - 275f_{yy}P$$

$$+ 12f_yT^3 + 117f_y^2T^2 - 798f_y^3T + 798f_yTS) + O(h^6).$$

EXAMPLE 4. For Heun's method we have

$$z_1 = y_0 + h(81k_1 + 46k_2 + 117k_3 + 237k_4 - 92k_5 - 93k_6 + 42k_7$$

$$+ 46k_8 - 24k_9)/360,$$

$$z_2 = y_0 + h(187k_1 - 81k_2 + 558k_3 + 505k_4 + 162k_5 - 495k_6$$

$$+ 808k_7 - 81k_8 - 63k_9)/750,$$

$$z_3 = y_0 + 3h(87k_1 - 186k_2 + 523k_3 - 110k_4 + 372k_5 - 710k_6$$

$$+ 823k_7 - 186k_8 + 187k_9)/800,$$

where

$$z_3 - y(x_3) = (h^5/5!)(-181T^4 - 807TS^2 - 54T^2S - 264f_{yy}P$$

$$+ 60f_yT^3 + 96f_y^2T^2 - 804f_y^3T + 798f_yTS)/60 + O(h^6).$$

3.3. Case r=4

For the method of order 4 the following equations must be satisfied:

$$(3.8)\quad a_3(a_3-a_2)=2(1-2a_2)c_3,\ (1-a_3)c_4=(3-4a_3)c_3b_{43},\ a_4=1,$$

$$(1-a_2)(1-a_3)=2[3-4(a_2+a_3)+6a_2a_3]c_3b_{43},$$

$$\textstyle\sum_{i=1}^4 q_i=1,\ \sum_{i=2}^4 a_iq_i=1/2,\ 24(1-a_3)c_3q_3=1,\ 24c_3b_{43}q_4=1.$$

From these it follows that $(1-a_3)c_3b_{43}\neq 0$, and the condition (3.2) with $p=3$ yields the equations:

$$p_1+p_5+p_9=t,\ p_2+p_6+p_{10}=0,\ p_3+p_7+p_{11}=0,$$

$$p_4+p_8+p_{12}=0,\ p_5+p_6+p_7+p_8+2p_9+2p_{10}+2p_{11}+2p_{12}=t^2/2,$$

$$a_2^2p_6+(a_3^2-2c_3)p_7+(1-2c_4)p_8=0,$$

$$2(a_3-1)c_3p_7+a_2p_{10}+[a_3+4(a_3-1)c_3]p_{11}+p_{12}=t^2(t-2)^2/24,$$

$$(a_3-1)p_7+b_{43}p_8+2(a_3-1)p_{11}+2b_{43}p_{12}=0,$$

$$p_9+(1+6a_2)p_{10}+(1+6a_3)p_{11}+7p_{12}=t^2(3t^2-10t+9)/12,$$

$$a_2^2p_{10}+(a_3^2-2c_3)p_{11}+(1-2c_4)p_{12}=0,$$

$$c_3p_{11}+c_4p_{12}=t^2(3t^3-15t^2+25t-15)/360.$$

From these p_j $(j=1, 2,\dots, 11)$ are determined uniquely for any given p_{12}. The choice $p_{tk}=0$ $(k=10, 11, 12;\ t=1, 2)$ is impossible because $3t^3-15t^2+25t-15\neq 0$ for $t=1, 2$. Thus we have the following

THEOREM 3. *For each one-step method of order* 4 *the formulas* (3.1) *satisfying* (3.2) *exist only for* $p\geqq 3$ *and the formulas* (3.3) *satisfying* (3.4) *do not exist for* $q=2$.

EXAMPLE 5. For the Runge-Kutta method we have

$$z_1=y_0+h(71k_1+90k_2+90k_3+55k_4+138k_5-76k_6-76k_7$$
$$-58k_8+151k_9-14k_{10}-14k_{11}+3k_{12})/360,$$

$$z_2=y_0+h(41k_1+30k_2+30k_3+25k_4+168k_5-16k_6-16k_7$$
$$-28k_8+151k_9-14k_{10}-14k_{11}+3k_{12})/180,$$

$$z_3 = y_0 + h(101k_1 + 38k_2 + 38k_3 + 57k_4 + 508k_5 - 120k_6 - 120k_7 - 136k_8 + 591k_9 + 82k_{10} + 82k_{11} + 79k_{12})/400,$$

where

$$z_3 - y(x_3) = (h^6/6!)(3/80)(-33T^5 - 330TS^3 - 428T^2S^2 - 350T^3S - 143f_{yy}TT^2 - 462PR - 528TQ + 176f_yf_{yy}P - 386f_yTS^2 + 328f_yT^2S + 744f_y^2TS - 746f_yT^4 + 10f_y^2T^3 + 244f_y^3T^2 - 656f_y^4T) + O(h^7).$$

EXAMPLE 6. For the method with $a_2=1/3$, $a_3=2/3$, $b_{21}=a_2$, $b_{31}=-1/3$, $b_{32}=b_{41}=b_{43}=1$, $b_{42}=-1$, $q_1=q_4=1/8$, $q_2=q_3=3/8$ we have

$$z_1 = y_0 + h(167k_1 + 249k_2 + 285k_3 + 107k_4 + 392k_5 - 192k_6 - 264k_7 - 112k_8 + 401k_9 - 57k_{10} - 21k_{11} + 5k_{12})/960,$$

$$z_2 = y_0 + h(13k_1 + 9k_2 + 15k_3 + 7k_4 + 52k_5 - 12k_7 - 8k_8 + 55k_9 - 9k_{10} - 3k_{11} + k_{12})/60,$$

$$z_3 = y_0 + h(43k_1 + 5k_2 + 25k_3 + 15k_4 + 210k_5 - 34k_6 - 74k_7 - 38k_8 + 227k_9 + 29k_{10} + 49k_{11} + 23k_{12})/160,$$

where

$$z_3 - y(x_3) = (h^6/6!)(-152T^5 - 1716TS^3 - 1992T^2S^2 - 920T^3S - 1548f_{yy}TT^2 - 3048PR - 1800TQ - 864f_yf_{yy}P - 2124f_yTS^2 + 1161f_yT^2S + 3024f_y^2TS - 92f_yT^4 + 72f_y^2T^3 - 252f_y^3T^2 - 1872f_y^4T)/72 + O(h^7).$$

EXAMPLE 7. For the method with $a_2=1/3$, $a_3=1/2$, $b_{21}=a_2$, $b_{31}=1/8$, $b_{32}=3/8$, $b_{41}=1/2$, $b_{42}=-3/2$, $b_{43}=2$, $q_1=q_4=1/6$, $q_2=0$ and $q_3=2/3$ we have

$$z_1 = y_0 + h(109k_1 + 260k_3 + 75k_4 + 227k_5 - 228k_7 - 77k_8 + 204k_9 - 32k_{11} + 2k_{12})/540,$$

$$z_2 = y_0 + h(178k_1 + 240k_3 + 95k_4 + 744k_5 - 136k_7 - 104k_8 + 608k_9 - 104k_{11} + 9k_{12})/765,$$

$$z_3 = y_0 + h(159k_1 + 108k_3 + 81k_4 + 807k_5 - 372k_7 - 201k_8 + 894k_9 + 264k_{11} + 120k_{12})/620,$$

where

$$z_3 - y(x_3) = (h^6/6!)(9/248)[39(T^5 + 10TS^3 + 10T^2S^2 + 10f_{yy}TT^2 + 15PR) - 208T^3S + 284TQ + 113f_yf_{yy}P - 176f_yTS^2 + 656f_yT^2S + 704f_y^2TS - 21f_yT^4 - 32f_y^2T^3 - 84f_y^3T^2 - 704f_y^4T] + O(h^7).$$

3.4. Numerical examples

The following six problems are solved by the five methods in Examples 3–7.

Problem I. $y' = 2xy,\ y(1) = 1.$
Problem II. $y' = -5y,\ y(0) = 1.$
Problem III. $y' = 2y/x^3,\ y(1) = 1.$
Problem IV. $y' = 1 - y^2,\ y(0) = 0.$
Problem V. $y' = -y^2,\ y(0) = 1.$
Problem VI. $y' = y - 2x/y,\ y(0) = 1.$

Two approximations $z(x)$ and $u(x)$ of $y(x)$ are computed for comparison. $z(x)$ is obtained by the following program:

(i) compute y_j and z_j $(j=1, 2, 3)$;
(ii) if $|y_3 - z_3| > \varepsilon \max(|y_3|, 1)$, halve the step-size and go to (i);
(iii) if $|y_3 - z_3| \leqq \delta \max(|y_3|, 1)$, double the step-size;
(iv) replace x_0 and y_0 by x_3 and z_3 respectively. (Initially $h=1$.)

$u(x)$ is computed by the usual process with the corresponding step-size. The errors of $z(5)$ and $u(5)$ are listed in Tables 1 and 2, where $\varepsilon = 10^{-5}$, $\delta = \varepsilon/32$ when $r=3$ and $\varepsilon = 10^{-6}$, $\delta = \varepsilon/64$ when $r=4$. It seems that this method of correction and step-size control works fairly well.

TABLE 1. Methods of order 3

M / P	3		4	
	z	u	z	u
I	−9.283+05	−9.583+06	−5.529+05	−9.383+06
II	2.662−09	−3.442−11	9.950−10	−3.442−11
III	−3.160−06	2.184−05	1.302−05	1.534−05
IV	−4.420−07	9.527−07	−2.657−07	9.459−07
V	4.689−07	−2.757−06	−1.041−08	−3.910−06
VI	−9.082−03	2.092−02	−4.223−03	3.291−02

TABLE 2. Methods of order 4

P \ M	5		6		7	
	z	u	z	u	z	u
I	−9.522+04	−6.780+05	−1.082+05	−6.944+05	−9.987+04	−6.770+05
II	−3.972−11	1.558−10	−5.580−11	1.558−10	−5.211−11	1.558−10
III	−8.789−08	1.263−06	−2.528−07	2.205−06	1.402−06	1.870−06
IV	2.768−08	−8.610−08	2.301−08	−8.606−08	3.244−08	−8.607−08
V	−7.944−09	8.633−08	−5.080−08	3.154−08	−2.641−08	1.433−07
VI	1.326−02	2.289−02	2.106−03	3.191−03	1.508−02	1.880−02

4. Block methods with two points

We shall show the following

THEOREM 4. *For $p=2$, 3 there exist the formulas*

(4.1) $$y_1 = y_0 + h\sum_{i=1}^{2p} q_i k_i,\ y_2 = y_0 + h\sum_{i=1}^{2p} p_i k_i,$$

$$m_1 = h\sum_{i=1}^{2p} r_i k_i,\ m_2 = h\sum_{j=1}^{2p+1} s_j k_j,$$

such that

(4.2) $$y_1 - y(x_1) = O(h^{p+2}),\ y_2 - y(x_2) = O(h^{p+3}),$$

$$m_1 = O(h^{p+1}),\ m_2 = O(h^{p+2}),$$

where $k_{2p+1} = f(x_2, y_2)$.

The methods $z_j = y_2 + m_j$ $(j=1, 2)$ are of orders $p+j-1$. If y_2 is accepted as an approximation to $y(x_2)$, then k_{2p+1} can be used as k_1 in the next step of integration.

4.1. Case p=2

The condition (4.2) yields the following equations:

(4.3) $$\sum_{i=1}^{4} p_i = 2,\ \sum_{i=2}^{4} a_i p_i = 2,\ 3(2 - a_3)c_3 p_3 = 2,\ 3c_3 b_{43} p_4 = 2,$$

$$a_4 = 2,\ a_3(a_3 - a_2) = 2(1 - a_2)c_3,\ 2(2 - a_2)(2 - a_3) = Kc_3 b_{43},$$

$$(2 - a_3)c_4 = (3 - 2a_3)c_3 b_{43},$$

(4.4) $$\sum_{i=1}^{4} q_i = 1,\ \sum_{i=2}^{4} a_i q_i = 1/2,\ 6(2 - a_3)c_3 q_3 = 5 - 3a_3,\ 6c_3 b_{43} q_4 = -1,$$

(4.5) $$\sum_{i=1}^{4} r_i = 0,\ \sum_{i=2}^{4} a_i r_i = 0,$$

(4.6) $$\sum_{j=1}^{5} s_j = 0,\ \sum_{j=2}^{5} a_j s_j = 0,\ c_3 s_3 + c_4 s_4 + 2s_5 = 0,$$

$$c_3 b_{43} s_4 + 2s_5 = 0,$$

where

$$K = 6 - 4X + 3Y,\ X = a_2 + a_3,\ Y = a_2 a_3.$$

From (4.3) it follows that $(2-a_3)c_3 b_{43} \neq 0$, and we have

$$\text{(4.7)}\quad y_1 - y(x_1) = (h^4/4!)(F_1 T^3 + 3F_2 TS + F_3 f_y T^2 + F_4 f_y^2 T) + O(h^5),$$

$$y_2 - y(x_2) = 8(h^5/5!)(G_1 T^4 + G_2 TS^2 + G_3 T^2 S + G_4 f_{yy} P + G_5 f_y T^3 + G_6 f_y^2 T^2 + G_7 f_y^3 T + G_8 f_y TS) + O(h^6),$$

$$m_1 = (h^3/2)(\tilde{A}_3 T^2 + 2\tilde{A}_4 f_y T) + O(h^4),$$

$$m_2 = 2s_5(h^4/3!)(B_1^* T^3 + 3B_2^* TS + B_3^* f_y T^2 + B_4^* f_y^2 T) + O(h^5),$$

where

$$\text{(4.8)}\quad F_1 = -5 + 4X - 4Y,\ F_2 = 4a_3 - 5,\ F_3 = 6a_2 - 5,\ F_4 = -5,$$

$$G_1 = (6 - 5X + 5Y)/6,\ G_2 = 6 - 5a_3,\ G_3 = 4 - 5a_2,\ G_5 = -4G_1,$$

$$G_6 = -G_3,\ G_7 = -4,\ G_8 = 2(5a_3 - 4),$$

$$G_4 = 5[c_3 + (3 - 2a_3)c_4]/(2 - a_3) - 12,$$

$$\tilde{A}_3 = 2(1 - a_2)\tilde{r}_3 + K\tilde{r}_4,\ \tilde{A}_4 = \tilde{r}_3 + (3 - 2a_3)\tilde{r}_4,\ \tilde{r}_3 = c_3 r_3,$$

$$\tilde{r}_4 = c_3 b_{43} r_4/(2 - a_3),\ B_1^* = 2(1 - a_2)(a_3 - 1),\ B_2^* = 3(a_3 - 1),$$

$$B_3^* = 3a_2 - 2,\ B_4^* = -2.$$

Since $2(1-a_2)(3-2a_3)-K=a_2(a_3-2)\neq 0$, it is seen that $\tilde{A}_3=\tilde{A}_4=0$ if and only if $\tilde{r}_3=\tilde{r}_4=0$, namely $r_i=0$ $(i=1, 2, 3, 4)$. Hence there exists no formula $m_1\not\equiv 0$ such that $m_1=O(h^4)$. The method y_1 cannot be of order 4 because $F_4\neq 0$.

EXAMPLE 8. For the choice $a_2=4/5$, $a_3=6/5$, $r_3=-5r_4$, $r_4=1/36$ and $s_5=1/3$ we have $b_{21}=a_2$, $b_{31}=-3/10$, $b_{32}=3/2$, $b_{41}=19/22$, $b_{42}=-15/22$, $b_{43}=20/11$,

$$y_1 = y_0 + h(55k_1 + 65k_2 + 35k_3 - 11k_4)/144,$$

$$y_2 = y_0 + h(11k_1 + 25k_2 + 25k_3 + 11k_4)/36,$$

$$m_1 = h(-k_1 + 5k_2 - 5k_3 + k_4)/36,$$

$$m_2 = h(-k_1 + 5k_2 - 5k_3 - 11k_4 + 12k_5)/36,$$

where

$$y_1 - y(x_1) = -(h^4/4!)(21T^3 + 15TS + 5f_yT^2 + 125f_y^2T)/25 + O(h^5),$$

$$y_2 - y(x_2) = (h^5/5!)(16/15)[T^4 + (135/11)f_{yy}P - 4f_yT^3 - 30f_y^3T + 30f_yTS] + O(h^6),$$

$$m_1 = -(h^3/3!)8f_yT/5 + (h^4/4!)16[T^3/75 - (9TS + 3f_yT^2 - 5f_y^2T)/55] + O(h^5),$$

$$m_2 = (h^4/4!)(16/75)(2T^3 - 15TS + 5f_yT^2 - 25f_y^2T) + O(h^5).$$

4.2. Case p=3

In this section we impose the condition (2.19). Then the condition (4.2) yields the following equations:

(4.9) $\sum_{i=1}^6 p_i = 2,\ \sum_{i=3}^6 a_ip_i = 2,\ \sum_{i=4}^6 a_i(a_i - a_3)p_i = 2(4 - 3a_3)/3,$

$\sum_{i=5}^6 a_i^j\alpha_ip_i = A_j \quad (j = 0, 1),\ w_5p_5 + w_6p_6 = 4(1 - a_3)/3,$

$\alpha_5b_{65}p_6 = 4(6 - 5X + 5Y)/15,$

$(a_6 - a_5)w_6p_6 = 32/15 - 2a_3 - 4(1 - a_3)a_5/3,$

$w_5b_{65}p_6 = 2(4 - 5a_3)/15,$

(4.10) $\sum_{i=1}^6 q_i = 1,\ \sum_{i=3}^6 a_iq_i = 1/2,\ \sum_{i=4}^6 a_i(a_i - a_3)q_i = (2 - 3a_3)/6,$

$\sum_{i=5}^6 \alpha_iq_i = B,\ w_5q_5 + w_6q_6 = (1 - 2a_3)/12,$

(4.11) $\sum_{i=1}^6 r_i = 0,\ \sum_{i=3}^6 a_i^kr_i = 0 \quad (k = 1, 2),$

(4.12) $\sum_{j=1}^7 s_j = 0,\ \sum_{j=3}^7 a_j^ks_j = 0 \quad (k = 1, 2, 3),\ 3\sum_{i=4}^6 l_is_i + 4s_7 = 0,$

where

$$p_2 = q_2 = r_2 = s_2 = 0,\ a_7 = 2,\ X = a_3 + a_4,\ Y = a_3a_4,$$

$$\alpha_i = a_i(a_i - a_3)(a_i - a_4),\ w_i = \sum_{j=4}^{i-1} a_j(a_j - a_3)b_{ij} \quad (i = 5, 6),$$

$$A_0 = 2(6 - 4X + 3Y)/3,\ A_1 = 4(24 - 15X + 10Y)/15,$$

$$B = (3 - 4X + 6Y)/12.$$

From these it follows that

$$(a_6 - 2)\sigma\alpha_5 = 0,\ \sigma = (5a_3^2 - 8a_3 + 4)a_4 - 2a_3,$$

$$(A_1 - a_5A_0)w_6 = [32/15 - 2a_3 - 4(1 - a_3)a_5/3]\alpha_6,$$

$$(A_1 - a_6A_0)w_5 = [32/15 - 2a_3 - 4(1 - a_3)a_6/3]\alpha_5.$$

EXAMPLE 9. For the choice $a_3=1/2$, $a_4=6/5$, $a_5=8/5$, $r_6=-22r_5/75$, $r_5=125/264$ and $s_7=-5/7$ we have $a_2=b_{21}=1/3$, $a_6=2$, $b_{31}=1/8$, $b_{32}=3/8$, $b_{41}=132/125$, $b_{42}=-486/125$, $b_{43}=504/125$, $b_{51}=-148/125$, $b_{52}=5208/875$, $b_{53}=-3872/875$, $b_{54}=44/35$, $b_{61}=9/5$, $b_{62}=-294/35$, $b_{63}=3336/385$, $b_{64}=-10/7$, $b_{65}=15/11$,

$$y_1 = y_0 + h(2233k_1 + 10880k_3 + 1650k_4 + 175k_5 - 154k_6)/14784,$$

$$y_2 = y_0 + h(847k_1 + 4096k_3 + 2750k_4 + 2625k_5 + 770k_6)/5544,$$

$$m_1 = 5h(-77k_1 + 256k_3 - 550k_4 + 525k_5 - 154k_6)/5544,$$

$$m_2 = 5h(-77k_1 + 256k_3 - 550k_4 + 525k_5 + 638k_6 - 792k_7)/5544,$$

where

$$y_2 - y(x_2) = (h^6/6!)(16/5)(T^3S + 3TQ + f_yf_{yy}P + f_yTS^2 + f_yT^2S - 12f_y^2TS - f_y^2T^3 - f_y^3T^2 + 7f_y^4T) + O(h^7),$$

$$m_2 = -(h^5/5!)(2/21)[7(T^4 + 6TS^2 + 4T^2S + 3f_{yy}P) - 16(f_yT^3 + f_y^2T^2) + 396f_y^3T - 216f_yTS] + O(h^6).$$

EXAMPLE 10. For the choice $a_3=1/2$, $a_4=1$, $a_5=3/2$, $r_6=-r_5/4$, $r_5=16/315$ and $s_7=1/7$ we have $a_2=b_{21}=1/3$, $a_6=2$, $b_{31}=1/8$, $b_{32}=3/8$, $b_{41}=1/2$, $b_{42}=-3/2$, $b_{43}=2$, $b_{51}=3/8$, $b_{52}=b_{53}=0$, $b_{54}=9/8$, $b_{61}=-8/7$, $b_{62}=6/7$, $b_{63}=24/7$, $b_{64}=-24/7$, $b_{65}=16/7$,

$$y_1 = y_0 + h(k_1 + 4k_3 + k_4)/6,$$

$$y_2 = y_0 + h(7k_1 + 32k_3 + 12k_4 + 32k_5 + 7k_6)/45,$$

$$m_1 = -4h(k_1 - 4k_3 + 6k_4 - 4k_5 + k_6)/315,$$

$$m_2 = h(-4k_1 + 16k_3 - 24k_4 + 16k_5 - 49k_6 + 45k_7)/315,$$

where

$$y_2 - y(x_2) = (h^6/6!)8[T^3S + 3TQ - (f_yf_{yy}P + f_yTS^2)/2 + f_yT^2S - 3f_y^2TS - f_y^2T^3 - f_y^3T^2 + f_y^4T] + O(h^7),$$

$$m_2 = -(h^5/5!)(2/21)[T^4 + 6TS^2 + 4T^2S + 3f_{yy}P + 26(f_yT^3 + f_y^2T^2) - 54f_y^3T + 72f_yTS] + O(h^6).$$

4.3. Numerical examples

Problems I–VI are solved by the three methods in Examples 8–10. Two approximations $u(x)$ and $v(x)$ of $y(x)$ are computed for comparison. $u(x)$ is obtained by the following program:

(i) compute y_1, y_2, m_2 and z_2;
(ii) if $|m_2|>\varepsilon\max(|z_2|, 1)$, halve the step-size and go to (i);
(iii) if $|m_2|\leqq\delta\max(|z_2|, 1)$, double the step-size;
(iv) set $u(x_j)=y_j$ $(j=1, 2)$ and replace x_0 and y_0 by x_2 and y_2 respectively. (Initially $h=1$.)

$v(x)$ is computed with the corresponding step-size by Kutta's method (K) when $p=2$ and by the Runge-Kutta method (RK) when $p=3$. The errors of $u(5)$ and $v(5)$ are listed in Table 3, where $\varepsilon=10^{-5}$, $\delta=\varepsilon/32$ when $p=2$ and $\varepsilon=10^{-6}$, $\delta=\varepsilon/64$ when $p=3$. It seems that these block methods compare favorably with two steps of integration by one-step methods of order $p+1$.

TABLE 3. Block methods

P \ M	8	K	9	RK	10	RK
I	−1.538+06	−7.308+06	9.172+03	−9.068+04	6.768+03	−6.781+05
II	7.222−08	−1.299−11	6.379−10	7.561−12	6.639−10	1.075−11
III	1.466−05	2.924−05	−4.045−09	6.255−07	4.244−07	3.948−06
IV	−2.670−07	2.890−07	−7.101−09	−1.021−08	−5.137−09	−1.543−08
V	2.076−07	−1.710−06	1.295−09	1.050−08	1.623−09	6.683−08
VI	1.342−02	1.844−02	−2.950−05	1.409−03	−5.964−05	1.676−03

5. Four-stage methods

We shall show the following

THEOREM 5. *For each one-step method* (2.23) *of order* 4 *there exists a formula* $m=h\sum_{j=1}^{5}s_jk_j$ *such that* $m=O(h^4)$, *which is unique apart from a constant factor, where* $k_5=f(x_1, y_1)$.

The condition in the theorem yields (3.8) and the equations:

$$s_1+s_2+s_3+s_4+s_5=0,\tag{5.1}$$

$$a_2s_2+a_3s_3+s_4+s_5=0,$$

$$2c_3s_3+2c_4s_4+s_5=0,$$

$$4c_3b_{43}s_4+s_5=0.$$

Since $a_2(1-a_3)c_3b_{43}\neq 0$, s_i $(i=1, 2, 3, 4)$ are determined uniquely for any given s_5, and we have

$$(5.2)\quad y_1 - y(x_1) = (h^5/5!)(G_1T^4 + G_2TS^2 + G_3T^2S + G_4f_{yy}P + G_5f_yT^3 + G_6f_y^2T^2 + G_7f_y^3T + G_8f_yTS) + O(h^6),$$

$$(5.3)\quad m = 2s_5(h^4/4!)(B_1^*T^3 + 3B_2^*TS + B_3^*f_yT^2 + B_4^*f_y^2T) + s_5(h^5/4!)(C_1^*T^4 + 6C_2^*TS^2 + 4C_3^*T^2S + 3C_4^*f_{yy}P + C_5^*f_yT^3 + C_6^*f_y^2T^2 + C_7^*f_y^3\,T + C_8^*f_yTS) + O(h^6),$$

where

$$(5.4)\quad G_1 = (3 - 5X + 10Y)/12,\ G_2 = (3 - 5a_3)/2,\ G_3 = (2 - 5a_2)/2,$$

$$G_5 = -4G_1,\ G_6 = -G_3,\ G_7 = -1,\ G_8 = 5a_3 - 2,$$

$$G_4 = (5/2)[c_3 + (3 - 4a_3)c_4]/(1 - a_3) - 3,\ X = a_2 + a_3,\ Y = a_2a_3,$$

$$B_1^* = (1 - 2a_2)(2a_3 - 1),\ B_2^* = 2a_3 - 1,\ B_3^* = 3a_2 - 1,\ B_4^* = -1,$$

$$C_1^* = (1 - 2a_2)(2a_3 - 1)(1 + X)/2,\ C_2^* = (1 + a_3)(2a_3 - 1)/2,$$

$$C_3^* = (6Y + 3a_2 - 2)/4,$$

$$C_4^* = [1 - a_3 + (1 - 2a_3)c_3 + (4a_3 - 3)c_4]/(1 - a_3),$$

$$C_5^* = 1 - 2X + 4Y + 2a_2^2,\ C_6^* = 1 - 3a_2,\ C_7^* = 1,\ C_8^* = 1 - 6a_3.$$

The case $a_2=a_3=1/2$ has been treated in [6].

EXAMPLE 11. For the choice $a_2=1/3$, $a_3=2/3$ and $s_5=1/6$ we have $b_{21}=a_2$, $b_{31}=-1/3$, $b_{32}=1$, $b_{41}=b_{43}=-b_{42}=1$,

$$y_1 = y_0 + h(k_1 + 3k_2 + 3k_3 + k_4)/8,$$

$$m = h(-k_1 + 3k_2 - 3k_3 - 3k_4 + 4k_5)/24,$$

where

$$y_1 - y(x_1) = (h^5/5!)(T^4 - 9TS^2 + 9T^2S + 18f_{yy}P - 4f_yT^3 - 9f_y^2T^2 - 54f_y^3T + 72f_yTS)/54 + O(h^6),$$

$$m = (h^4/4!)(T^3 + 9TS - 9f_y^2T)/27 + (h^5/5!)(5/54)(T^4 + 15TS^2 + 3T^2S + 9f_{yy}P + f_yT^3 + 9f_y^3T - 27f_yTS) + O(h^6).$$

EXAMPLE 12. The choice $a_2=2/5$, $a_3=3/5$ and $s_5=1/6$ yields $b_{21}=a_2$, $b_{31}=-3/20$, $b_{32}=3/4$, $b_{41}=19/44$, $b_{42}=-15/44$, $b_{43}=10/11$,

$$y_1 = y_0 + h(11k_1 + 25k_2 + 25k_3 + 11k_4)/72,$$

$$m = h(-k_1 + 5k_2 - 5k_3 - 11k_4 + 12k_5)/72,$$

$$y_1 - y(x_1) = (h^5/5!)(T^4/30 + 9f_{yy}P/22 - 2f_yT^3/15 - f_y^3T + f_yTS) + O(h^6),$$

$$m = (h^4/4!)(T^3 + 15TS + 5f_yT^2 - 25f_y^2T)/75 + (h^5/5!)(T^4 + 24TS^2 + 16T^2S + 195f_{yy}P/11 + 7f_yT^3 - 5f_y^2T^2 + 25f_y^3T - 65f_yTS)/30 + O(h^6).$$

The method $z=y_1+m$ is of order 3. If y_1 is accepted as an approximation to $y(x_1)$, then k_5 can be used as k_1 in the next step of integration.

Numerical examples

Problems I–VI are solved with $h=2^{-s}$ by the two methods in Examples 11 and 12. The values s, m and the error e of z are listed in Table 4.

TABLE 4. Four-stage methods

P \ M	11			12	
	s	m	e	m	e
I	5	−1.620−07	−1.675−07	−1.815−07	−1.884−07
II	6	−5.376−07	−5.137−07	−5.376−07	−5.137−07
III	5	2.641−07	2.743−07	1.908−07	1.963−07
IV	3	2.768−07	4.456−07	5.376−07	5.364−07
V	5	−5.302−08	−5.241−08	−6.376−08	−6.277−08
VI	4	−3.502−07	−3.530−07	1.065−07	1.248−07

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