

On One-step Methods for Ordinary Differential Equations

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1. Introduction

Let us consider the initial value problem

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

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

$$(2.1) \quad x_j = x_0 + jh \quad (j = 1, 2, \dots),$$

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

where

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

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

Put

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

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

Let D be the differential operator defined by

$$(2.7) \quad D = \frac{\partial}{\partial x} + k_1 \frac{\partial}{\partial y}$$

and put

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

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

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

where

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

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

$$(2.12) \quad A_4 = \sum_{i=3}^s c_i p_i, \quad B_2 = \sum_{i=3}^s a_i c_i p_i, \quad B_3 = \sum_{i=3}^s d_i p_i, \quad C_2 = \sum_{i=3}^s a_i^2 c_i p_i,$$

$$C_3 = \sum_{i=3}^s a_i d_i p_i, \quad C_4 = \sum_{i=3}^s c_i^2 p_i, \quad C_5 = \sum_{i=3}^s e_i p_i, \quad D_2 = \sum_{i=3}^s a_i^3 c_i p_i,$$

$$D_3 = \sum_{i=3}^s a_i^2 d_i p_i, \quad D_4 = \sum_{i=3}^s a_i e_i p_i, \quad D_5 = \sum_{i=3}^s c_i d_i p_i, \quad D_6 = \sum_{i=3}^s a_i c_i^2 p_i,$$

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

$$C_8 = \sum_{i=4}^s (a_i l_i + g_i) p_i, \quad D_7 = \sum_{i=4}^s a_i g_i p_i,$$

$$\begin{aligned}
 (2.14) \quad D_8 &= \sum_{i=4}^s (2c_i l_i + \sum_{j=3}^{i-1} c_j^2 b_{ij}) p_i, \quad D_9 = \sum_{i=4}^s (a_i^2 l_i + \sum_{j=3}^{i-1} a_j^2 c_j b_{ij}) p_i, \\
 D_{10} &= \sum_{i=4}^s (a_i m_i + \sum_{j=3}^{i-1} a_j d_j b_{ij}) p_i, \\
 D_{11} &= \sum_{i=5}^s [\sum_{j=4}^{i-1} (a_i l_j + a_j l_j + g_j) b_{ij}] p_i, \\
 D_{12} &= \sum_{i=3}^s (\sum_{j=2}^{i-1} a_j^4 b_{ij}) p_i, \quad D_{13} = \sum_{i=4}^s (\sum_{j=3}^{i-1} e_j b_{ij}) p_i, \\
 D_{14} &= \sum_{i=5}^s (\sum_{j=4}^{i-1} m_j b_{ij}) p_i, \quad D_{15} = \sum_{i=6}^s [\sum_{j=5}^{i-1} (\sum_{k=4}^{j-1} l_k b_{jk}) b_{ij}] p_i.
 \end{aligned}$$

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

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

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

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

$$\begin{aligned}
 (2.18) \quad D_1 &= 2D_2 = 3D_3 = 4D_4 = 6D_5 = 4D_6 = 8D_7 = 60D_8/13 \\
 &= 15D_9/4 = 20D_{10}/3 = 10D_{11} = 5D_{12} = 20D_{13} = 60D_{14} \\
 &= 120D_{15} = t^6/6.
 \end{aligned}$$

If we impose the condition

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

then it follows that

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

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

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

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

Suppose that

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

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

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

where

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

Since

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

we have

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

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

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

Making use of the conditions

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

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

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

$$(2.28) \quad c_{nr+i} = n^2/2 + na_i + c_i \quad (r \geq 2),$$

$$d_{nr+i} = n^3/3 + n^2 a_i + 2nc_i + d_i \quad (r \geq 3),$$

$$e_{nr+i} = n^4/4 + n^3 a_i + 3n^2 c_i + 3nd_i + e_i \quad (r = 4),$$

$$l_{nr+i} = n^3/6 + n^2 a_i/2 + nc_i + l_i \quad (r = 4),$$

$$m_{nr+i} = n^4/12 + n^3 a_i/3 + n^2 c_i + 2nl_i + m_i \quad (r = 4)$$

$$(i = 1, 2, \dots, r; n = 0, 1, \dots),$$

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

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

such that

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

and the formulas

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

such that

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

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

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:

$$\begin{aligned} p_1 + p_2 + p_3 + p_4 &= t, \\ a_2 p_2 + p_3 + (1 + a_2) p_4 &= t^2/2, \\ a_2^2 p_2 + p_3 + (1 + a_2)^2 p_4 &= t^3/3, \\ p_3 + (1 + 2a_2) p_4 &= t^3/3 \quad (t = 1, 2), \end{aligned}$$

which can be reduced to

$$p_1 + p_3 = t, \quad p_2 + p_4 = 0, \quad p_3 + p_4 = t^2/2, \quad a_2 p_4 = t^2(2t - 3)/12.$$

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

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

where

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

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

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

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 $p \geq 2$ 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 $a_2=1/2$,

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

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:

$$a_3(a_3 - a_2) = (2 - 3a_2)c_3, \quad \sum_{i=1}^3 q_i = 1, \quad \sum_{i=2}^3 a_i q_i = 1/2, \quad 6c_3 q_3 = 1.$$

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

$$\begin{aligned} p_1 + p_4 + p_7 &= t, \quad p_2 + p_5 + p_8 = 0, \quad p_3 + p_6 + p_9 = 0, \\ p_4 + p_5 + p_6 + 2p_7 + 2p_8 + 2p_9 &= t^2/2, \\ a_2p_5 + a_3p_6 + p_7 + (1 + 2a_2)p_8 + (1 + 2a_3)p_9 &= t^2(2t - 3)/12, \\ c_3p_6 - 2a_2p_8 + 2(c_3 - a_3)p_9 &= -t^2(t - 2)^2/12, \\ p_7 + (1 + 6a_2)p_8 + (1 + 6a_3)p_9 &= t^2(3t^2 - 10t + 9)/12. \end{aligned}$$

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

$$\begin{aligned} (3.6) \quad w_1 &= y_0 + h(4k_1 + k_4 + k_7)/6 - hp_2(k_1 - k_2 - k_4 + k_5) \\ &\quad - hp_3(k_1 - k_3 - k_4 + k_6), \end{aligned}$$

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

where

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

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

$$- 30a_2a_3 - 13)f_yT^3 + (30a_2 - 13)f_y^2T^2 - 13f_y^3T \\ + (60a_3 - 31)f_yTS] + O(h^6).$$

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 $p\geq 3$. 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:

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

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

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

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

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

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

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

$$2(a_3 - 1)c_3 p_7 + a_2 p_{10} + [a_3 + 4(a_3 - 1)c_3]p_{11} + p_{12} = t^2(t - 2)^2/24,$$

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

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

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

$$c_3 p_{11} + c_4 p_{12} = t^2(3t^3 - 15t^2 + 25t - 15)/360.$$

From these p_j ($j=1, 2, \dots, 11$) are determined uniquely for any given p_{12} . The choice $p_{1k}=0$ ($k=10, 11, 12$; $t=1, 2$) 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 $p \geq 3$ and the formulas (3.3) satisfying (3.4) do not exist for $q=2$.*

EXAMPLE 5. For the Runge-Kutta method we have

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

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

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

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 $|y_3 - z_3| \leq \delta \max(|y_3|, 1)$, 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

P \ M	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

$$(4.1) \quad y_1 = y_0 + h \sum_{i=1}^{2p} q_i k_i, \quad y_2 = y_0 + h \sum_{i=1}^{2p} p_i k_i, \\ m_1 = h \sum_{i=1}^{2p} r_i k_i, \quad m_2 = h \sum_{j=1}^{2p+1} s_j k_j,$$

such that

$$(4.2) \quad y_1 - y(x_1) = O(h^{p+2}), \quad y_2 - y(x_2) = O(h^{p+3}), \\ m_1 = O(h^{p+1}), \quad m_2 = O(h^{p+2}),$$

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:

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

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

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

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

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

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

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

where

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

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

$$\begin{aligned} (4.7) \quad y_1 - y(x_1) &= (h^4/4!)(F_1 T^3 + 3F_2 TS + F_3 f_y T^2 + F_4 f_y^2 T) + O(h^5), \\ y_2 - y(x_2) &= 8(h^5/5!)(G_1 T^4 + G_2 TS^2 + G_3 T^2 S + G_4 f_{yy} P \\ &\quad + G_5 f_y T^3 + G_6 f_y^2 T^2 + G_7 f_y^3 T + G_8 f_y TS) + O(h^6), \\ m_1 &= (h^3/2)(\tilde{A}_3 T^2 + 2\tilde{A}_4 f_y T) + O(h^4), \\ m_2 &= 2s_5(h^4/3!)(B_1^* T^3 + 3B_2^* TS + B_3^* f_y T^2 + B_4^* f_y^2 T) + O(h^5), \end{aligned}$$

where

$$\begin{aligned} (4.8) \quad F_1 &= -5 + 4X - 4Y, \quad F_2 = 4a_3 - 5, \quad F_3 = 6a_2 - 5, \quad F_4 = -5, \\ G_1 &= (6 - 5X + 5Y)/6, \quad G_2 = 6 - 5a_3, \quad G_3 = 4 - 5a_2, \quad G_5 = -4G_1, \\ G_6 &= -G_3, \quad G_7 = -4, \quad G_8 = 2(5a_3 - 4), \\ G_4 &= 5[c_3 + (3 - 2a_3)c_4]/(2 - a_3) - 12, \\ \tilde{A}_3 &= 2(1 - a_2)\tilde{r}_3 + K\tilde{r}_4, \quad \tilde{A}_4 = \tilde{r}_3 + (3 - 2a_3)\tilde{r}_4, \quad \tilde{r}_3 = c_3 r_3, \\ \tilde{r}_4 &= c_3 b_{43} r_4 / (2 - a_3), \quad B_1^* = 2(1 - a_2)(a_3 - 1), \quad B_2^* = 3(a_3 - 1), \\ B_3^* &= 3a_2 - 2, \quad B_4^* = -2. \end{aligned}$$

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 $m_1 \neq 0$ 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 $b_{21} = a_2$, $b_{31} = -3/10$, $b_{32} = 3/2$, $b_{41} = 19/22$, $b_{42} = -15/22$, $b_{43} = 20/11$,

$$\begin{aligned} y_1 &= y_0 + h(55k_1 + 65k_2 + 35k_3 - 11k_4)/144, \\ y_2 &= y_0 + h(11k_1 + 25k_2 + 25k_3 + 11k_4)/36, \\ m_1 &= h(-k_1 + 5k_2 - 5k_3 + k_4)/36, \\ m_2 &= h(-k_1 + 5k_2 - 5k_3 - 11k_4 + 12k_5)/36, \end{aligned}$$

where

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

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

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

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

4.2. Case $p=3$

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

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

$$\sum_{i=5}^6 a_i^j \alpha_i p_i = A_j \quad (j = 0, 1), \quad w_5 p_5 + w_6 p_6 = 4(1 - a_3)/3,$$

$$\alpha_5 b_{65} p_6 = 4(6 - 5X + 5Y)/15,$$

$$(a_6 - a_5)w_6 p_6 = 32/15 - 2a_3 - 4(1 - a_3)a_5/3,$$

$$w_5 b_{65} p_6 = 2(4 - 5a_3)/15,$$

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

$$\sum_{i=5}^6 \alpha_i q_i = B, \quad w_5 q_5 + w_6 q_6 = (1 - 2a_3)/12,$$

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

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

where

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

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

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

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

From these it follows that

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

$$(A_1 - a_5 A_0)w_6 = [32/15 - 2a_3 - 4(1 - a_3)a_5/3]\alpha_6,$$

$$(A_1 - a_6 A_0)w_5 = [32/15 - 2a_3 - 4(1 - a_3)a_6/3]\alpha_5.$$

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

$$y_2 - y(x_2) = (h^6/6!)(16/5)(T^3S + 3TQ + f_y f_{yy}P + f_y TS^2 + f_y T^2S$$

$$- 12f_y^2 TS - f_y^2 T^3 - f_y^3 T^2 + 7f_y^4 T) + O(h^7),$$

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

$$+ f_y^2 T^2) + 396f_y^3 T - 216f_y TS] + O(h^6).$$

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

$$y_2 - y(x_2) = (h^6/6!)8[T^3S + 3TQ - (f_y f_{yy}P + f_y TS^2)/2 + f_y T^2S - 3f_y^2 TS$$

$$- f_y^2 T^3 - f_y^3 T^2 + f_y^4 T] + O(h^7),$$

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

$$- 54f_y^3 T + 72f_y TS] + O(h^6).$$

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 $|m_2| \leq \delta \max(|z_2|, 1)$, 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 $m = h \sum_{j=1}^5 s_j k_j$ 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:

$$\begin{aligned}
 (5.1) \quad & s_1 + s_2 + s_3 + s_4 + s_5 = 0, \\
 & a_2 s_2 + a_3 s_3 + s_4 + s_5 = 0, \\
 & 2c_3 s_3 + 2c_4 s_4 + s_5 = 0, \\
 & 4c_3 b_{43} s_4 + s_5 = 0.
 \end{aligned}$$

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

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

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

where

$$(5.4) \quad G_1 = (3 - 5X + 10Y)/12, \quad G_2 = (3 - 5a_3)/2, \quad G_3 = (2 - 5a_2)/2, \\ G_5 = -4G_1, \quad G_6 = -G_3, \quad G_7 = -1, \quad G_8 = 5a_3 - 2, \\ G_4 = (5/2)[c_3 + (3 - 4a_3)c_4]/(1 - a_3) - 3, \quad X = a_2 + a_3, \quad Y = a_2a_3, \\ B_1^* = (1 - 2a_2)(2a_3 - 1), \quad B_2^* = 2a_3 - 1, \quad B_3^* = 3a_2 - 1, \quad B_4^* = -1, \\ C_1^* = (1 - 2a_2)(2a_3 - 1)(1 + X)/2, \quad C_2^* = (1 + a_3)(2a_3 - 1)/2, \\ C_3^* = (6Y + 3a_2 - 2)/4, \\ C_4^* = [1 - a_3 + (1 - 2a_3)c_3 + (4a_3 - 3)c_4]/(1 - a_3), \\ C_5^* = 1 - 2X + 4Y + 2a_2^2, \quad C_6^* = 1 - 3a_2, \quad C_7^* = 1, \quad C_8^* = 1 - 6a_3.$$

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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