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ONE-STEP MULTIDERIVATIVE METHODS FOR SOLVING DIFFERENTIAL EQUATIONS OF THE FIRST ORDER

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The subject of this paper is the problem of obtaining coefficients for a special class of numerical methods for solving ordinary differential equations.

1. Introduction.

One-step multiderivative methods are a means for numerical solution of a first-order differential equation

$$\begin{aligned} y' &= f(x, y) \\ y(x_0) &= y_0 \end{aligned} \tag{1}$$

at the point x_n. In this paper we suppose that the function $f(x, y)$ satisfies the conditions of existence and unit theorem of the solution of the differential equation. This theorem has been proved in [1]. Numerical methods for solving the above mentioned problem are using also derivatives of the function $f(x, y)$. The problem is solved in the interval $\langle a, b \rangle$. Interval $\langle a, b \rangle$ is divided into parts separated by points $x_0, x_1, x_2, \ldots, x_n$, where $x_0 = a$, $x_n = b$. A step we define as $h_n = x_{n+1} - x_n$ and in this paper we suppose $h_n = h$.

The basic idea of these methods is very simple. To find the next value of the solution, the values of the function $f(x, y)$ and the derivatives of this function in the points (x_n, y_n) and (x_{n+1}, y_{n+1}) have to be used. This can be written as follows,

$$y_{n+1} = y_n + \sum_{i=0}^{k} h^{i+1}(a_i f_n^{(i)} + b_i f_{n+1}^{(i)}) \tag{2}$$

where a_i, b_i for $i = 0, 1, \ldots, k$ are unknown coefficients of the method,

h is a step, $h = x_{n+1} - x_n$

and

$$f_n^{(i)} = \frac{d^i}{dx^i} f(x, y(x)) \bigg|_{x = x_n} \tag{3}$$

are total derivatives of the right-hand side of initial value problem (1) in the point x_n.
As can be seen the method defined by (2) is implicit. We suppose, that coefficients a_i, b_i, for $i = 0, 1, \ldots, k$ are derived by scheme (2) in order to obtain the maximal order of accuracy. This sort of methods are A-stable, so this property predestinates this methods as a corrector of an explicit one-step methods.

2. The general formula for finding the unknown coefficients

In this part we shall find the general formula for counting the unknown coefficients a_i, b_i for $i = 0, 1, \ldots, k$ for any value of k. If we expand $y_{n+1}, f_n^{(i)}, f_{n+1}^{(i)}$ to the Taylor's series in the point x_n, compare the coefficients of the derivatives of $f(x, y)$ and powers of h, we get the linear equations system of the following form:

$$Qt = s, \tag{4}$$

where t is the unknown coefficients vector in the form

$$t = (a_0, a_1, \ldots, a_k, b_0, b_1, \ldots, b_k)^T,$$

S is the vector of the right-hand side of the linear equations system and can be written in the form:

$$s_i = \frac{1}{i!} \qquad \text{for } i = 1, 2, \ldots, 2k + 2$$

Q denotes the matrix of dimension $2k + 2$ and has the form:

$$\begin{aligned}
Q_{ij} &= \delta_{ij} && \text{for } i = 1, 2, \ldots, 2k + 2 \\
& && \phantom{\text{for }} j = 1, 2, \ldots, k + 1 \\
Q_{ij} &= \frac{1}{(i - j + k + 1)!} && \text{for } i \geq j - k - 1 \\
& && \phantom{\text{for }} i = 1, 2, \ldots, 2k + 2 \\
& && \phantom{\text{for }} j = k + 2, \ldots, 2k + 2 \\
Q_{ij} &= 0 && \text{for } i < j - k - 1 \\
& && \phantom{\text{for }} i = 1, 2, \ldots, 2k + 2 \\
& && \phantom{\text{for }} j = k + 2, \ldots, 2k + 2
\end{aligned} \tag{5}$$

$$
\left[\begin{array}{ccccc|ccccc}
1 & 0 & 0 & \dots & 0 & 1 & 0 & 0 & \dots & 0 \\
0 & 1 & 0 & \dots & 0 & 1 & 0 & 0 & \dots & 0 \\
0 & 0 & 1 & \dots & 0 & \frac{1}{2} & 0 & 0 & \dots & 0 \\
 & & & & & & & & & \\
0 & 0 & 0 & \dots & 1 & \frac{1}{k!} & \frac{1}{(k-1)!} & \dots & & 1 \\
\hline
 & & & & & \frac{1}{(k+1)!} & \frac{1}{k!} & & \dots & 1 \\
 & & \mathbf{0} & & & & & & & \\
 & & & & & \frac{1}{(2k+1)!} & \frac{1}{(2k)!} & & \dots & \frac{1}{(k+1)!}
\end{array}\right]
$$

Figure 1

Figure 1 shows the matrix Q. The general form of the solution of the linear equations system can be written in the form:

$$a_j = \frac{(k+1)!\,(2k+1-j)!}{(2k+2)!\,(k-j)!\,(j+1)!} \tag{6}$$

and

$$b_j = (-1)^j a_j . \tag{7}$$

Let us prove this hypothesis. First we shall prove this for the unknowns b_j, so we use the right-down quadrant of the matrix Q and the solution must satisfy the equations for all $i = k+2, \ldots, 2k+2$. So we have to prove this implication:

The equality

$$\sum_{j=1}^{k} (-1)^j \frac{(k+1)!\,(2k+1-j)!}{(k-j)!\,(j+1)!\,(2k+2)!} \cdot \frac{1}{(i-j-1)!} = \frac{1}{i!} \tag{8}$$

is correct only for $i = k+2,\ k+3,\ \ldots,\ 2k+2$.

In order to prove the equality (8) we step-wise modify left side as follows

$$\sum_{j=1}^{k} (-1)^j \frac{(k+1)!\,(2k+1-j)!}{(k-j)!\,(j+1)!\,(2k+2)!\,(i-j-1)!} \cdot \frac{i!\,(j+1)!}{i!\,(j+1)!} =$$

$$= \sum_{j=1}^{k} (-1)^j \binom{k+1}{j+1} \cdot \binom{i}{j+1} \cdot \binom{2k+2}{j+1}^{-1} \frac{1}{i!} =$$

$$= \sum_{j=1}^{k} (-1)^{j+1} \binom{k+1}{j} \cdot \binom{i}{j} \cdot \binom{2k+2}{j}^{-1} \frac{1}{i!} =$$

$$= \frac{-1}{i!} \sum_{j=1}^{k} (-1)^j \binom{k+1}{j} \cdot \binom{i}{j} \cdot \binom{2k+2}{j}^{-1} + \frac{1}{i!} =$$

$$= \frac{-1}{i!} \binom{2k+2-i}{k+1} \cdot \binom{2k+2}{k+1}^{-1} + \frac{1}{i!} = \frac{-1}{i!} \frac{(2k+2-i)_{[k+1]}}{(2k+2)_{[k+1]}} + \frac{1}{i!}$$

where $n_{[k]}$ denotes the decreasing factorial. The previous equality was proved in a general form in [4]. If one writes the equality (8) in the form

$$\frac{-1}{i!} \frac{(2k+2-i)_{[k+1]}}{(2k+2)_{[k+1]}} + \frac{1}{i!} = \frac{1}{i!}$$

can be easily seen that the equality can be written

$$(2k+2-i)_{[k+1]} = 0 \tag{9}$$

and that is what we had to prove.

Now let us show that the unknown coefficients a_i, b_i for $i = 0, 1, \dots k$ satisfy also the first $k+1$ equations. This can be written in the form:

$$\frac{(2k+2-i)!\,(k+1)!}{(k-i+1)!\,i!\,(2k+2)!} + \sum_{j=1}^{k} (-1)^j \frac{(2k+1-j)!\,(k+1)!}{(k-j)!\,(j+1)!\,(2k+2)!\,(i-j-1)!} = \frac{1}{i!}$$

The equality we denote as (10), and it is true for $i = 1, 2, 3, \dots, k+1$. It is correct because of the factorial $(k+1-i)!$, so i must not decrease to $k+1$. Now let us prove the equality (10). The first member can be written as follows:

$$\frac{(2k+2-i)!\,(k+1)!}{(k+1-i)!\,(2k+2)!\,i!} \cdot \frac{(k+1)!}{(k+1)!} = \binom{2k+2-i}{k+1} \cdot \binom{2k+2}{k+1}^{-1} \cdot \frac{1}{i!}$$

The second member of (10) can be written in the form:

$$\frac{1}{i!} \cdot \binom{2k+2-i}{k+1} \cdot \binom{2k+2}{k+1}^{-1} + \frac{1}{i!}$$

So the equality has the form:

$$\frac{1}{i!} \cdot \binom{2k+2-i}{k+1} \binom{2k+2}{k+1}^{-1} - \frac{1}{i!} \binom{2k+2-i}{k+1} \binom{2k+2}{k+1}^{-1} + \frac{1}{i!} = \frac{1}{i!}$$

Therefore the equality (10) is true for all $i = 1, 2, \ldots, k+1$. By this two parts of the proof, formule (6) and (7) can be considered as the solution of the linear equations system (4). The equality (7) is very important, since the coefficients computation requires only the solution of a smaller linear equations system of the form:

$$Pb = z, \tag{11}$$

where b is the vector of unknowns

$$b = (b_0, b_1 \ldots b_k)^T,$$

vector z can be written as follows:

$$z_i = s_{i+k+1} \qquad \text{for } i = 1, 2, \ldots, k+1$$

and matrix P is a reduced matrix from matrix Q, i.e.:

$$P_{i,j} = Q_{i+k+1, j+k+1} \qquad \text{for } i, j = 1, 2, \ldots, k+1$$

That means that for finding the unknown coefficients the right down quadrant of matrix Q is used.

3. The local truncation error and the aproximation order

Suppose we have a general form of the one-step method:

$$y_{n+1} = hG_f(x_n, y_n, y_{n+1}, h) \tag{12}$$

Then the local truncation error T_{n+1} in the point x_{n+1} is given by:

$$T_{n+1} = y(x_n + h) - h\,G_f(x_n, y(x_n), y(x_n + h), h),$$

where $y(x)$ is the exact solution of differential equation (1). In our case, the methods defined by (2), the local truncation error is given

$$T_{n+1} = c_k \frac{h^{2k+3}}{(k+2)!} y^{(2k+3)}(x_n) + O(h^{2k+4}) \tag{13}$$

where the constant term c_k is

$$c_k = \frac{1}{(k+3)^{[k+1]}} - \sum_{i=0}^{k} (-1)^{k-i} \frac{(k+1)!\,(k+1+i)!}{(2k+2)!\,i!\,(k-i+1)!\,(k+3)^{[i]}} \tag{14}$$

and $n^{[k]}$ is the k-th increasing factorial from n.
Approximation order can be as simple as possible defined as the greatest power of polynom $G(x) = 1 + x + x^2 + \ldots + x^n$ which excatly satisfies the method. From expresion (13) we can see that the methods described in this paper are of order $2k + 2^{nd}$.

Table 1

k	a_0	a_1	a_2	a_3	a_4	a_5	a_6	a_7	a_8	c_k
1	$\frac{1}{2}$									$\frac{1}{6}$
1	$\frac{1}{2}$	$\frac{1}{12}$								$\frac{1}{120}$
2	$\frac{1}{2}$	$\frac{1}{10}$	$\frac{1}{120}$							$\frac{1}{4200}$
3	$\frac{1}{2}$	$\frac{3}{28}$	$\frac{1}{84}$	$\frac{1}{1680}$						$\frac{1}{211680}$
4	$\frac{1}{2}$	$\frac{1}{9}$	$\frac{1}{72}$	$\frac{1}{1008}$	$\frac{1}{30240}$					$\frac{1}{13970880}$
5	$\frac{1}{2}$	$\frac{5}{44}$	$\frac{1}{66}$	$\frac{1}{792}$	$\frac{1}{15840}$	$\frac{1}{665280}$				$\frac{1}{1141620480}$
6	$\frac{1}{2}$	$\frac{3}{26}$	$\frac{5}{312}$	$\frac{5}{3432}$	$\frac{1}{11440}$	$\frac{1}{308880}$	$\frac{1}{1729280}$			$\frac{1}{111307996800}$
7	$\frac{1}{2}$	$\frac{7}{60}$	$\frac{1}{60}$	$\frac{1}{624}$	$\frac{1}{9360}$	$\frac{1}{205920}$	$\frac{1}{7207200}$	$\frac{1}{518918400}$		$\frac{1}{12614906304000}$
8	$\frac{1}{2}$	$\frac{2}{17}$	$\frac{7}{408}$	$\frac{7}{4080}$	$\frac{1}{8160}$	$\frac{1}{159120}$	$\frac{1}{4455360}$	$\frac{1}{196035840}$	$\frac{1}{17643225600}$	$\frac{1}{1629845894476800}$

4. Particular methods

In the case when $k = 0$, we have to do with a well-known Euler's method. When $k = 1$ we get the method described in [2], but the procedure for finding the coefficients does not exist.

The coefficients from $k = 0$ to $k = 8$ are tabulated in Table 1. Here only the coefficients a_i for $i = 0, 1, \ldots, k$ and the coefficients b_i for $i = 0, 1, \ldots, k$, multipled by 1 or -1 are written in Table 1 consists also of the constant term c_k for the local truncation error, but the exact local truncation error is given by (13).

There are three possibilites for the unknown coefficients a_i, b_i ($i = 0, 1, \ldots, k$) to find.

The first possibility is to solve the linear equation system as given by (4) and a_i, b_i for $i = 0, 1, \ldots, k$ are obtained. The second possibility is to solve the reduced linear equations system specified by (11) from whicch only b_i coefficients for $i = 0, 1, \ldots, k$ are found and coefficients a_i for $i = 0, 1, \ldots, k$ from equation (7) can be determined.

The above mentioned a_i coefficients starting $k = 0$ up to $k = 8$ are given in *Table 1.* A computation program in FORTRAN was prepared for generating matrices Q and P as well as the right-hand sides of the linear equation systems (4) and (11) also a special computer program has been written for solving the linear equations system. The algorithm used for this purpose is a Gaussian elimination method using fractions. More abouth this method as well as the computer program can be found in [5]. Also a separate computer program was written for obtaining the constant c_k of the equation (14) from local truncation error.

The third possibility is to get the unknown coefficients as given in (6) and (7). This way is the simpliest one. Also for this third possibility a special computer program was written for finding the unknown coefficients. For the case where $k = 8$, the last unknown denominator of the coefficients is so great that it is impossible represent it in the full range in the computer. Therefore all the numbers are cut into parts and represented in a vector form. After this "number cuts" it is possible to get coefficients a_i and b_i for any value of k.

4. Numerical results

The methods described in this paper are acceptable for solving the stiff differential equations as a correctors for one-step methods. As a predictor the clasic Runge—Kutta method of the 4-th order could be used. The Runge—Kutta method can be written as follows.

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

By this method we find the predicted value of y_{n+1}. Then by using the methods presented in this paper the predicted value of y_{n+1} can be corrected. General formula of these methods is as follows:

$$P(E^{k+1}C)^m,$$

where P denotes the predictor (in our example the classic Runge—Kutta method of the 4-th order)
E is the evaluation of the ringt-hand side of the differential equation and the derivatives (evaluated $k + 1$ times)
C is the corrector of the method (corrector of the predictor)
m is the number of repeated uses of the corrector

Certain disadvantage of these methods is that we have to find the derivatives of the right-hand side of the diferential equation. The first derivative is:

$$\frac{d}{dx}(f(x, y)) = \frac{\partial f}{\partial x} + f \cdot \frac{\partial f}{\partial y} = f^{(1)}$$

and the remaining derivative formula can be written

$$\frac{d^i}{dx^i} f(x, y) = \frac{\partial f^{(i-1)}}{\partial x} + f \cdot \frac{\partial f^{(i-1)}}{\partial y}.$$

Example:

Suppose we have a differential equation

$$y' = 10y$$
$$y(0) = 1$$

with the exact solution $y(x) = \exp(10x)$. Function $y(x)$ is sharply increasing in x. The one-step explicit methods are not able to take into account this sharp increase. If the methods described in this paper are used for solution of differential equation with step $h = 0.1$ in the interval $\langle 0, 1\rangle$ the accuracy of solution substintially differs. *Tables 2—4* demonstrate the error terms in absolute value at the end point of interval $\langle 0, 1\rangle$ as well as the advantage of the described

Table 2

The Runge—Kutta methods

Method	The order	Inacouracy
Euler's	2	0.125 E 5
King's	3	0.384 E 4
Merson's	4	0.242 E 3
Clasical	4	0.793 E 3
Nyström's	5	0.121 E 3
Huťa's	6	0.363 E 1
Huťa-Peniak's	7	0.383

methods for the mentioned initial value problem. The numbers are given in the following form:

$$0.765\,E\,5 = 0.765\ 10^5 .$$

The methods described in this paper

Table 3

The method order	Inaccuracy
4	0.322 E 3
6	0.227 E 1
8	0.893 E −2
10	0.184 E −4
12	0.379 E −5

In the following the predictor-corector pairs were used to solve the initial value problem. The Adam's—Bashforth's method was used as a predictor and Adam's—Moulton's method as a corector and this predictor-corrector pairs is identified as ABM.

Table 4

Method	The order	Inaccuracy
ABM	2	0.272 E 5
ABM	3	0.530 E 4
ABM	4	0.186 E 4
Milne's	4	0.585 E 3
Hemming's	4	0.191 E 4
ABM	5	0.817 E 3
ABM	6	0.333 E 3

The methods proposed in this paper are a bit complicated ones, because of derivatives, but by this algorithm more accurate results could be obtained for some kind of initial value problems (stiff or when the solution is sharply increasing).

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SÚHRN

JEDNOKROKOVÉ METÓDY RIEŠENIA DIFERENCIÁLNYCH ROVNÍC PRVÉHO RÁDU VYUŽÍVAJÚCE DERIVÁCIU PRAVEJ STRANY DIFERENCIÁLNEJ ROVNICE

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V práci sa uvádza postup odvodenia koeficientov jednokrokových metód, ktoré využívajú deriváciu pravej strany diferenciálnej rovnice. Tieto metódy majú tvar:

$$y_{n+1} = y_n + \sum_{i=0}^{k} h^{i+1}(a_i f_n^{(i)} + b_i f_{n+1}^{(i)})$$

Súčasne s koeficientami je odvodená i chyba metódy. V závere práce sú uvedené konkrétne metódy pre $k = 0$ až $k = 8$ a riešená jednoduchá začiatočná úloha prvého rádu.

РЕЗЮМЕ

ОДНОШАГОВЫЕ МЕТОДЫ РЕШЕНИЯ ДИФФЕРЕНЦИАЛЬНЫХ УРАВНЕНИЙ ПЕРВОГО ПОРЯДКА, ИСПОЛЬЗУЮШИХ ПРОИЗВОДНЫЕ ПРАВОЙ СТОРОНЫ ДИФФЕРЕНЦИАЛЬНОГО УРАВНЕНИЯ

В работе изучается метод получения коэффициентов одношаговых методов, использующих производную правой стороны дифференциального уравнения. Эти методы имеют вид:

$$y_{n+1} = y_n + \sum_{i=1}^{k} h^{i+1}(a_i f_n^{(i)} + b_i f_{n+1}^{(i)})$$

Одновременно выводится тоже погрешность аппроксимации методов. В конце работы приводятся конкретне методы для $\kappa = 0$ до $\kappa = 8$ и пример одной конкретной начальной задачи, решаемой при помощи описанных методов.