

About One Multistep Multiderivative Method of Predictor-Corrector Type Constructed for Solving Initial-Value Problem for ODE of Second Order

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Abstract: - Considering the wide application of the initial-value problem for Ordinary Differential Equations second-order with a special structure, here for solving this problem constructed the special Multistep Multiderivative Methods. Many scientists studied this problem, but the most distinguishing is the Štörmer. To solve this problem here is proposed to use the Multistep Second derivative Method with a special structure. This method has been generalized by many authors, which is called as the linear Multistep Multiderivative Methods with the constant coefficients. Many authors have shown that the Multistep Second derivative Method can be applied to solve the initial-value problem for ODEs of the first order. Euler himself using his famous method discovered that, in his method when moving from one point to another local truncation errors add up, the results of which reach a very large value. To solve this problem, he suggested using more accurate methods. For this aim, Euler proposed calculating the next term in the Taylor series of the solutions of the investigated problem. Developing this idea and population of the Multistep Multiderivative Methods here to solve the named problem it is suggested to use Multistep Thriedderivative Methods, taking into account that methods of this type are more accurate. For the demonstration above, receiving results here have constructed some concrete methods. Also by using some of Dahlquist's and Ibrahimov's results for Multistep Methods with the maximum order of accuracy were compared. Proven that the Multistep Thriedderivative Methods are more accurate than the others. By using model problems have illustrated some results received here.

Key-Words: - Initial-value problem for ODEs, Stability and Degree, Multistep Multiderivative Methods (MMM), Local Truncation Error, Štörmer Method, Multistep Secondderivative Methods (MSM).

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1 Introduction

As was noted above, here considering the construction of more exact stable methods and their application them to solve the initial-value problem for the ODEs of the second order, which can presented as follows:

$$\begin{aligned} y''(x) &= F(x, y(x), y'(x)), \\ y(x_0) &= y_0, \quad y'(x_0) = y'_0, \quad x_0 \leq x \leq X. \end{aligned} \quad (1)$$

As is known, Newton's second law of motion leads to systems of second-order differential equations. Hence, the problem (1) was studied by many specialists. The problem in fundamental form was investigated by Štörmer using the numerical method, which is popular as a Štörmer method. Suppose that the problem (1) has the unique continuous solution defined in the segment $[x_0, X]$.

The function $F(x, y, z)$ is defined in some closed set which has the continuous partial derivatives to the totality of arguments to some p , inclusively. As was noted above, the aim of this work is to construct some simple numerical method for finding the values of the solution of problem (1) at the mesh points defined as the $x_{i+1} = x_i + h$ ($i = 0, 1, \dots, N$), $0 < h$ is the step-size. Note that usually the approximate values of the solution at the point x_i are denoted by the y_i , but the corresponding exact values by the $y(x_i)$ ($i = 0, 1, \dots, N$). For solving problem (1) have constructed approximate methods, such as analytical, analitico-numerical and numerical methods. Among them, the most popular are numerical methods, the application of which is associated with the development of computer technology. As is known the initial-value problem for ODE of the highest order by using the method of undetermined coefficients can be reduced to a system of ODEs of the first order. In this case, to solve this system one can apply the following method:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h \sum_{i=0}^k \beta_i y'_{n+i}; \quad n = 0, 1, \dots, N - k; \quad \alpha_k \neq 0. \quad (2)$$

This method has been investigated by many authors, [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14]. Noted that method (2) fundamentally has investigated by Dahlquist (see for example [3]). Some authors for solving the problem (1), have used the following method:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h \sum_{i=0}^k \beta_i y'_{n+i} + h^2 \sum_{i=0}^k \gamma_i F_{n+i}; \quad (3)$$

$$n = 0, 1, 2, \dots, N - k; \quad \alpha_k \neq 0,$$

which is generalized of the method (2) and the Štörmer method. Noted that the Štörmer method in our case can be presented as the followers, [1], [2], [5], [6], [10], [15], [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29]:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h^2 \sum_{i=0}^k \gamma_i F_{n+i}; \quad n = 0, 1, 2, \dots, N - k; \quad \alpha_k \neq 0. \quad (4)$$

By taking into account that the method (4) is a partial case of the method (3), one can consider the method (4) as the some parts of the method (3). Therefore one might think that if method (3) is stable, then the Štörmer method is also stable. We will show later that this is not so. Here the goal research is in the application of the Multistep

Thirdderivative Methods to solve problem (1), given that these methods are more accurate.

§1. The Multistep Thirdderivative Methods and its application to solve problem (1).

The Multistep Thirdderivative Methods in one version can presented as follows:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h \sum_{i=0}^k \beta_i y'_{n+i} + h^2 \sum_{i=0}^k \gamma_i y''_{n+i} + h^3 \sum_{i=0}^k l_i y'''_{n+i};$$

$$n = 0, 1, \dots, N - k; \quad \alpha_k \neq 0. \quad (5)$$

If applied this method to solve the problem (1), then received the following:

$$\sum_{i=0}^k \alpha_i y_{n+i} = h \sum_{i=0}^k \beta_i y'_{n+i} + h^2 \sum_{i=0}^k \gamma_i F_{n+i}$$

$$+ h^3 \sum_{i=0}^k l_i g_{n+i}; \quad n = 0, 1, \dots, N - k. \quad (6)$$

Obviously, a method (6) is a partial case of a method (5).

Here, function $g(x, y, y') = dF(x, y, y') / dx$. In other words, the function of $g(x, y, y')$ is defined as the first full derivative from the function $F(x, y, y')$. The methods, which are presented here, takes as given if are known of the values of k and the coefficients $\alpha_i, \beta_i, \gamma_i, l_i$ ($i = 0, 1, \dots, k$). Therefore, let us consider the definition of the values of the coefficients $\alpha_i, \beta_i, \gamma_i, l_i$ ($i = 0, 1, 2, \dots, k$). To do this, it is proposed to use the method of undetermined coefficients. Typically the use of this method is accompanied by the use of a function decomposition Taylor series. In our case one can suggest using the following Taylor series:

$$y^{(j)}(x+h) = y^{(j)}(x) + hy^{(j+1)}(x) + \frac{h^2}{2!} y^{(j+2)}(x) + \dots$$

$$+ \frac{h^{p-j}}{(p-j)!} y^{(p)}(x) + O(h^{p-j+1}), \quad h \rightarrow 0, \quad j = (0, 1, 2, 3) \quad (7)$$

here, $y^{(0)}(x) = y(x)$.

By using Taylor series (7) in the following equality

$$\sum_{i=0}^k (\alpha_i y(x+ih) - h\beta_i y'(x+ih) - h^2 \gamma_i y''(x+ih) - h^3 l_i y'''(x+ih)) = O(h^{p+1}), \quad h \rightarrow 0, \quad (8)$$

receive the following asymptotic equality:

$$\sum_{i=0}^k \alpha_i y(x) - h \sum_{i=0}^k (\beta_i - i \alpha_i) y'(x) - h^2 \sum_{i=0}^k (\gamma_i + i \beta_i - \frac{i^2}{2!} \alpha_i) y''(x) - \dots - h^p \sum_{i=0}^k (\frac{i^{p-3}}{(p-3)!} l_i + \frac{i^{p-2}}{(p-2)!} \gamma_i + \frac{i^{p-1}}{(p-1)!} \beta_i - \frac{i^p}{p!} \alpha_i) y^{(p)}(x) = O(h^{p+1}), h \rightarrow 0. \tag{9}$$

Note that for the comparison of the Multistep Methods usually are used the conceptions of the degree and stability.

Definition1. The integer value p is called as the degree for the method (6), if the asymptotic relation (8) is held.

Definition2. The method (6) is called as stable, if the roots of the polynomial

$$\rho(\lambda) = \alpha_k \lambda^k + \alpha_{k-1} \lambda^{k-1} + \dots + \alpha_1 \lambda + \alpha_0,$$

located in the unit circle on the boundary of which there are no multiple roots.

Noted that methods (2) and (3) were investigated by many authors, [27], [28], [29], [30], [31], [32], [33], [34].

As follows from the above mentioned the conception of stability is defined by using the values of the coefficients $\alpha_i (i = 0, 1, \dots, k)$. Therefore, one can say that with the help of the selection of coefficients $\alpha_i (i = 0, 1, 2, \dots, k)$ it is possible to construct stable and instable methods of types (2)-(5). We later will show that this is not always true for the methods (3) and (4). The conception of stability and degree very important for the comparison of above mentioned Multistep Methods. By using these conceptions, let us compare the methods (2) and (3). As is known, stability is the necessary and sufficient condition for the convergence of the Multistep Multiderivative Methods (see for example [1]). Therefore let us compare stable methods of types (2),(3), and (5). Dahlquist proves that in a class of method (2) there are stable methods with the degree $p \leq 2[k/2] + 2$, if $\beta_k \neq 0$ and if $\beta_k = 0$ then there are stable methods with the degree $p \leq k$ and there are stable methods with a degree p_{max} for all the values of order k . And now let us investigate the method (3). Let the method(3) have the degree of p , in the case: $|\beta_k| + |\beta_{k-1}| + \dots + |\beta_0| \neq 0$ and $\gamma_k \neq 0$. Then in the class of method (3), there are stable methods with the degree $p \leq 2k + 2$ and for all the k , there are stable methods with the degree $p_{max} = 2k + 2$, if $\beta_k = \gamma_k = 0$ and method (3) is stable then $p \leq 2k$. In the case $\beta_i = 0 (i = 0, 1, \dots, k)$, there is not stable method in

the class of (3). Therefore in this case, the following definition of stability.

Definition3. Method (3) in the case $\beta_i = 0 (i = 0, 1, \dots, k)$ called as the stable, if the roots of the polynomial $\rho(\lambda)$ located in the unit circle on the boundary of which there is not multiply root, except double root $\lambda = 1$.

Let us suppose that method (3) is stable for the case $\beta_i = 0 (i = 0, 1, \dots, k)$, then in class (4), there are methods with the degree $p_{max} = 2[k/2] + 2$ for all the order of k . And now let us to consider the investigation of a method (5). The maximum order for the stable methods of type (5), one can find by using the following theorems. In first let us consider the case, when $|\beta_k| + |\beta_{k-1}| + \dots + |\beta_0| = 0$ and $|\gamma_k| + |\gamma_{k-1}| + \dots + |\gamma_0| = 0$. In this case method (5) is called stable if the roots of the polynomial located in unit circle on the boundary of which, there is not multiplied root in addition to the three-fold root $\lambda = 1$.

If the stable method from the above mentioned class has the degree p , then in the receiving class methods there are stable methods with the degree $p_{max} = 2[k/2] + 2$. And now to consider the case, when $|\beta_k| + |\beta_{k-1}| + \dots + |\beta_0| \neq 0$. Let us consider the following theorem.

Theorem. If method (5) is stable, and has the degree of p , then in the class of method (5), there are methods with the degree $p \leq 3k + 4$. If $\beta_k = \gamma_k = l_k = 0$, then in the receiving class of methods, there are stable methods with the degree $p \leq 3k + 1$.

As is known, one of the main problems in the study of Multistep Methods is the ways of finding the coefficients of the method (5), so in the next paragraph we will consider finding the coefficients of the method (5).

§2. About some ways for the definition of the values of the coefficients in the method (5).

Let's consider finding coefficients for the construction a Multistep Thirdderivative Methods having appropriate precision. For this aim from the asymptotic equality of (9) one can receive the following linear system of algebraic equations:

$$\sum_{i=0}^k \alpha_i = 0; \sum_{i=0}^k \beta_i = \sum_{i=0}^k i \alpha_i; \sum_{i=0}^k (\gamma_i + i \beta_i) = \sum_{i=0}^k \frac{i^2}{2!} \alpha_i; \dots; \sum_{i=0}^k \left(\frac{i^{p-3}}{(p-3)!} l_i + \frac{i^{p-2}}{(p-2)!} \gamma_i + \frac{i^{p-1}}{(p-1)!} \beta_i \right) = \sum_{i=0}^k \frac{i^p}{p!} \alpha_i (\alpha_k \neq 0). \tag{10}$$

The amount of the unknowns in this system of (10) is equal to $4k+4$ and the amount of the equations is equal to $p+1$. By taking into account that the system (10)-is the homogenous, therefore if $p + 1 < 4k + 4$, then it follows from here that the solution of system (10) will be a unit for the case $p=4k+2$. Noted that some of the authors suggested replacing the system of (10) with the following, in the case $L_i = 0 (i = 0,1,...k)$:

$$\begin{aligned} g(1) &= 0; \quad g'(1) = \rho(1); \quad g''(1) = 2\rho'(1) - \rho(1) + 2\gamma(1); \\ g(\lambda)(\ln \lambda)^{-1} &= \sum_{m=0}^{\infty} c_m (\lambda - 1)^m; \\ \rho(\lambda) + \gamma(\lambda) \ln \lambda &= \sum_{i=0}^p c_i (\lambda - 1)^i, \end{aligned} \tag{11}$$

here

$$\begin{aligned} g(\lambda) &\equiv \sum_{i=0}^k \alpha_i \lambda^i; \quad \rho(\lambda) \equiv \sum_{i=0}^k \beta_i \lambda^i; \quad \gamma(\lambda) \equiv \sum_{i=0}^k \gamma_i \lambda^i, \\ c_i &= \frac{1}{i!} \int_0^1 u(u-1)\dots(u-i+1)du, \quad i = 0,1,2,\dots \end{aligned}$$

Let us note that the system of algebraic equations (10) and (11) are equivalent, so these systems are the necessary and sufficient conditions in order for these methods to have a degree p . As is known, every necessary and sufficient condition can be taken as a definition for some conception.

And now let us consider construction some examples for the case $k=3$. In this case, by solving the system (10) one can construct the following methods:

$$\begin{aligned} y_{n+3} &= (y_n + y_{n+1} + y_{n+2})/3 + \\ &h(10781y'_{n+3} + 22707y'_{n+2} + 16659y'_{n+1} + \\ &+ 4285y'_n)/27216 \\ &- h^2(2099F_{n+3} - 7227F_{n+2} - 2853F_{n+1} - 979F_n)/45360. \end{aligned} \tag{12}$$

The local truncation error for the method (12) can be presented as follows:

$$R_n = 3h^9 y_n^{(9)} / 156800 + O(h^{10}), \quad h \rightarrow 0.$$

As is known for the application of implicit methods one can use the predictor-corrector methods. For this aim usually are used implicit method as the

corrector, but as the predictor methods are used explicit method. And let us note that usually a predictor method selected the explicit method with the maximum degree. applying this theory to our case, the following method can be taken as the predictor method:

$$\begin{aligned} y_{n+3} &= (245y_n - 702y_{n+1} + 459y_{n+2})/2 \\ &- h(-87y'_n + 108y'_{n+1} + 189y'_{n+2})/2 \\ &+ h^2(9F_n - 108F_{n+1} + 27F_{n+2})/2 \\ &+ h^9 y_n^{(9)} / 1680 + O(h^{10}). \end{aligned} \tag{13}$$

It is known, that the predictor method can be taken as unstable. Noted that there are numerous works dedicated to the investigation of the methods (2)-(5), [35], [36], [37], [38], [39], [40], [41], [42], [43], [44].

In the application of methods (12) and (13) to solve some problems arises necessary calculation of the values y_{n+1} and y_{n+2} , since y_n - can be determined from the initial value condition. One can be suggested for finding the value y_{n+1} by using the initial-values y_n and y'_n . But in this case the rate of approximation will be low. By using this, here is recommended to use some sequence of methods, as the simple algorithm.

It is obvious that y_0, y'_0 and y''_0 -are known.

Let us consider the following algorithm.

Step 1. Input $(x_0, y_0, y'_0, y''_0; h)$;

Step 2. For $i := 0$ step 1 to $N-1$ do begin

$$y'_{i+2/3} = y'_i + \frac{2}{3} h y''_i;$$

$$y_{i+2/3} := y_i + h(y'_i + y'_{i+2/3})/2;$$

$$y_{i+1} := y_i + h(y'_i + 3y'_{i+2/3})/4;$$

$$\begin{aligned} y'_{i+1} &= y'_i + h(F(x_i, y_i, y'_i) \\ &+ 3F(x_{i+2/3}, y_{i+2/3}, y'_{i+2/3}))/4; \end{aligned}$$

print (y_{i+1}, y'_{i+1}) ;

Step 3: $j := i + 1$; $y'_{j+2/3} = y'_j + \frac{2}{3} h F(x_j, y_j, y'_j)$;

$$y_{j+2/3} := y_j + h(y'_j + y'_{j+2/3})/3 \text{ (Trapezoidal method);}$$

$$y_{j+1} := y_j + h(y'_j + 3y'_{j+2/3})/4;$$

$$y'_{j+1} = y'_j + h(F(x_j, y_j, y'_j) + 3F(x_{j+2/3}, y_{j+2/3}, y'_{j+2/3}))/4;$$

Print (y_{j+1}, y'_{j+1}) ; $i := i + 1$; go to step 2;

Step 4: Stop.

Here have used the Hybrid method with a simple structure. The degree for this method can be defined as the $p = 3$.

Note that these methods can be taken as the one-step methods and can applied to the calculation of

definite integrals, by the one and the same form. For this aim, one can use the following method:

$$y_{n+1} = y_n + h(y'_n + y'_{n+1})/12 + 5h^2(F_n + F_{n+1})/12, \tag{14}$$

here $F_i = F(x_i, y_i, y'_i)$, ($i = 0,1,2,\dots, N$).

Note that in using the method (14), the question of calculating the first derivatives of the original solutions also arises. How does it follow from here, that in the application of method (14), it becomes necessary to calculate of the values y_j and y'_j ($j = n, n+1$). If y'_j ($j \geq 0$) are known, then by using method (14) one can calculate the values of the solution of the problem (1). Noted that method (14) also has the degree $p = 4$.

It is not difficult to understand that for the receiving best results, one can use the above proposed methods (12) and (13).

Each method has its advantages and disadvantages, so here the proposed methods also have some advantages and disadvantages. However, depending on the problem being selected one of the above-suggested methods. Method (6) is more accurate and easily adapts to solve the problem (1). Taking into account that method (6) is more accurate, one can use the stable explicit methods as type (6).

2 Numerical Methods

Let us consider the following model problem:

$$y''(x) = \lambda^2 y(x), y(0) = 1, y'(0) = \lambda. \tag{15}$$

The exact solution for which can be presented as:

$$y(x) = \exp(\lambda x).$$

For the simplicity to solve this problem, let us use the following known method:

$$y_{n+2} = 2y_{n+1} - y_n + h^2(y''_{n+2} + 10y''_{n+1} + y''_n)/12. \tag{16}$$

The receiving results are tabulated in Table 1.

Table 1. Results for the step-size $h = 0.01$

x	$\lambda = 1$	$\lambda = -1$	$\lambda = 5$	$\lambda = -5$
0.20	5.66E-13	4.92E-13	1.28E-08	6.5E-09
0.60	6.23E-12	4.17E-12	4.31E-07	8.13E-08
1.00	2.12E-11	1.10E-11	5.76E-06	6.11E-07

Now let us consider the case, when λ is constant, but h -receive different values.

Table 2. Results obtained for the case $\lambda = 1$ and $h = 0.1; 0.05; 0.01$.

Variable x	Step size $h = 0.1$	Step size $h = 0.05$	Step size $h = 0.01$
0.20	4.45E-09	3.8E-10	7.32E-13
0.60	5.29E-08	3.45E-09	5.68E-12
1.00	1.2E-07	7.51E-09	1.2E-11

In order to describe the properties of the solutions of problem (16) in an accessible form decided here, take into account the value of the parameter λ and the arguments x , which are tabulated in Table 1 and Table 2.

Noted that, above-given method can be applied to solve Volterra integral and Volterra integrodifferential equations, [45], [46], [47], [48], [49]

For this aim let us consider the following.

Example:

$$y'' = \lambda^2(1 + a(1 - y(x)) + (1 + a)\lambda^2 \int_0^x y(s)ds, y(0) = 1; \tag{17}$$

$$y'(0) = \lambda, x \in [0,1]$$

The exact solution for this example: $y(x) = \exp(\lambda x)$.

From the example 2 it follows the example 1 for the case $a = -1$.

Receiving results are tabulated in Table 3.

Table 3. Error for method (15) at $a = 1; h = 0.01$

x	$\lambda = 1$	$\lambda = -1$	$\lambda = 5$	$\lambda = -5$
0.20	2.04E-12	2.16E-12	2.53E-08	3.26E-08
0.60	1.7E-12	2.05E-12	1.17E-08	1.17E-08
1.00	4.1E-11	5.53E-11	2.86E-06	1.97E-07

The results are corresponding theoretical.

By results receive that method can be taken as the normal.

3 Conclusion

There are some classes of methods constructed to solve problems (1). This problem is usually investigated in two forms. One of them investigates problem (1) in the given form and the others follows:

$$y'' = f(x, y), y(x_0) = y_0, y'(x_0) = y'_0, x_0 \leq x \leq X. \tag{18}$$

Solving as many problems are reduced to solving the problem (18), therefore the problem (18) is called the special presentation of the ODEs of second order. Many known specialists have investigated the problem (18). Have proven that Multistep Secondderivative Method (3)-(6) can apply to solve problem (1), with one and the same success. But these methods have different properties. The problem (18) is intersected with the above-investigated problems. Therefore, by using the above-presented methods one can solve problem (1) and all the partial cases of this problem. For the sake of objectivity, let us note that all the above-noted methods can be applied to solve problems (18). In this case, there is a need to calculate values y'_m ($m \geq 1$) at every step. On the other side the function $f(x, y)$ independent from the $y'(x)$. Therefore, there is no need for calculation values y'_i ($i > 0$).

Štörmer by using this property, suggested for the calculated the values y'_i ($i > 0$) of the solution of problem (14), by using method (4). Note that the definition of the conception of stability for method (4) can use the definition3.

Let us note that method (14) has the degree of $p=4$ and the method used in the algorithm, has the degree $p=3$ and is stable. To increase the accuracy of which one can use in the above-constructed method is the half sum of the following methods:

$$\bar{y}_{n+1} = y_n + h(y'_{n+1} + 3y'_{n+1/3})/4, \quad (19)$$

$$\hat{y}_{n+1} = y_n + h(y'_n + 3y'_{n+2/3})/4. \quad (20)$$

Method (20) was used in the algorithm. By simple comparison of the method (14) and half sum of the method (19) and (20) receive that, the use of methods (19) and (20) is preferable. One by using the method of (6) can be construct the stable method with the high order. By using the higher accuracy of the method (12), one can recommend an application to solve some problems by using the method (13) as the predictor method. Method (20) and method (13) are representatives of different classes of methods. Methods (19) and (20) are usually called as the hybrid or fractional step method. Here given one way to construct numerical methods with the new properties. We hope that this method described here will find its followers.

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