A-STABLE METHOD FOR THE SOLUTION OF THE CAUCHY PROBLEM FOR STIFF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

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For the solution of the Cauchy problem for the system of equations

$$\dot{y} = f(y) \tag{1}$$

there is constructed the Rosenbrock type method accurate to the fifth local order with a single computation of a Jacobian matrix per step of integration. Numerical experiments have shown high efficiency of the proposed method. The following approximation of the exponential function is taken as the basis of the method

$$e^x \approx \varphi_4(x) \equiv 1 + \frac{x}{1-x} - \frac{1}{2}\frac{x^2}{(1-x)^2} + \frac{1}{6}\frac{x^3}{(1-x)^3} + \frac{1}{24}\frac{x^4}{(1-x)^4} \; . \tag{2}$$

From the results of papers [1,2] it immediately follows that

$$|\varphi_4(x)| \le 1, \quad \text{at} \quad \mathrm{Re}\, x \le 0 \; . \tag{3}$$

One of the possible versions of the Rosenbrock type formulae based on approximation (2) is of the form

$$y_{n+1} = y_n + \sum_{i=1}^{4} p_i k_i \; , \tag{4}$$

$$k_i = h\,[1 - hf_y]^{-1} f(\eta_i) \; , \tag{5}$$

$$\eta_i = y_n + \sum_{j=1}^{i-1} \beta_{ij} k_j, \quad i = 2,3,4,$$
$$\eta_1 = y_n, \tag{6}$$

where f_y is the Jacobian matrix of system (1) calculated in the point y_n. Method (4)-(6) is of the fifth local order of accuracy and A-stable provided that the coefficients p_i, β_{ij} satisfy the following system of nonlinear algebraic equations:

$$\sum_{i=1}^{4} p_i = 1, \tag{7}$$

$$\sum_{i=2}^{4} p_i c_i = -\frac{1}{2}, \tag{8}$$

$$\sum_{i=2}^{4} p_i c_i^2 = \frac{1}{3}, \tag{9}$$

$$\sum_{i=2}^{4} p_i c_i^3 = \frac{1}{4}, \tag{10}$$

$$\beta_{32} c_2 p_3 + (\beta_{42} c_2 + \beta_{43} c_3)\, p_4 = \frac{1}{6}, \tag{11}$$

$$\beta_{32} c_2^2 p_3 + (\beta_{42} c_2^2 + \beta_{43} c_3^3)\, p_4 = -\frac{1}{4}, \tag{12}$$

$$\beta_{32} c_2 c_3 p_3 + (\beta_{42} c_2 + \beta_{43} c_3)\, c_4 p_4 = -\frac{5}{24}, \tag{13}$$

$$\beta_{32}\, \beta_{43} c_2 p_4 = \frac{1}{24}, \tag{14}$$

$$c_i = \sum_{j=1}^{i-1} \beta_{ij}, \quad i = 2,3,4. \tag{15}$$

All the solutions (7)-(15) are exhausted by the general solution depending on the two parameters c_2, c_3 and by the singular solution depending on one parameter p_4.

The general solution where $(c_3 \neq c_4)$: c_2, c_3 are parameters, is given by

$$\beta_{32}=\frac{c_3(c_2-c_3)}{c_2(6+4c_2)},\ c_4=-\frac{6+7c_2}{8+7c_2},$$

$$p_4=\frac{3-4c_2-c_3(4+6c_2)}{12c_4(c_4-c_3)(c_4-c_2)},\ p_3=\frac{1}{c_3(c_3-c_2)}\left[\frac{1}{3}+\frac{c_2}{2}-p_4c_4(c_4-c_2)\right],$$

$$p_2=-\frac{1}{c_2}\left[\frac{1}{2}+c_3p_3+c_4p_4\right],\ p_1=1-p_2-p_3-p_4,$$

$$\beta_{43}=\frac{1}{24p_1c_2\beta_{32}},\ \beta_{42}=\frac{1}{c_2p_4}\left[\frac{1}{6}-p_3c_2\beta_{32}-p_4c_3\beta_{43}\right], \qquad (16)$$

$$\beta_{21}=c_2,\quad \beta_{31}=c_3-\beta_{32},\quad \beta_{41}=c_4-\beta_{42}-\beta_{43}.$$

The singular solution ($c_3=c_4$), where p_4 is a parameter, is given by

$$c_2=-\frac{16}{7},\ c_3=-\frac{5}{4},\quad c_4=-\frac{5}{4},\ p_2=-\frac{7^3}{6\cdot16\cdot29},$$

$$p_3=\frac{17\cdot16}{3\cdot5\cdot29}-p_4,\quad p_1=1-p_2-p_3-p_4,$$

$$\beta_{32}=\frac{5\cdot7\cdot29}{2\cdot(16)^2\cdot11},\quad \beta_{43}=-\frac{4\cdot11}{3\cdot5\cdot29}\cdot\frac{1}{p_4}, \qquad (17)$$

$$\beta_{42}=\frac{\left(\frac{1}{6}-\beta_{32}c_2p_3\right)-p_4\beta_{43}c_3}{c_2p_4},\quad \beta_{21}=c_2,$$

$$\beta_{31}=c_3-\beta_{32},\quad \beta_{41}=c_4-\beta_{42}-\beta_{43}.$$

From this set of solutions we distinguish the variant of the general solution with $c_2 = -1$, $c_3 = 1/2$:

$$c_2 = 1 , \quad c_3 = \frac{1}{2} , \quad c_4 = 1,$$

$$p_1 = \frac{13}{6} , \; p_2 = \frac{1}{6} , \quad p_4 = -2, \quad p_4 = \frac{2}{3} , \tag{18}$$

$$\beta_{21} = -1, \quad \beta_{31} = \frac{1}{8} , \quad \beta_{32} = \frac{3}{8} , \quad \beta_{41} = \frac{3}{8} ,$$

$$\beta_{42} = \frac{19}{24} , \quad \beta_{43} = -\frac{1}{6} .$$

Method (4)-(6), (18) has the following remarkable properties. In the first place, the domain of influence is reduced to the minimal possible one:

$$|\beta_{ij}| \le 1, \quad |c_j| \le 1. \tag{19}$$

In the second place, accumulation of round-off errors characterized by the value ξ :

$$\xi = \sum_{i=1}^{4} |p_i| = 5 \tag{20}$$

is close to the minimal one. If the condition (19) is fulfilled, the minimal $\xi \approx 4.8$, but the coefficients β_{ij}, p_i have a more complicated form. We assume that the fulfilment of condition (19) must ensure high accuracy on smooth slowly changing variables. Tests of the method (4)-(6),(18) on examples of the small stiffness show that it achieves the same accuracy as the Runge-Kutta method with steps two times smaller than those required by the Runge-Kutta method. The global volume of work in comparison with the Runge-Kutta method, is approximately ten times as large. The method suggested will be more effective than the Runge-Kutta method, if stiffness of the system (the relation of the maximal module of eigenvalues of the Jacobian matrix to the minimal one) exceeds one hundred.

Numerical trials of the method on typical test stiff type problems [3] have shown its high efficiency in comparison with the methods of Runge-Kutta, Hamming [4], Brayton, Gustavson, Hachtel [5], and Liniger [6]. We used the standard programs of the "Dubna" monitor system [7] for method of Runge-Kutta and Hamming in numerical experiments, in algorithm [5] changes were introduced in the variation strategy of the step and the order of the method; method [6] was used in the form linearized according to Newton (non-iterative Rosenbrock type algorithm) was used.

R e f e r e n c e s

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