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RATIONAL-FRACTIONAL METHODS FOR SOLVING STIFF SYSTEMS OF DIFFERENTIAL EQUATIONS

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Abstract. This paper proposes new numerical methods for solving stiff systems of first-order differential equations not resolved with respect to the derivative. These methods are based on rational-fractional approximations of the vector-valued function of solution of the system considered. The authors study the stability of the constructed methods of arbitrary finite order of accuracy. Analysis of the results of experimental studies of these methods by test examples of various types confirms their efficiency.

In many cases, modern numerical methods for solving the Cauchy problem for systems of differential equations are based on the Taylor formula. The process of construction of numerical methods by using these formulas consists in the choice of the method for approximating the derivative of the desired solution. However, these so-called explicit methods have a number of deficiencies. In their implementation, there arise certain computational difficulties, and they have a bounded stability region and cannot be applied to solving stiff systems.

In this paper, we propose new numerical methods for the solution of stiff systems of first-order differential equations not resolved with respect to the derivative. These methods are based on rational-fractional approximation of the vector-valued function of solution of the system considered.

We consider the Cauchy problem for the following system of differential equations not resolved with respect to the derivative:

$$F(x,y,y')=0,\quad y(x_0)=y_0,\quad x_0\le x\le x_k, \tag{1}$$

where F is a smooth S-dimensional vector-valued function, $x\in\mathbb{R}$, $y\in\mathbb{R}^S$, and $y'\in\mathbb{R}^S$.

We assume that in a certain closed domain

$$D=\{x_0\le x\le x_k,\ \|y\|_D\le M_1<\infty,\ \|y'\|_D\le M_2<\infty\},$$
$$\|y\|_D=\max_x\|y(x)\|_{R^S},\quad \|y'\|_D=\max_x\|y'(x)\|_{R^S},$$

the function $F(x,y,y')$ is continuous and differentiable in all its arguments, the derivative $F_{y'}=\frac{\partial F}{\partial y'}$ exists and is a nonsingular positive-definite matrix, and there exists the derivative $\left\|\frac{\partial F}{\partial y}\right\|_D\le N_1$, which also is a bounded positive-definite matrix.

Moreover, assume that

$$y'(x_0)=y'_0 \tag{2}$$

is a known root of the equation $F(x_0,y_0,y')=0$. Starting from the above conditions, we assume that there exists a unique solution of problem (1) defined on the whole closed interval $[x_0,x_k]$ of the range of x.

The reduction of the initial system (1) to the form resolved with respect to the derivative requires the solution of a nonlinear system with respect to the variable y'; in most of the cases, this leads to large computational expenditures at each step of integration.

Let us consider the methodology for constructing approximations of the solution (1), which uses the rational-fractional structure of the approximations, allows us to construct an approximation of arbitrary concordance order, and does not require the solution of the nonlinear system (1) with respect to y'.

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Taking into account the obvious relation $F_x+F_y y'+F_{y'}y''=0$, where $F_x=\frac{\partial F}{\partial x}$, we transform problem (1), (2) to the form

$$y''=-F_{y'}^{-1}(F_y y'+F_x),\quad y(x_0)=y_0,\quad y'(x_0)=y'_0. \tag{3}$$

We represent problem (3) in the form of the following extended first-order system:

$$\begin{cases} y'=z,\ y(x_0)=y_0,\ z(x_0)=y'_0, \\ z'=f(x,y,z), \end{cases} \tag{4}$$

where $f(x,y,z)=-F_{y'}^{-1}(F_y z+F_x)$.

We construct rational-fractional approximations of problem (4) for y_{n+1} and $z_{n+1}=y'_{n+1}$ separately. It is known that rational-fractional approximations of solutions of stiff systems are described by the expression

$$y_{n+1}^{[p]}=\frac{\sum\limits_{j=0}^{p}(-1)^j C_p^j a_p^j h^j J_n^j T_{p-j,n}}{(E-a_p hJ_n)^p}, \tag{5}$$

where $T_{k,n}$ is the Taylor approximation of the solution of the kth order with respect to the grid node, C_p^i is the binomial coefficient, a_p is the parameter of approximation of the pth order of concordance, and J_n is the Jacobi matrix of the initial system of equations defined by $J_n=-F_{y'_n}^{-1}F_{y_n}$, which is common for finding y_{n+1} and z_{n+1}. In this case, an additional computational expenditure for finding the inverse matrix $F_{y'_n}^{-1}$ arises. For approximations of the first and second order, we can avoid this deficiency. In relation (5), the division must be understood as the premultiplication of the inverse matrix of the denominator by the vector of the numerator.

To reduce the computational expenditures, let us transform (5). Extract the summand y_n from the Taylor approximations $T_{k,n}$ by introducing the notation

$$y_{n+1}^{[p]}=y_n+F_{kn},$$

where

$$F_{kn}=\sum_{i=1}^{k}\frac{h^i}{i!}y_n^{(i)}.$$

Then we can represent (5) in the form

$$y_{n+1}^{[p]}=y_n+\frac{\sum\limits_{j=0}^{p-1}(-1)^j C_p^j a_p^j h^j J_n^j F_{p-j,n}}{(E-a_p hJ_n)^p}. \tag{6}$$

Expand the fractional part of this relation into the sum of elementary fraction in powers of the denominator:

$$y_{n+1}^{[p]}=y_n+\sum_{i=1}^{p}\frac{A_i}{(E-a_p hJ_n)^i}, \tag{7}$$

where A_i are vectors of the expansion.

For the concordance of (5) with (4), find the vector coefficients A_i from the system of linear vector equations

$$\sum_{i=1}^{p-k}C_{p-i}^k A_i=C_p^k F_{p-k,n},\quad k=\overline{0,p-1}. \tag{8}$$

The solution of system (8) has the form

$$A_i=C_p^i\sum_{j=0}^{i-1}(-1)^j C_i^j F_{i-j,n},\quad i=\overline{1,p}.$$

Then (7) transforms to the form

$$y_{n+1}^{[p]} = y_n + \sum_{i=1}^{p} \frac{C_p^i \sum\limits_{j=0}^{i-1} (-1)^j C_i^j F_{i-j,n}}{(E - a_p h J_n)^i}. \tag{9}$$

Let us consider first-order concordance rational-fractional transformations of the solution of the problem (3) for $y_{n+1}^{[1]}$ and $z_{n+1}^{[1]}$ separately, taking into account that $J_n = -F_{y_n'}^{-1} F_{y_n}$:

$$y_{n+1}^{[1]} = y_n + \frac{F_{1ny}}{E + a_1 h F_{y_n'}^{-1} F_{y_n}}, \quad z_{n+1}^{[1]} = z_n + \frac{F_{1nz}}{E + a_1 h F_{y_n'}^{-1} F_{y_n}}, \tag{10}$$

where, according to (4), $F_{1ny} = hz_n$ and $F_{1nz} = -hF_{y_n'}^{-1}(F_{y_n} z_n + F_{x_n})$. Premultiplying the fractional part of (10) by the matrix F'_{y_n}, we obtain

$$y_{n+1}^{[1]} = y_n + \frac{hF_{y_n'} z_n}{F_{y_n'} + a_1 h F_{y_n}}, \quad z_{n+1}^{[1]} = z_n - \frac{h(F_{y_n} z_n + F_{x_n})}{F_{y_n'} + a_1 h F_{y_n}}. \tag{11}$$

From the restriction imposed on the function $F(x, y, y')$, we conclude that the matrix $Q_n = F_{y_n'} + a_1 h F_{y_n}$ of denominators (11) is positive-definite and invertible.

Consider the stability conditions for approximations (11) by examining the model system

$$y' + AY = 0, \quad y(0) = y_0, \quad y'(0) = -Ay_0, \tag{12}$$

where A is a constant positive-definite matrix, $F_y = A$, $F'_y = E$, and $F_x = 0$. For this model system, approximations (11) become

$$y_{n+1}^{[1]} = y_n + \frac{hz_n}{E + a_1 hA}, \quad z_{n+1}^{[1]} = z_n - \frac{hAz_n}{E + a_1 hA}. \tag{13}$$

If $z_0 = -Ay_0$, then we obtain by induction $z_n^{[1]} = -Ay_n^{[1]}$. Then we can represent (13) in the form

$$y_{n+1}^{[1]} = \frac{(E + (a_1 - 1)hA) y_n}{E + a_1 hA}, \quad z_{n+1}^{[1]} = \frac{(E + (a_1 - 1)hA) z_n}{E + a_1 hA}. \tag{14}$$

Approximations (14) has the following common operator function:

$$D(hA) = \frac{E + (a_1 - 1)hA}{E + a_1 hA}. \tag{15}$$

It follows from the definition of L- and A-stability that for $a_1 = 1$, approximations (11) are L-stable, and for $a_1 = \frac{1}{2}$, approximations (11) are A-stable.

Similarly, for the solution y_{n+1}, we can construct the second-order concordance approximation using the first-order concordance approximation z_{n+1} for this purpose.

With account for (3) and (4), the values of the second-order accuracy Taylor approximation of y_{n+1} are defined by the relation

$$F_{2ny} = hz_n - \frac{h^2}{2} F_{y_n'}^{-1} (F_{y_n} z_n + F_{x_n}). \tag{16}$$

Then the second-order concordance approximation has the form

$$y_{n+1}^{[2]} = y_n + \frac{F_{y_n'}}{F_{y_n'} + a_2 h F_{y_n}} \left(2hz_n - \frac{hF_{y_n'} z_n + \frac{h^2}{2}(F_{y_n} z_n + F_{x_n})}{F_{y_n'} + a_2 h F_{y_n}} \right), \quad z_{n+1}^{[1]} = z_n - \frac{h(F_{y_n} z_n + F_{x_n})}{F_{y_n'} + a_2 h F_{y_n}}. \tag{17}$$

In the process of defining $y_{n+1}^{[2]}$, the use of the first-order concordance approximations $y'_n = z_n$ does not reduce the concordance order of y_{n+1}.

Let us find the stability conditions of approximations (17) by examining the model system (12). The approximations of solutions of this system are described by the relations

$$y_{n+1}^{[2]} = y_n + \frac{h(E + (2a_2 - \frac{1}{2})hA)}{(E + a_2 hA)^2} z_n, \quad z_{n+1}^{[1]} = \frac{E + (a_2 - 1)hA}{E + a_2 hA}. \tag{18}$$

If $a_2 = \frac{1}{2}$, then approximations (15) have the A-stability property with the common operator function

$$D(hA) = \frac{E - \frac{h}{2}A}{E + \frac{h}{2}A}$$

and have the form

$$y_{n+1}^{[2]} = \frac{E - \frac{h}{2}A}{E + \frac{h}{2}A} y_n, \quad z_{n+1}^{[1]} = \frac{E - \frac{h}{2}A}{E + \frac{h}{2}A} z_n.$$

As a test problem, let us consider the equation $y = ay'(y'^2 - 1)$ with the initial conditions $y(0) = 0$. Differentiating with respect to the argument x, we transform this implicit differential equation to the explicit second-order differential equation

$$y'' = \frac{y'}{a(3y'^2 - 1)}. \tag{19}$$

To ensure the uniqueness of solution, we complement the initial conditions by the condition $y'(0) = 1$, which is a root of the initial equation. To solve the second-order equation (19), we reduce it to a system of two first-order equations

$$\begin{cases} y_1' = y_2, & y_1(0) = 0, \\ y_2' = \dfrac{y_2}{a(3y_2^2 - 1)}, & y_2(0) = 1. \end{cases} \tag{20}$$

In the process of solution using explicit linear numerical methods of Runge–Kutta type on the closed interval $[0; 1]$, it turned out that when the solution approaches the right endpoint of the closed interval, the stiffness of the system increases and the integration step sequentially decreases. In this connection, the solution of the transformed system (20) was performed using the rational-fractional numerical methods for solving stiff systems. As a result, the approximate solution of system (20) was obtained on the whole interval of integration with a sufficiently large step whose maximum value is $h_{\max} = 0{,}4096$ and ensures the required accuracy. The real error of the approximate solution, which was estimated using the given exact solution of the test example in the parametric form

$$x = a\left(\frac{3}{2}(p-1)^2 - \ln p\right), \quad y = ap(p^2 - 1),$$

does not exceed the admissible error on the whole interval of integration.

The study of other test examples also confirms the effectivity of using the rational-fractional numerical methods of the order indicated above for solving stiff implicit differential equations with their transformation to explicit equations of enlarged order.

To construct numerical methods on the basis of formulas of rational-fractional approximations of higher order, it is necessary to point out the method for finding a sequence of partial sums of the Taylor formula of accuracy from the first to the pth order. If for finding these sums, we use known methods of Runge–Kutta type, then applying the formulas of rational-fractional approximations, it is easy to construct one-step rational-fractional numerical methods.

If for approximating the partial sums of the Taylor series, we use linear multi-step methods, then using the formulas of rational-fractional approximations, it is possible to construct multi-step rational-fractional numerical methods. For this purpose, we can use, for example, the Adams–Bushford methods or linear multi-step methods with a variable step of integration. It is appropriate to find higher-order approximations by using multi-step methods.

The stability of the constructed methods of arbitrary finite order of accuracy was studied. Analysis of the results of experimental studies of these methods by examining various types of test examples justifies their effectiveness.

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