Numerical Algorithm for Design of Stability Polynomials for the First Order Methods

E. A. Novikov
Institute of Computational Modelling
Siberian Branch of Russian Academy of Sciences
Krasnoyarsk, Russia
novikov@icm.krasn.ru

M. V. Rybkov
Institute of Mathematics and Fundamental Informatics
Siberian Federal University
Krasnoyarsk, Russia
mixailrybkov@yandex.ru

A. E. Novikov
Institute of Mathematics and Fundamental Informatics
Siberian Federal University
Krasnoyarsk, Russia
aenovikov@bk.ru

Abstract — **The algorithm for coefficients determination for stability polynomials of degree up to m = 35 is developed. The coefficients correspond to explicit Runge-Kutta methods of the first accuracy order. Dependence between values of a polynomial at the points of extremum and both size and form of a stability domain is shown. Numerical results are given.**

Keywords - stiff problem; explicit methods; stability polynomials;

I. INTRODUCTION

Heterogeneous algorithms are applied to solving stiff problems in a number of situations. Such algorithms are designed using the fact that on the settling and transition regions the integration stepsize is limited according to the requirements of stability and accuracy, respectively. Efficiency growth can be achieved by applying an explicit scheme over the transition region and a *L*-stable scheme over the settling region. Switch between methods is performed using an inequality for stability control. The problem is that the size of stability domains of the known methods is too small. Some monographs and papers present explicit methods with extended stability domains [1, 2]. The way how to obtain stability polynomials providing the maximal length of a stability domain is considered in [3]. In [2] there is proposed the algorithm for obtainment of polynomials coefficients that allows to design explicit methods with predefined form and size of a stability domain. Furthermore, stability polynomials coefficients of degree up to *m*=13 are found there. Here is developed the algorithm for obtainment of the coefficients of stability polynomials of degree up to *m*=27. The coefficients correspond to the Runge-Kutta methods of the first accuracy order. It is shown that the form, size, and structure of a stability domain depend on position of the roots of stability polynomial on the complex plane.

II. EXPLICIT METHODS OF THE RUNGE-KUTTA TYPE

To solve a stiff problem

$$y' = f(t, y),\ y(t_0) = y_0,\ t_0 \le t \le t_k,$$

where y and f are smooth real N-dimensional vector-functions, t is an independent variable, in [2] explicit methods

$$y_{n+1} = y_n + \sum_{i=1}^{m} p_{mi} k_i,\ k_i = hf\left(t_n + \alpha_i h, y_n + \sum_{j=1}^{i-1} \beta_{ij} k_j\right)$$

are considered, where k_i, $1 \le i \le m$, are stages of the method, h is the integration stepsize, p_{mi}, α_{ij}, and β_{ij} are numerical coefficients defining accuracy and stability properties of this numerical scheme. For simplicity, let us consider the following Cauchy problem for the autonomous system of ODEs

$$y' = f(y),\ y(t_0) = y_0,\ t_0 \le t \le t_k. \quad (1)$$

We apply methods of the form

$$\begin{gathered} y_{n,i} = y_n + \sum_{j=1}^{i} \beta_{i+1,j} k_j, 1 \le i \le m-1, \\ y_{n+1} = y_n + \sum_{i=1}^{m} p_{mi} k_i, \end{gathered} \quad (2)$$

to solve (1), where $k_i = hf(y_{n,i-1})$, $1 \le i \le m$, $y_{n,0} = y_n$. All the findings those are to obtained below can be used for non-autonomous problems, if

$$\alpha_1 = 0,\ \alpha_i = \sum_{j=1}^{i-1} \beta_{ij},\ 2 \le i \le m.$$

Stability of one-step methods is widely studied on the Dahlquist equation $y'=\lambda y$, $y(0) = y_0$, $t \ge 0$ with complex λ, $\mathrm{Re}(\lambda) < 0$ (see [4]). Applying the second formula from (2) to solve $y'=\lambda y$, we get

$$y_{n+1} = Q_m(z) y_n,\ Q_m(z) = 1 + \sum_{i=1}^{m} c_{mi} z^i,$$
$$c_{mi} = \sum_{j=i}^{m} b_{ij} p_{mj},\ 1 \le i \le m,$$

where $z = h\lambda$. Hence, the stability function of a m-stage explicit Runge-Kutta method is polynomial $Q_m(z)$ of degree m. Order conditions for methods of form (2) are given in [2] and, particularly, a method has the first accuracy order, if $p_{m1} + \ldots + p_{mm} = c_{m1} = 1$. Further, consider the problem of finding such coefficients that a stability domain had the predefined form and size.

III. Stability Polynomials Over Interval $[\gamma_M, 0]$

Let k and m be given integers, $k \le m$. Consider polynomials

$$Q_{m,k}(x) = 1 + \sum_{i=1}^{k} c_i x^i + \sum_{i=k+1}^{m} c_i x^i, \tag{3}$$

where c_i, $1 \le i \le k$, are defined, and c_i, $k + 1 \le i \le m$, are arbitrary. Usually c_i, $1 \le i \le k$, are determined according to the requirements of accuracy. Therefore, let us assume that $c_i = 1/i!$, $1 \le i \le k$.

Denote points of extremum of (3) by $x_1, \ldots, x_{m-1}$, at that $x_1 > x_2 > \ldots > x_{m-1}$. Define unknown coefficients c_i, $k + 1 \le i \le m$, so that polynomial (3) has predefined values in extreme points x_i, $k \le i \le m-1$, i.e. $Q_{m,k}(x_i) = F_i$, $k \le i \le m-1$, where $F(x)$ is some given function, $F_i = F(x_i)$. For this purpose, consider the system of algebraic equations

$$Q_{m,k}(x_i) = F_i, Q'_{m,k}(x_i) = 0, k \le i \le m-1,$$
$$Q'_{m,k} = \sum_{i=1}^{m} i c_i x^{i-1}, \tag{4}$$

in variables x_i, $k \le i \le m - 1$, and c_j, $k + 1 \le j \le m$.

Rewrite (4) in the form, suitable for calculations on the computer. Denote through y, z, g, and r vectors with components

$$y_i = x_{k+i-1},\ z_i = c_{k+i},\ g_i = F_{k+i-1} - 1 - \sum_{j=1}^{k} c_j y_i^j,$$
$$r_i = -\sum_{j=1}^{k} j c_j y_i^{j-1},\ 1 \le i \le m-k,$$

through E_1, E_2, E_3 − diagonal matrices with elements

$$e_1^{ii} = k+i,\ e_2^{ii} = 1/y_i,$$
$$e_3^{ii} = (-1)^{k+i-1},\ 1 \le i \le m-k,$$

and through A − a matrix with elements $a_{ij} = y_i^{k+j}$, $1 \le i, j \le m-k$. Using these notations problem (4) can be written as follows

$$Az - g = 0,\ E_2 A E_1 z - r = 0. \tag{5}$$

System (5) is ill-conditioned that leads to some difficulties while solving it with the fixed point iteration method. For convergence of the Newton's method is necessary to somehow obtain good initial conditions (in this case is a separate difficult problem). If we assume in (4) that $F_i = (-1)^i$, $k \le i \le m-1$, we find the polynomial with the maximal length of stability interval. In this case the problem of computation of initial value y^0 is solved by using values of the Chebyshev polynomial at extreme points over interval $[-2m^2, 0]$, where m is degree of polynomial (3). That values can be computed using the formula

$$y_i = m^2[\cos(i\pi/m) - 1],\ 1 \le i \le m-1. \tag{6}$$

Substituting (6) in the system (5), get coefficients of the Chebyshev polynomial, for that $|Q_{m1}(x)| \le 1$ on $x \in [-2m^2, 0]$. For any k (6) can be taken as initial values and, as numerical results show, there is good convergence rate in this case. If $F_i \ne (-1)^i$, $k \le i \le m-1$, then the choice of initial values is a separate difficult problem.

Let us describe a way to solve (5) that does not require good initial values. Apply the relaxations for the numerical solution of (5). The main idea of the relaxations is that for a steady-state problem we run unsteady-state process which solution settles to the solution of the initial problem. Consider the Cauchy problem

$$y' = E_3(E_2 A E_1 A^{-1} g - r),\ y(0) = y_0. \tag{7}$$

Apparently, after the determination of stationary point of (7) the stability polynomial coefficients can be computed from the system (5). Notice, that due to using matrix E_3 all the eigenvalues of the Jacobi matrix of (7) have negative real components, i.e. problem (7) is stable. From the numerical results follows that (7) is a stiff problem. Applying methods that require evaluation of the Jacobi matrix may cause difficulties while solving (7). Therefore, let us apply the second accuracy order method using numerical computation and freezing (i.e. using same matrix over several steps) the Jacobi matrix [5] to solve (7). When this method is applied to the problem $y' = f(y)$, $y(0) = y_0$ it takes the form

$$y_{n+1} = y_n + ak_1 + (1-a)k_2,\ D_n = E - ah_n A_n,$$
$$D_n k_1 = h_n f(y_n), D_n k_2 = k_1. \tag{8}$$

Here, $a = 1 - 0.5\sqrt{2}$, k_1 and k_2 are stages of the method, E is the identity matrix, h_n is the integration stepsize, A_n is a matrix representable in the form $A_n = f_n' + h_n R_n + O(h_n^2)$, $f_n' = \partial f(y_n)/\partial y$ is the Jacobi matrix of (7), R_n is the integration stepsize independent matrix. Since matrix R_n is arbitrary, then problems of numerical integration and freezing the Jacobi matrix can be concerned simultaneously. To control accuracy of (8) the inequality

$$\varepsilon(j_n) = \| D_n^{-j_n}(k_2 - k_1) \| \le a\varepsilon / |a - 1/3|, \ 1 \le j_n \le 2, \quad (9)$$

can be applied, where ε is the required accuracy of calculations, $\|\cdot\|$ is some norm in R^N, and integer variable j_n is chosen minimum for which inequality (9) is satisfied. The numerical differentiation step s_j, $1 \le j \le N$, is chosen using the formula $s_j = \max\{10^{-14}, 10^{-7}|y_j|\}$. In this case j-th column a_n^j of matrix A_n is computed using the formula

$$a_n^j = [f(y_1, .., y_j + s_j, .., y_N) - f(y_1, .., y_j, .., y_N)]/s_j,$$
$$1 \le j \le N,$$

i.e. it is required to perform N computations of the right part of problem (7) to define A_n. An attempt to use previous matrix D_n is performed after each successful integration step. To preserve stability properties of the numerical scheme, on freezing matrix D_n the integration stepsize is kept permanent. Recomputation of the matrix is carried out in the following cases: 1) accuracy of calculations is degenerated, 2) quantity of steps with frozen matrix has reached maximal number I_h, 3) the predicted step is greater than the previous successful one in Q_h times.

IV. Stability Polynomials Over Interval [–1, 1]

It is not difficult to see that the coefficients of a stability polynomial approach zero as m increases. Coefficients c_i, $k+1 \le i \le m$, for polynomials of degree up to m=13 are presented in [2]. Now consider the algorithm for the obtainment of polynomials with predefined properties over the interval [−1, 1]. In this case coefficients c_i grow not that much, and it is possible to derive polynomials for m>13. Denote through $|\gamma_m|$ the length of stability interval of m-stage explicit formula of the Runge-Kutta type, i.e. the inequality $|Q_{m,k}(x)| \le 1$ over interval $[\gamma_m, 0]$ is satisfied. Then, substituting $x = 1 - 2z/\gamma_m$ we can map $[\gamma_m, 0]$ into [−1, 1] and obtain the polynomial

$$Q_m(z) = \sum_{i=0}^{m} d_i z^i . \quad (10)$$

Coefficients d_i, $0 \le i \le m$ of polynomial (10) and coefficients c_i, $0 \le i \le m$, of (3) satisfy the relation

$$c = UVd, \quad (11)$$

where $d = (d_0, \dots, d_m)^T$, $c = (c_0, \dots, c_m)^T$, U is a diagonal matrix with elements $u^{ii} = (-2/\gamma_m)^{i-1}$, $1 \le i \le m+1$. Elements v^{ij} of V are defined by

$$v^{1j} = 1, \ 1 \le j \le m+1; \ v^{ij} = v^{i,j-1} + v^{i-1,j-1},$$
$$2 \le i \le j \le m+1; \ v^{ij} = 0, \ i > j.$$

It is easy to see that V represents the Pascal's triangle which elements are easily computed using a recurrent formula. Therefore, after deriving the polynomial (10) over interval [–1, 1], using (11) it is easy to compute coefficients of polynomial (3).

Now let us construct polynomial (10). We denote the extreme points of (10) through $z_1, \dots, z_{m-1}$, at that $z_1 > z_2 > \dots > z_{m-1}$. We determine coefficients d_i, $0 \le i \le m$, under condition that polynomial (10) has predefined values in extreme points z_i, $1 \le i \le m-1$, i.e.

$$Q_m(z_i) = F_i, \ 1 \le i \le m-1,$$

where $F(z)$ is some given function, $F_i = F(z_i)$. For that, consider the following system of algebraic equations

$$Q_m(z_i) = F_i, Q'_m(z_i) = 0, 1 \le i \le m-1,$$
$$Q'_m(z) = \sum_{i=1}^{m} i d_i z^{i-1}, \quad (12)$$

here the normality conditions $Q_m(-1) = (-1)^m$ and $Q_m(1) = 1$ are satisfied.

Rewrite (12) in the form, suitable for calculations on the computer. For this purpose, denote through y, w, g, and r vectors with components

$$y_j = z_j, \ r_j = 0, \ 1 \le j \le m-1; \ w_i = d_{i-1}, \ 1 \le i \le m+1,$$
$$g_i = F_i, \ 1 \le i \le m-1; \ g_i = 1, \ i = m; \ g_i = (-1)^m,$$
$$i = m+1;$$

through E_1 and E_2 matrices of dimension $(m+1)\times(m+1)$ and $(m-1)\times(m+1)$, respectively, with elements of the form

$$e_1^{jj} = j-1, \ 1 \le j \le m+1; \ e_2^{ii} = 1/y_i, \ 1 \le i \le m-1,$$

and through A – a matrix of dimension $(m+1)\times(m+1)$ with elements

$$a^{ij} = y_i^{j-1}, \ 1 \le i \le m-1, \ 1 \le j \le m+1; \ a^{m,j} = 1,$$
$$a^{m+1,j} = (-1)^{j+1}, \ 1 \le j \le m+1.$$

Now problem (12) can be written as follows

$$Aw - g = 0, \ E_2 A E_1 w - r = 0. \quad (13)$$

For the numerical solution of (13) we use the relaxations [2]. After the determination of polynomial (10) coefficients, compute the coefficients of polynomial (3) using relation (11). Find value γ_m under assumption that the polynomial to be obtained corresponds to the first order method, i.e. $c_1 = 1$. Having written the second relation and having made necessary transformations, we get

$$\gamma_m = \left\{-2\sum_{j=1}^{m+1} \nu_{2j} d_j\right\} / c_1, \;\; \gamma_m^0 = -2m^2.$$

V. Form and Size of Stability Domains

Let us describe how the choice of values F_i affects the size and form of the stability domain. If we let $F_i = (-1)^i$, $k \le i \le m-1$, then the stability interval length is known and computed using the formula $|\gamma_m| = 2m^2$. In this case for given m we get the maximal length of a stability domain along the real axis. Level curves $|Q_{m,k}(x)| = 1$, $|Q_{m,k}(x)| = 0.8$, $|Q_{m,k}(x)| = 0.6$, $|Q_{m,k}(x)| = 0.4$, and $|Q_{m,k}(x)| = 0.2$ in complex plane $\{h\lambda\}$ for the stability domain of the four-stage method on $m = 4$, $k = 1$, $F = \{-1, 1, -1\}$ is shown in fig. 1. The stability interval length of the method equals $|\gamma_m| = 32$. In case if the stability interval length is maximal, the stability domain is almost multiconnected, so rounding errors may lead to stepping out of the stability domain.

To solve this problem it is necessary to stretch the stability domain along the imaginary axis in tangency points of parts of the stability domain. For this purpose, we can let $F_i = (-1)^i\mu$, $1 \le i \le m - 1$, $0 < \mu < 1$. Numerical results show that if $\mu = 0.9$, then the length of stability interval decreases by 5–8% comparing to maximal possible length equal to $2m^2$. At that, the stability domain stretches along imaginary axis at the tangency points. This provides better stability properties of method to rounding errors on significant reducement of the stability interval length. If we assume $\mu = 0.95$, then the length of stability interval reduces by 3–4%. The stability domain of the five-stage method on $\mu = 0.9$ is shown in fig. 2. The length of stability interval of the method equals $|\gamma_m| = 30.00$.

As μ decreases from 1 to 0, roots of polynomial (3) get closer to each other on the real axis. Therefore, the length of stability interval regularly reduces. The ellipsises, those are well-defined on $\mu = 1$ get closer not providing sufficiently significant stretch of the stability domain along the imaginary axis. Therefore, depending on the problem to be solved it is reasonable to choose value μ from 0.8 to 0.95.

On solving problems, which Jacobi matrices have eigenvalues with imaginary components and which solutions have oscillating behavior, the extension of a stability interval often is not necessary. In this case the integration stepsize is rather small due to the accuracy requirements and thus it is more reasonable to extend a stability domain along the imaginary axis. If the Jacobi matrix have pure imaginary eigenvalues it is necessary to have the condition $|Q_{m,k}(x)| = 1$ satisfied over some region on the imaginary axis. This requirement is satisfied as k increases.

For the first order methods, i.e. for $k = 1$, it is possible to make the requirement satisfied choosing appropriate values of function F. For instance, on $m = 4$, $k = 1$, $F = \{0.75, 0.80, 0.75\}$ we obtain a polynomial, satisfying this requirement (see fig. 3). Since m is even and all the values F_i are positive, the graph of the polynomial does not cross the real axis, at that, polynomial has two pairs of complex conjugate roots. Therefore, the stability domain stretches along the imaginary axis and some region of the imaginary axis belongs to the stability domain. At that, length of the stability domain is not big along the real axis and equals $|\gamma_m| = 2.89$.

On reducing values F_i the length of a stability domain along the real axis gets greater. On the further reducement of values F_i the length of stability interval $|\gamma_m|$ also grows but the region on the imaginary axis belonging to the stability domain becomes less. Therefore, on developing the first order methods aimed at solving oscillating problems, it is reasonable to choose stability polynomials those have a couple of complex conjugate roots in a complex plane $\{h\lambda\}$ nearby the origin of coordinates. At that, values F_i that correspond to these roots are need to be chosen close to 1, so that the stability domain has the maximal region of the imaginary axis in it.

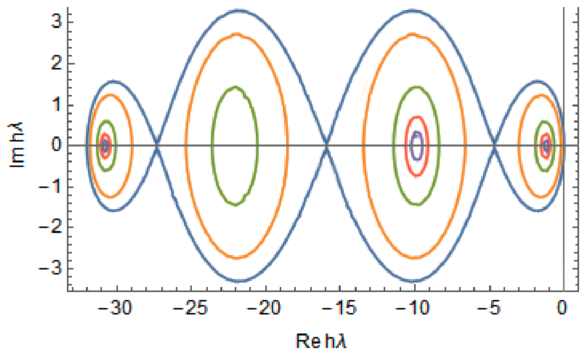

Figure 1. Stability domain on parameters m=4, k=1, F={–1, 1, –1}.

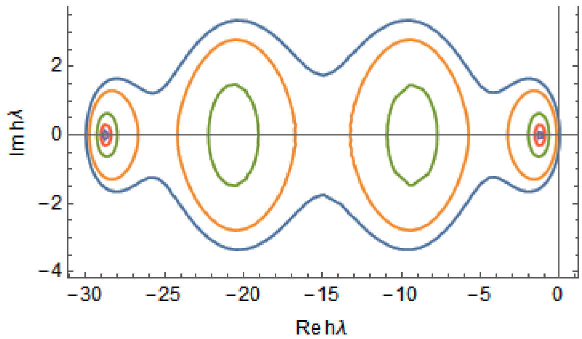

Figure 2. Stability domain on parameters m=4, k=1, F={–0.9, 0.9, –0.9}.

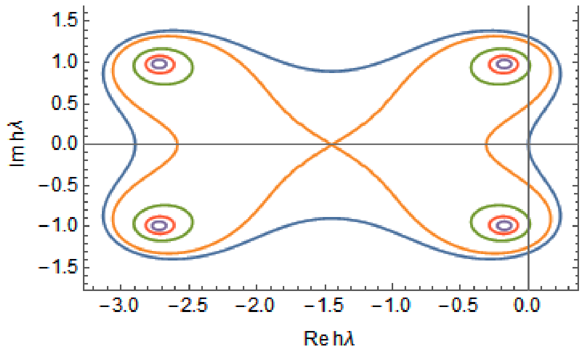

Figure 3. Stability domain on parameters m=4, k=1, F={0.75, 0.80, 0.75}.

VI. NUMERICAL RESULTS

From the numerical results it follows that coefficient c_m of polynomial (3) reduces as m grows and, in particular, on $m = 13$ and $k = 1$ value c_m is of the order of 10^{-26}. Due to rounding errors it is difficult to solve problem (7) for $m > 13$. Numerical results of solving (11) show that coefficients d_i, $0 \le i \le m$ of polynomial (8) grow in magnitude with growth of m. In particular, on $m = 13$ value $\max_{0\le i\le m}|d_i|$ is of the order of 10^5, and on $m = 25$ of the order of 10^9, i.e. d_i grow slower. Transition from coefficients of polynomial (8) to coefficients of (3) using (9) is performed after the solution of (11), that allows to compute the coefficients of stability polynomials of degree up to $m = 27$.

It is difficult to solve problem (11) with double precision for $m > 27$ due to the appearing rounding errors. To compute the coefficients of a stability polynomial for higher degrees m the algorithm using tools of the Quade-Double precision library (described in [6]) was developed.

The QD precision library allows performing calculations with higher accuracy. While the standard data type 'double', allowing to represent numbers with double precision, is confined to 53 bits of the binary mantissa and provides precision about 16 decimal numerals, numbers of the data type 'dd_real' from the library QD has the 106-bit mantissa that provides precision about 32 decimal numerals. In fact, the number of the type dd_real is the software-implemented sum of two numbers of the type 'double'. At that, the mantissa of the sum elongates in two times, but the range of values, presentable in new data type does not change and the possible values vary from about 10^{-308} to 10^{308}, as for the standard 'double'. Despite the confinement, accuracy of the representation of numbers in this diapason increases.

On the implementation of the algorithm for computation of the coefficients of (8) using the data type 'dd_real' the main input parameters of the algorithm − accuracy of calculations ε and differentiation stepsize s_j did not change. The Chebyshev polynomial values at the extreme points were chosen for initial conditions. The improved precision of the numbers representation allowed to compute polynomial coefficients for degree $m > 27$.

VII. CONCLUSION

Using the algorithm for obtainment of polynomials over interval $[-1, 1]$ with the predefined properties there were computed coefficients of stability polynomials of degree up to $m = 35$. These coefficients correspond to the first order methods. It is shown that choice of the values F_i affects the form and size of a stability domain. The proposed algorithm for design of stability domains increases efficiency of explicit methods. Furthermore, it allows to develop algorithms of alternating order and step for solving problems of moderate stiffness. If the solution behavior of a problem which is to be solved is known, then it is possible to design an integration algorithm with stability domain suitable for the given class of problems. From our point of view, one of the main future applications of our results is using the proposed algorithm for design of numerical methods for solution of ODEs systems. These methods can be included in libraries for software aimed at computer simulation.

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