Theory of Approximation and Applications, 2022, Volume 16, No.2 : 43-53, DOR: 20.1001.1.25382217.2022.16.2.7.5

Investigating the Stability of Various Implicit Runge-Kutta Methods

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ARTICLE INFO

Keywords
Implicit Runge Kutta method,
Kronecker product,
A - stability,
Orthogonal polynomial

Article history
Received: 2022 August 25
Accepted: 2022 November 15

ABSTRACT

In this article, the aim is to study the non-explicit Runge-Kutta methods. The following is the classification of these methods and how to implement them. To reduce the functions associated with their implementation, the concepts of sustainability related to such methods have been compared computationally with an emphasis on the non-explicit single method.

1 Introduction

Consider the following first-order differential equation with the initial condition:

$$y' = f\big(x, y(x)\big)$$
$$y(x_0) = y_0$$

Such that $f: [a,b] \times R^m \to R^m$,$y: [a,b] \to R^m$.

One of the one-step methods as usual for solving ordinary differential equations is Runge- Kutta (RK) method. In general, any RK method with s stage can be expressed as follows:

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i \qquad (1)$$
$$k_i = f\left(x_n + c_i h, y_n + h\sum_{j=1}^{s} a_{ij}k_j\right) \quad , i = 1, \dots, s$$

Such that $c_i = \sum_{j=1}^{s} a_{ij}$.

The coefficients $\{a_{ij}\}$, $\{b_i\}$ and $\{c_i\}$ in formula (1), can be expressed as:

C	A
	b^T

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The matrix and vector are also represented in the following form:

$$A = \left(a_{ij} \right)_{s\times s} \ , b = [b_1, \dots, b_s]^T \ , \qquad C = [c_1, \dots, c_s]^T$$

Definition 1. If the matrix A is strictly triangular below, then the Runge- Kutta method will be explicit, otherwise the method is non-explicit.
In this group, matrix A is not triangular, more parameters are calculated for the method. Explicit methods were considered more until the 1960s. but later due to the inefficiency of such methods for non-explicit problems, non-explicit methods with an infinite stability region were considered. The cost of implementing these methods increases compared to explicit methods, but the advantages of implicit methods in terms of accuracy and stability compared to peer-to-peer methods of explicit type were the incentive to use these methods by creating conditions to reduce costs.

2 Preliminaries

Definition 2. If $A = \left[a_{ij} \right]_{s\times s}$ and B= $\left[b_{ij} \right]_{m\times m}$ are matrixes, then Kronecker product of two matrixes with the symbol A⊗ B and a matrix sm ×sm will be defined as follows:[3]

$$\mathrm{A} \otimes \mathrm{B} = \begin{bmatrix} a_{11}B & a_{12}B & \dots & a_{1s}B \\ a_{21}B & a_{22}B & \dots & a_{2s}B \\ \dots & \dots & \dots & \dots \\ a_{s1}B & a_{s2}B & \dots & a_{ss}B \end{bmatrix}$$

Rung-Kutta method, relation (1) can be written using direct multiplication for the first step (n = 1) as follows:

$$Y = e \otimes y_0 + h(A \otimes I_N)F \tag{2}$$

$$y_1 = y_0 + h(b^T \otimes I_N)F \tag{3}$$

where:

$$e = [1, \dots,1]^T, Y = [Y_1, \dots, Y_s]^T, F = [f(Y_1), \dots, f(Y_s)]^T \ and \ \ b^T e = 1 \ , Ae = e$$

We have the assumptions of simplifying the John-Butcher order C (η), B(p), D (ξ) is defined as follows [12]:

$$B(p): \quad \sum_{i=1}^{s} b_i \ c_i^{q-1} = \frac{1}{q} \ , \quad q = 1, \dots, p \tag{4}$$

$$C(\eta): \quad \sum_{j=1}^{s} a_{ij} \ c_j^{q-1} = \frac{c_i^q}{q} \ , \quad i = 1,..,s \ \ q = 1, \dots, \eta \tag{5}$$

$$D(\xi): \quad \sum_{i=1}^{s} b_i \; c_i^{q-1} a_{ij} = \frac{b_j}{q}\left(1 - c_j^{q}\right), \quad j = 1, \dots, s \quad q = 1, \dots, \xi \tag{6}$$

Theorem 1. According to the simplification assumptions where p is the order and s is the number of stages, if the coefficients a_{ij}, b_i, c_i are in the condition C(η), B(p), D (ξ) is true, so that $p \leq \eta + \xi + 1$ and $p < 2\eta + 2$, then the method will be of order p.

Definition 3. The method is A-Stable. Whenever $\{h|\, Re(h) \leq 0\} \subseteq R$ where R is the region of stability [3].

Definition 4. In the one-step numerical method, the stability function $z = h\lambda, R(z)$ is expressed as
a ratio $\frac{y_n}{y_n - 1}$. The method is L-Stable When:
(I) The method is A-Stable.
(II) The stability function applies $\lim_{|z|\to\infty} R(z) = 0$

3 Classification of implicit methods

Among the implicit methods are methods based on Gaussian quantitative formulas, Butcher was invented in 1964. The general state of the IRK method for the problem $y' = f(x)$ should be checked as a quadratic form:

$$\int_{x_n}^{x_{n+1}} f(x)dx \approx y_{n+1} - y_n = h \sum_{j=1}^{s} b_j \, f\left(x_n + c_j h\right)$$

in which $x_n + c_j h$, and $b_j \;\; j = 1, \dots, s$ are points and coefficients of the quadratic formula.

1. Gauss Legendre method

orthogonal polynomial of Gauss Legendre is $P_n(x) = \frac{1}{2^n n!}\left(\frac{d^n}{dx^n}(x^2 - 1)^2\right)$ in the interval $[-1,1]$ with weight function $\omega = 0$. In this method, the values of coefficients are Legendre polynomial zeros are transferred from degree S to the interval [0,1]. [10]

2 - Radau methods

RadauIA methods are two groups of these methods that provide grounds for this The method set was made in 1964.

3. The Lobatto Methods

The LobattoIIIA and LobattoIIIB methods by Ehle in 1969, the LobattoIIIC method by Chipman in 1971, which are among the most important Lobatto methods.

Definition 5. the maximum of value q in equation (5), is true is called the "stage order". [10]

Definition 6. If the "stage order" is less than the method order, then the method error will be affected by the calculation error of the stages, and accuracy of the calculations may be obtained that is not inharmony with the order of the method. This phenomenon is called "order reduction". [10]

The following tables provide explanations of implicit methods. [1,7].

Method	Simplifying assumptions	order	Stage order
Gauss	B(2s), C(s), D(s)	2s	s
Radaua IA	B(2s-1), C(s-1), D(s)	2s-1	s-1
Radaua IIA	B(2s-1), C(s), D(s-1)	2s-1	s
Lobatto IIIA	B(2s-2), C(s), D(s-2)	2s-2	s
Lobatto IIIB	B(2s-2), C(s-2), D(s)	2s-2	s-2
Lobatto IIIC	B(2s-2), C(s-1), D(s-1)	2s-2	s-1

One way to eliminate "Rank reduction" is to use methods that have "Stiffly accurate", in which the assumption $\forall j\ a_{sj} = b_j$ considered. In such methods, in the case where $|z| = |\lambda h| \to \infty$ computational error disappears in stages, it causes L-stability of the method.

Method	Stiffly accurate	order
Gauss	-	-
Radaua IA	-	✔
Radaua IIA	✔	✔
Lobatto IIIA	✔	-
Lobatto IIIB	-	-
Lobatto IIIC	✔	✔

Implicit methods can also be divided according to the concept of “collection methods”. To solve the differential equation (6) with step length h to approximate the function f, a polynomial P with degree s is used, where the set of points $\{x_n + c_i h: i = 1,2, \dots, s\}$ is considered.

Theorem 2. The implicit RK method, a 5-stage and order 5 in which the c_i are different and distinct, is the collection m method if the coefficients of the method in condition (5) to $\eta = s$ apply.

4 Implementation of implicit methods

Non-explicit Rang-Kutta non-explicit methods According to Equation (2), the time vector Y will need to be calculated at each time step. Equation (2) is a nonlinear system that has the sN equations. modified Newton iteration equation used to solve the Jacobite matrix $J = f_y\ (e \otimes y_0)$ for each iteration in a time step. This matrix is small if the length is small. Step h can be assumed to be constant in several time steps. If $z = Y - e \otimes y_0$ is assumed, Equation (2) is as follows:

$$G(z) = z - hAf(z + e \otimes y_0) = 0 \quad (7)$$

Newton's method for the above nonlinear system is as follows

$$\Delta z = z^{(L+1)} - z^{(L)}$$

$z^{(L)}$ is the value in the L-amine iteration and $F = f(z + e \otimes y_0)$.

$$[(I_s \otimes I_N) - hA \otimes J]\Delta z = -z + h(A \otimes I_N)F \quad (8)$$

To decompose its LU in each iteration of the matrix sN × sN requires $s^3N^3 + o(N^2)$ It has computational costs, the computational cost for replacing the posterior is also $s^2N^2 + o(N)$ [3]. In 1979, Butcher reduced the computational cost by proposing the use of Jordan A form instead of matrix A. If matrix A is $s \times s$ and $\lambda_1, \lambda_2, \dots, \lambda_s$ are eigenvalues, the non-singular matrix T is found to be:

$$\bar{A} = T^{-1}AT = \begin{bmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ \mu_1 & \lambda_2 & 0 & \dots & 0 \\ 0 & \mu_2 & \lambda_3 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & \mu_{s-1} & \lambda_s \end{bmatrix}$$

$\bar{A}$ is the Jordan form matrix A. If the λ_i are distinct, then the μ_i have zero values, otherwise the μ_i have nonzero values. This transfer is well known, Butcher's transfer, relation (8) is as follows:

$$[(I_s \otimes I_N) - h\bar{A} \otimes J]\Delta\bar{z} = -\bar{z} + h(\bar{A} \otimes I_N)\bar{F} \quad (9)$$

Where:

$$\bar{z} = (T^{-1} \otimes I_N)z \ , \bar{F} = (T^{-1} \otimes I_N)F \ , \Delta z = (T \otimes I_N)\Delta\bar{z}$$

In this case, d is the number of distinct eigenvalues of interest in form of matrix $\bar{A}$ in the computational cost of LU decomposition of matrix $\bar{A}$ is dN^3.But the computational cost of transformation becomes s^2N for each $\Delta\bar{z}$ and $\bar{z}$ [3].

If the matrix A has a repeated eigenvalue, the computational cost of its decomposition is reduced to N^3. This method is called SIRK.

These methods, on the other hand, had a high conversion computational cost. To reduce the conversion calculations, Butcher proposed the following conversion for SIRK methods in 1988. He considered the T matrix as a product of two triangular lower and upper triangular matrices:

$$T = LU, \quad \bar{A} = T^{-1}AT \ \Rightarrow \ (UL)^{-1}AUL = L^{-1}U^{-1}AUL = \bar{A} \Rightarrow U^{-1}AU = L\bar{A}L^{-1} = \hat{A}$$

Matrix $\widehat{\mathrm{A}}$ is a lower triangular matrix whose elements on the diameter are all eigenvalues of duplicate λ. Now by selecting U as the nonlinear system conversion matrix, relation (8) is as follows:

$$\left[(I_s \otimes I_N) - h\widehat{\mathrm{A}} \otimes J\right]\Delta\hat{z} = -\hat{z} + h\left(\widehat{\mathrm{A}} \otimes I_N\right)\hat{F} \tag{10}$$

where: $\hat{z} = (T^{-1} \otimes I_N)z$, $\widehat{F} = (T^{-1} \otimes I_N)F$, $\Delta z = (\mathrm{T} \otimes I_N)\Delta\hat{z}$

In this case, the computational cost of decomposition LU the same as the previous cost of N^3, but the computational cost of replacing the backward due to the low triangularity of the matrix $\widehat{\mathrm{A}}$ to and the computational cost Convert to $sN^3 + \frac{s(s-1)N^2}{2}$, decreases $\frac{1}{2}s(s-1)N$ [11].

If in the relation (10) $M = \lambda\hat{A}^{-1}$ is assumed, the matrix M is as follows:

$$\mathrm{M} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ m_{21} & 1 & 0 & \dots & 0 \\ m_{21} & m_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{s1} & m_{s2} & m_{s3} & \cdots & 1 \end{bmatrix}$$

By multiplying the sides of relation (10) in M, we have:

$$[(\mathrm{M} \otimes I_N) - h\lambda I_s \otimes J]\Delta\hat{z} = -\tilde{z} + (h\lambda I_s \otimes I_N)\hat{F} \tag{11}$$

Where $\tilde{z} = (\mathrm{M} \otimes I_N)\hat{z}$.

This modification reduces the number of operators in recursive substitution. The elements of the lower triangular matrix in the non-linear system (10) change from the values of $\hat{a}_{ij}h_j$ to $m_{ij}I_N$, so the number of inverse substitution operators decreases from $\frac{s^2N^2}{2}$ to $\frac{S^2N}{2}$. In this case, too the transformation matrix is a triangular matrix. The following table shows the approximate number of operators (computational cost) for solving the N-dimensional system, using the solution methods (9), (10) and (11) for different N for methods 3-stages has been compared: [10]

Method(s=3)	N=2	N=10	N=50	N=250
IRK	252	27900	3397500	422437500
SIRK (9)	86	1870	141350	16006750
SIRK (10)	62	1750	140750	16003750
SIRK (11)	56	1480	133400	15817000

Example 1. the following system have exact solution $y_1(x) = e^{-2x}$, $y_2(x) = e^{-x}$.

$$\begin{cases} y_1'(x) = -1002y_1(x) + 1000y_2(x)^2 \quad , x\epsilon[0,10] \\ y_2'(x) = y_1(x) - y_2(x)\big(1 + y_2(x)\big) \\ y_1(0) = 1 \ , \\ y_2(0) = 1 \end{cases}$$

If the number of steps is considered 100 and the interval is integral [0,10], the table below shows that the conversions used in equations (9), (10) and (11) reduce the computational cost while maintaining accuracy.

Method(s=2)	Number of flops	Global error
IRK	89274	1.852×10^{-7}
SIRK (9)	46198	1.852×10^{-7}
SIRK (10)	42166	1.852×10^{-7}
SIRK (11)	41414	1.852×10^{-7}

5 Stability of SIRK Methods

As mentioned, a special family of implicit methods Introduced in 1978, SIRK methods have lower computational costs than other methods and have the following conditions:

1. Matrix A has a special value of repetition.
2. Standard method s -stage SIRK is of order s and therefore will be "step order" s and this method is in the category of Collation methods.

The stability function is the SIRK method $R(z) = \frac{P(z)}{(1-\lambda z)^s}$ in which the λ is eigenvalues of the matrix A and P (z) is polynomials of maximum degree s.

Lemma 1. if $L_s^{(n)}, n = -1, -2, \dots$ is $L_s^{(-1)}(0) = L_s^{(-2)}(0) = \cdots = 0$ and derivative $L_s^{(n-i)}$ is always equal $L_s^{(n)}$. If $L_s^{(0)}$ is expressed by L_s, then:

$$(1-z)^s exp(\theta z) = (-1)^s \sum_{k=0}^{\infty} L_s^{(s-k)}(\theta) z^k \tag{12}$$

Where:

$$L_s(z) = \sum_{k=0}^{s} \frac{s!}{k!(s-k)!} \frac{(-z)^k}{k!} \tag{13}$$

Laguerre orthogonal polynomial is of degree s. [Refer to reference 11 for further explanation]. The choice is closely related to the property of stability and error constant [11]. The error constant for z^s is given in the following form:

$$C_s = (-1)^s \lambda^s L_s\left(\frac{1}{\lambda}\right)$$

If $\frac{1}{\lambda}$ is the root of Laguerre orthogonal polynomial L_s ,degree of $P(z)$ will be less than s, according to the A-stability of SIRK method, it will be L-stable. In this case $P(z)$ will be as follows:

$$P(z) = (-1)^s \sum_{k=0}^{s-1} \lambda^k L_s^{(s-k)}(\tfrac{1}{\lambda}) z^k \qquad (14)$$

Approximation $P(z)$ through the exponential function, approximately λ for the stability of the method [11].

The following table shows approximate eigenvalues for L-Stability of SIRK Method with s-Stages:

s	λ
2	$1 \pm \sqrt{2}/_2$
3	0.4358665215084
4	0.5728160648213
5	0.2780538411364
6	0.3341423670680
8	0.2343731596055

Table (1)

6 Transformation matrix SIRK

As the method is collocation, the conditions B (s) and C(s) apply. Assuming the coefficients are separate, c_i can be used to calculate other coefficients. The following theorem expresses the relationship between the eigenvalue and the coefficients c_i.

Theorem 3. For the SIRK s-stage method with repetitive eigenvalue λ, $\sigma(A) = \{\lambda\}$ .The values of $c_1, \dots, c_s$ apply in the following condition: $c_i = \lambda\xi_i \quad , i = 1,2, \dots, s$,where ξ_i are the polynomial roots of the Laguerre L_s ,of degree s.

Condition $C(s)$, $\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \quad , k = 1,2, \dots, s$ is equivalent to:

$$\sum_{j=0}^{s} a_{ij} P(c_j) = \int_0^{\xi_i} P(c)dc \qquad (15)$$

where $P(x)$ is a polynomial with a maximum degree of s-1 and $c_i = \lambda\xi_i \quad , i = 1,2, \dots, s$,where ξ_i are the polynomial roots of the Laguerre L_s .

$L_k(0) = L_{k+1}(0) = 1$, using the Laguerre polynomial properties for $k = 0,1,2, \dots, s-1$ have:

$$\sum_{j=1}^{s} a_{ij} L_k(\xi_j) = \sum_{j=1}^{s} a_{ij} L_k\left(\frac{c_j}{\lambda}\right) = \int_0^{\xi_i} \lambda L_k(\xi)d\xi = \lambda \int_0^{\xi_i} \left(L_k'(\xi) - L_{k+1}'(\xi)\right)d\xi$$

$$= \lambda(L_k(\xi_i) - L_{k+1}(\xi_i))$$

Therefore, the transformation matrix can be considered as follows:

$T = [v_1, v_2, \dots., v_S]$

where:

$$v_k = \begin{bmatrix} L_{k-1}(\xi_1) \\ L_{k-1}(\xi_2) \\ \vdots \\ L_{k-1}(\xi_s) \end{bmatrix}$$

In this case, the matrix A with this transformation, which is calculated directly, becomes Jordan's form, which has λ elements in the main diameter and $-\lambda$ elements in the sub-diameter [10].

$$T^{-1}\mathrm{AT} = \begin{bmatrix} \lambda & 0 & 0 & \dots & 0 & 0 \\ -\lambda & \lambda & 0 & \dots & 0 & 0 \\ 0 & -\lambda & \lambda & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\lambda & \lambda \end{bmatrix}$$

Therefore, for the standard SIRK method, from L - stability the value of λ, which is true in condition $L_s\left(\frac{1}{\lambda}\right)$,is calculated. Using theorem (3) one of the values c_i is selected and the other c_i are calculated. In this method for $c_i = 1$,is assumed that: $b_j = a_{ij} \quad , j = 1,2, \dots, s.$

Structure procedure of the standard SIRK method s - stage by Order 5 is as follows:

1) Select suitable for stability from Table (1).

2) Calculate $c_i = \lambda\xi_i \quad , i = 1,2, \dots, s$, which ξ_i are the roots of L_s .

3) Calculate the matrix of coefficients A using the simplification C(s).

4) Calculate the vector b of the relation $b^T = e_j^T A$,in which e_j the vector j-element is one and the rest is zero.

5) Calculation of the corresponding transformation matrix T.

Example 1. In this example, the above steps are investigated for the 2-stage SIRK method. By selecting $\lambda = \frac{1}{\xi_2} = 1 - \frac{\sqrt{2}}{2}$,which has a lower error constant, it is continued.

$c_2 = 1$, $c_1 = \lambda\xi_1 = \lambda\left(2 - \sqrt{2}\right) = 3 - 2\sqrt{2}$, Using condition $C(2)$ the following equations are written:

$$a_{21} + a_{22} = c_2, a_{11} + a_{12} = c_1, a_{11}c_1 + a_{12}c_2 = \frac{c_1^2}{2}, a_{21}c_1 + a_{22}c_2 = \frac{c_2^2}{2}$$

In this way, matrix A is calculated and the vector b^T the last row of the matrix A. table are as follows:

$$\begin{array}{c|cc} 3-2\sqrt{2} & \frac{5-3\sqrt{2}}{4} & \frac{7-5\sqrt{2}}{4} \\ 1 & \frac{1+\sqrt{2}}{4} & \frac{3-\sqrt{2}}{4} \\ \hline & \frac{1+\sqrt{2}}{4} & \frac{3-\sqrt{2}}{4} \end{array}$$

Transformation matrix T is:

$$T = [v_1, v_2] = \begin{bmatrix} L_0(\xi_1) & L_1(\xi_1) \\ L_0(\xi_2) & L_1(\xi_2) \end{bmatrix} = \begin{bmatrix} 1 & -1+\sqrt{2} \\ 1 & -1-\sqrt{2} \end{bmatrix}$$

Example 2. In this example, the SIRK method is checked with order 3:

$$\lambda \approx \frac{1}{\xi_2} = 0.4358665, \qquad c_1 = \frac{\xi_1}{\xi_2} = 0.1812222 \ , c_3 = \frac{\xi_3}{\xi_2} = 2.741576 \, , \quad c_2 = 1.00000$$

Which ξ_1, ξ_2, ξ_3 are roots of L_3 .Similarly, the matrix of coefficients A is calculated by equations C (3), and the table of the method is as follows:

c_1	0.20863	-0.03087	0.00346
c_2	0.57438	0.44266	-0.01705
c_3	0.15442	1.93085	0.65629
	0.57438	0.44266	-0.01705

Transformation matrix T is:

$$T = [v_1, v_2, v_3] = \begin{bmatrix} L_0(\xi_1) & L_1(\xi_1) & L_2(\xi_1) \\ L_0(\xi_2) & L_1(\xi_2) & L_2(\xi_2) \\ L_0(\xi_3) & L_1(\xi_3) & L_2(\xi_3) \end{bmatrix} = \begin{bmatrix} 1 & 0.58422 & 0.25488 \\ 1 & -1.29428 & -0.95670 \\ 1 & -5.28994 & 8.20181 \end{bmatrix}$$

7 Discussion

As can be seen in the example above, the value c_3 for the method of order 3 is greater than one and causes one of the approximations to be out of the integral range. Imposing stability conditions. To be calculated for orders of magnitude greater than 2, more than one. The values of c_i up to the 6th order are given in the following table:

s	c_1	c_2	c_3	c_4	c_5	c_6
3	0.18122	1	2.74158			

4	0.18476	1	2.59865	5.38165		
5	0.07328	0.39300	1	1.97024	3.51482	
6	0.07446	0.39727	1	1.92972	3.28711	5.34056

To overcome this problem, it was tried to generalize the SIRK method maintain the advantages of the more freedom method to choose c_i arise. One of these generalized methods is ESIRK (effective SIRK), in this method using the concept of effective order and adding free and desirable parameters by creating disturbances in the initial approximations, while maintaining the appropriate stability of the SIRK method, the values of the C vector components in the interval [0,1] to calculate.

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