

Efficiency the Concept Effective Order and Combination of Runge-Kutta Methods

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ARTICLE INFO ABSTRACT

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In this paper, Runge-Kutta (RK) methods is introduced; The conditions of order p and its equations have been investigated by calculating Fréchet derivatives and displaying them graphically as rooted trees. The concept of effective order and combination of methods are introduced; The efficiency of the effective order method is explicitly compared to the RK method with the classical order in terms of computational speed and reduction of the number of ancient conditions.

1. Introduction

The Rung-Kuttta methods began with an introduction to the Euler method and were gradually generalized while maintaining the one-step method so that the linear form of the method was eliminated. In 1886, Carl David Tolmrang began research in the field of number theory and complex analysis. Runge's first paper on the numerical solution of differential equations was published in 1896. He considered Euler's approximation for the equation:

 $y' = f(x, y)$ $y_n = y_{n-1} + (x_n - x_{n-1})f(x_n, y_n)$

That expressed as $\int_{x_{n-1}}^{x_n} g(x) dx = (x_{n-1} - x_n)g(x_{n-1})$. He Calculate the recent integral mathematics using the midpoint and trapezoid method. In 1900, Heun, with a theory of Rang paper, proposed a more general method in the form of Gaussian quadratic formula:

$$
y_1 - y_0 = h \sum_{i=1}^{s} b_i k_i
$$

\n
$$
k_1 = f(x_0, y_0), \quad k_2 = f(x_0 + c_2 h, y_0 + c_2 h k_1)
$$

\n
$$
k_3 = f(x_0 + c_3 h, y_0 + c_3 h k_2), \quad \dots
$$

reached the algebraic conditions b_i and c_i using the Taylor expansion and the most famous Express the method with order3[7]. William Matterin Kutta from 1897 to 1909, studying the Runge and Heun methods, introduced a method for the fourth time in a 1901 paper, which was modified with the Heun method. So that all the values of the derivatives participated in the calculation:

$$
y_1 - y_0 = h \sum_{i=1}^{s} b_i k_i
$$

\n
$$
k_1 = f(x_0, y_0), \quad k_2 = f(x_0 + c_2 h, y_0 + a_{21} h k_1)
$$

\n
$$
k_3 = f(x_0 + c_3 h, y_0 + a_{32} h k_2), \quad \dots
$$

In later years around 1925 E.J.Nystrem published a paper on the efficiency of the Kutta idea for solving differential equations and extended it to quadratic equations, 1950s G Gill and Merson papers on how to calculate coefficients The first description of the condition was given by John Butcher, based on the early SIRA and generalization of these methods to stiff problems . Specialized Mathematical Journal of the first year has presented the second issue from year1964 until now [7] Consider the following first-order differential equation with the initial condition:

$$
y' = f(x, y(x))
$$

$$
y(x_0) = y_0
$$

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

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 [9]:

$$
y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i
$$

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

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:

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

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

If then from the solution during a time step h with the initial value $y(x_0)$ give the output value $y_1 - y_0 = O(h^{p+1})$,in this case the RK method will have an order of P. The concept of shear error is expressed [3]. With increasing order, the number of coefficients increases, and their calculation becomes more complicated. Fewer equations and calculations are needed to calculate the coefficients of the method, so that by combining the methods and increasing the order with fewer operators to calculate the coefficients of the method, numerical solutions can be obtained.

2 Preliminaries

One way to calculate coefficient is by obtaining sequential derivatives and equivalence of Taylor is the expansion of numerical solution and exact solution, which leads to equations, and by solving the equations, the coefficients are calculated. This method of calculation will make the calculation of consecutive derivatives more complicated as time increases. The RK method was explicitly considered until the 1960s, but in non-explicit methods the number of coefficients increases and requires more calculations.

In solving the differential equation $y' = (f(y(x))$ requires successive derivatives with which are calculated through the chain rule and as Férchet derivatives [9]; to represent the nth derivative, the graph of the root trees of nth vertex wind is used [4].

$$
y'(x) = f, y''(x) = f'f, y^{(3)}(x) = f''(f, f) + f'f'f,
$$

$$
y^{(4)}(x) = f^{(3)}(f, f, f) + 3f''(f, f', f) + f'f'''(f, f) + f'f'f'f
$$

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Definition 1. For any tree that $t \in T_n$ (T_n is a set of trees with n vertices.) $r(t)$ the number of tree nodes, $\sigma(t)$ tree symmetry and $\gamma(t)$ tree density is defined as follows [3]:

$$
r(\tau) = \sigma(\tau) = \gamma(\tau) = 1
$$

$$
r([t_1^{n_1} t_2^{n_2}, \dots]) = 1 + n_1 r(t_1) + n_2 r(t_2) + \dots
$$

$$
\gamma([t_1^{n_1} t_2^{n_2}, \dots]) = r([t_1^{n_1} t_2^{n_2}, \dots]) \gamma(t_1)^{n_1} \gamma(t_2)^{n_2} \dots
$$

$$
\sigma([t_1^{n_1} t_2^{n_2}, \dots]) = n_1! n_2! \dots (\sigma(t_1))^{n_1} (\sigma(t_2))^{n_2} \dots
$$

Definition 2. $\alpha(t)$ the number of different methods for gluing nodes from numbers the correct one is the order of the tree, which is calculated from the following equation [2]:

$$
\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)}
$$

Definition 3. primary differential function, $F(t)$ on the set of trees is defined as follows [9]:

$$
F([t_1, t_2, ..., t_m]) = F(t_1)F(t_2) ... F(t_m)
$$

$$
F(\tau) = f
$$

Definition 4. functions of initial weights on the set of trees is defined as follows [9]:

$$
\psi_i([t_1, t_2, ..., t_m]) = \sum_{j=1}^s a_{ij} \psi_j(t_1) ... \psi_j(t_m)
$$

$$
\psi_j(\tau) = \sum_{j=1}^s a_{ij} , i = 1, ..., s+1
$$

(In the above definition $a_{s+1} = b_i$ and $\psi_{s+1}(t) = c(t)$ is assumed.)

3 Conditions of order P

Theorem 1. If $y' = (f(y(x)), f: R^m \to R^m$ is shown in this case [3]:

$$
y^{(q)} = \sum_{r(t)=q} \alpha(t) F(t)
$$

If the Taylor expansion is solved, Consider the exact differential equation around x_n ;

$$
y(x_{n+1}) = y(x_n) + hy^{(1)}(x_n) + \frac{1}{2h^2}y^{(3)}(x_n) + \dots = y(x_n) + \sum_{q=1}^{\infty} \frac{h^q y^{(q)}(x_n)}{q!}
$$
 (2)

can be given according to the definition of $\alpha(t)$; the exact solution of the differential equation as B - series with, coefficients $\frac{1}{\gamma(t)}$:

$$
y(x_{n+1}) = y(x_n) + \sum_{q=1}^{\infty} h^q \sum_{r(t)=q} \frac{1}{\sigma(t)\gamma(t)} F(t) (y) = B(\frac{1}{\gamma(t)}, y)
$$
 (3)

Similar too Taylor Expansion Equation (1) can be written as B-series [3]:

$$
y_{n+1} = y_n + \sum_{q=1}^{\infty} h^q \sum_{r(t)=q} \frac{1}{\sigma(t)} c(t) F(t) (y) = B(c(t), y)
$$
 (4)

For existence the order P in RK method, they must be the same as the corresponding sentence in Equation (3), (4) until the P sentence, The following theorem states.

Theorem 2. The Runge-Kutta method has an order of P, whenever for all trees That $r(t) \leq P$ holds $c(t) = \frac{1}{\gamma(t)}$ $\frac{1}{\gamma(t)}$ and for some that $r(t) > P$. [3]

 Writing the order conditions will lead to equations that by solving the equations, the matrix of coefficients and vectors 5 and C are calculated, and the method is constructed with the desired order. As the deck increases the number of conditions increases and the calculation of coefficients becomes more complicated! The table below shows the number of conditions up to the order of 9 [9]:

4. **Combination of Rung-Kutta methods**

For the explicit method, $P = 1,2,3,4$ the number of stages will be $s = p$, and with increasing $p \geq 5$, number of stages will increase and $s > p$; As there is no explicit 5-stage method of order 5 [9] With the concept of effective order, it is possible to create an explicit method with effective order 5 which has only 5 stages, in such a method with the corrections that are made, the results obtained in terms of behavior Error works like a fifth-order method [9]. The concept of combining methods was introduced and pursued in 1969 by Butcher.

Definition 1. RK method with s stages with matrix of coefficients A and vectors b and up can be represented as a matrix of $(s + 1) \times s$, so that the last row of coefficients $\{b_i\}$ are located [9]:

$$
A' = \begin{bmatrix} a_{11} & \cdots & \cdots & a_{1s} \\ \cdots & \cdots & \cdots & \cdots \\ a_{s1} & \cdots & \cdots & a_{ss} \\ b_1 & \cdots & \cdots & b_s \end{bmatrix}
$$

RK method is called method a' , introduced as A' . If method b' with t stages is similarly defined by:

$$
B'=\begin{bmatrix} \tilde{a}_{11} & \cdots & \cdots & \tilde{a}_{1t} \\ \cdots & \cdots & \cdots & \cdots \\ \tilde{a}_{t1} & \cdots & \cdots & \tilde{a}_{tt} \\ \tilde{b}_1 & \cdots & \cdots & \tilde{b}_t \end{bmatrix}
$$

Definition 2. Combining the two methods a' with s-stages and method b' with t-stage is method likes c' Will has $(s + t)$ -stages and the matrix C' is defined as follows [9]:

$$
C' = \begin{bmatrix} D & 0 \\ M & B' \end{bmatrix}
$$

where the matrix M, $m_{ij} = b_j$, $\forall i$, $j = 1, ..., s$ and the matrix D is the same is matrix A whose last row has been deleted.

Definition 3. If method a' has s-stages, a'^{-1} which is defined as follows and has s-stages [9]:

$$
A'^{-1} = \begin{bmatrix} a_{11} - b_1 & \dots & \dots & a_{1s} - b_s \\ \dots & \dots & \dots & \dots \\ a_{s1} - b_1 & \dots & \dots & a_{ss} - b_s \\ -b_1 & \dots & \dots & -b_s \end{bmatrix}
$$

Methods $a'a'^{-1}$ and $a' a'$ will have 2s-stages; By observing a numerical result with the same initial value, it can be shown that in the above method $a'a'^{-1}$ and $a'^{-1}a'$ are two equivalent methods and acts as a member even in the combination of methods,

$$
b'(a'a'^{-1}) = (a'a'^{-1})b' = b'(a'^{-1}a') = (a'^{-1}a')b' = b'
$$

Definition 4. If method a' has an effective order of p, then the methods b' and c' can be calculated to solve any differential equation in such a way that, if method b' is used in the first time step of the method and method c' is used in the last step, and time steps are calculated between the time steps, the method a' is used.

5 Investigating the Effective Order Conditions

The concept of effective order in the numerical method Using the pre-operator and the postoperator methods on numerical results. For solving $y' = f(y)$, $y(a) = \alpha$, $x \in [a, b]$, consider onestep method such that $\psi_{h,f}$ (This numerical method is assumed to be RK). In this case, the numerical sequence $\{y_n\}_{n=0}^N$ is calculated as follows

$$
Y_{n+1} = \psi_{h,f}(Y_n)
$$
 $n = 0, ..., N-1$ $h = \frac{b-a}{N}$

 Y_n can be an approximation for $y(a + nh)$. With mapping $\pi_{h,f}$ such that $y_n = \pi_{h,f}(Y_n)$, y_n can be an approximation for $y(a + nh)$. This mapping is close to the same mapping and its inverse can be considered as follows:

$$
\pi_{h,f} = id + o(h) \Rightarrow \chi_{h,f}^{-1} = \pi_{h,f}
$$

So $y_0 = \chi_{h,f}^{-1}(Y_0)$, can be an approximation for $y(a) = \alpha$. In other words, the initial error $y_0 - \alpha$ and

$$
Y_0 = \chi_{h,f}(\alpha).
$$

In this way, the function can be expressed in three stages:

- 1. Pre-operator: Find the initial value for the time step $Y_0 = \chi_{h,f}(\alpha)$
- 2. Time step: Calculate Y_{n+1} by mapping the method $\psi_{h,f}$:

$$
Y_{n+1} = \psi_{h,f}(Y_n) \quad n = 0, ..., N-1
$$

3.post- operator: The value of $y_n = \chi_{h,f}^{-1}(Y_n)$ is an approximation for $y(a + nh)$, $n = 1, ..., N$.

$$
y_{n+1} = \chi_{h,f}^{-1}(Y_{n+1}) = \chi_{h,f}^{-1}(\psi_{h,f}(Y_n)) = \chi_{h,f}^{-1}\psi_{h,f}\chi_{h,f}(y_n)
$$
 (5)
So $\hat{\psi}_{h,f} = \chi_{h,f}^{-1}\psi_{h,f}\chi_{h,f}$

The above method is considered if $\hat{\psi}_{h,f}$ has a better accuracy than $\psi_{h,f}$,and post-operator cost is negligible. In this case, we can say that $\hat{\psi}_{h,f}$ method will be less expensive and more accurate than $\psi_{h,f}$.

Definition 1. Method $\hat{\psi}_{h,f}$ has an effective order of p, if operator $\chi_{h,f}$ exits, such that $\psi_{h,f}$ has an order p. Therefore, according to Equation (5) the method $\hat{\psi}_{h,f}\,$ has an effective order of p that

$$
\chi_{h,f}^{-1}\psi_{h,f}\chi_{h,f}=\varphi_{h,f}+o(h^{p+1})
$$

in which $\varphi_{h,f}$ is the exact solution of the differential equation.

$$
\psi_{h,f}\chi_{h,f}=\chi_{h,f}\varphi_{h,f}+o(h^{p+1})
$$

with the condition of existence $\chi_{h,f}$ and it can be expressed as B-series with coefficients $d(t)$ that these coefficients are defined in the second part of the set of trees to the set of real numbers (weight function).

$$
\chi_{h,f} = B(d(t),y) = y + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} d(t) F(t) (y) \tag{7}
$$

The exact solution of the differential equation $\varphi_{h,f}$ according to Equation (3) has the following Bseries expansion:

$$
\varphi_{h,f} = B(e(t), y) = y + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} e(t) F(t) (y)
$$
(8)

where $e(t) = \frac{1}{\sqrt{2}}$ $\frac{1}{\gamma(t)}$.

Method $\psi_{h,f}$ is similarly according to Equation (4) has the following B-series expansion, with coefficients $c(t)$:

$$
\psi_{h,f} = B(c(t), y) = y + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} c(t) F(t) (y)
$$
(9)

Definition 2. If G The set of maps of the set of trees are real numbers, the multiplication of such maps on the set G is defined as follows [9]:

$$
\alpha(t), \beta(t)\epsilon G \qquad \alpha\beta(t) = \alpha(t) + \sum_{u} \alpha(\frac{t}{u})\beta(u) + \beta(t)
$$

where u the set of all the sub-trees of the tree, which is the removal of the vertices and wings tree t are created.

Theorem 1. Combining two B-series with coefficients $a(t)$ and $b(t)$ will be a B-series with coefficients $ab(t)$.

 $B(b(t), B(a(t), y)) = B(ab(t), y)$

To prove, refer to the reference [3].

Using the above theorem, the relation (6) as two B-series in a simpler way and according to the consecutive sentences B-series up to p. Can be written:

$$
cd(t) = de(t) \quad , t \in T_n \quad , n = 1, 2, \dots, p \tag{10}
$$

where $e(t) = \frac{1}{\pi t}$ $\frac{1}{\gamma(t)}$.

If in relation (10) $p = 1$:

$$
cd(\tau) = c(\tau) + d(\tau) + \frac{1}{\gamma(\tau)} \Rightarrow c(\tau) = \frac{1}{\gamma(\tau)} \Rightarrow c(\tau) = 1
$$

 $c(\tau) = 1$ is the only condition for the effective order p, which is equivalent to the normal order condition? Now if $p = 2$:

$$
d([\tau])+c(\tau)d(\tau)+c([\tau])=\frac{1}{\gamma([\tau])}+d(\tau)\frac{1}{\gamma(\tau)}+d([\tau])\Rightarrow c([\tau])=\frac{1}{2}
$$

Therefore, the two conditions $c(\tau) = 1$ and $c([\tau]) = \frac{1}{2}$ $\frac{1}{2}$ are two conditions of the effective order 2, which is equivalent to the conditions of the normal order. For effective order 3 two conditions add to others.

$$
d([\tau^2]) + c(\tau)d(\tau)^2 + 2c([\tau])d(\tau) + c([\tau^2]) = \frac{1}{\gamma([\tau^2])} + d(\tau)\frac{1}{\gamma(\tau)^2} + 2d([\tau])\frac{1}{\gamma(\tau)} + d([\tau^2]) \quad (11)
$$

$$
d([\tau]]) + c(\tau)d([\tau]) + c([\tau])d(\tau) + c([\tau])] = \frac{1}{\gamma([\tau])} + d(\tau)\frac{1}{\gamma([\tau])} + d([\tau])\frac{1}{\gamma(\tau)} + d([\tau])
$$

$$
\Rightarrow c([\tau]]) = \frac{1}{24}
$$

Equation (11) does not create a condition by removing $d([\tau^2])$ from the parties to the relation and considering $c([\tau^2])$ and $d(\tau)$ as free parameters, so only the added condition $c([[\tau]]) = \frac{1}{2}$ $\frac{1}{24}$. To generalize the conditions of effective order, we need the following definition.

Definition 3. for $n \geq 3$ The set of T trees is divided into two sets. The set F_n consists of trees Which contains n nodes and can be written as $t\tau$ so that the tree has $n-1$ nodes, in other words, F_n is a set of trees whose roots have at least one end child. The set S_n is $S_n = T_n - F_n$.

 $#F_n = v_{n-1}$, $#S_n = v_n - v_{n-1}$, $n \ge 3$

For $n = 1,2$ define $F_1 = F_2 = \emptyset$ and $S_1 = T_1$, $S_2 = T_2$ [9].

For example, if $n = 4$, the above sets would be $F_4 = \{\lbrack \tau^3 \rbrack, \lbrack \tau \lbrack \tau \rbrack \rbrack, S_4 = \{\lbrack \tau^2 \rbrack, \lbrack \lbrack \tau \rbrack \rbrack \rbrack \} \rbrack$.

Theorem 2. For each arbitrary selection $c(t)$ for teF_n , $n = 1,2,...,p$ and arbitrary selection $d(\tau)$ from relation (10), unique values $c(t)$ for $t \in S_n$, $n = 1, 2, ..., p$ s n and $d(t)$ is obtained for $t \epsilon T_n$, $n = 1, 2, ..., p$. [9]

Corollary. For $p > 1$, $v_p + 1$ independence equations for Coefficients $c(t)$ for $t \in T_n$, $n =$ 1,2, ..., p press the effective order conditions

Proof: Assuming $d(\tau) = 0$ number of equations e_p , as unknowns $c(t)$, for $t \epsilon S_p$ are calculated:

$$
e_p = v_1 + v_2 + v_3 - v_2 + \dots + v_p - v_{p-1} = v_p + 1
$$

If the differential equation is linear $y' = f(y) = Ay$,in this case B - series related to $\psi_{h,f}$, $\chi_{h,f}$, $\varphi_{h,f}$ becomes the linear form of the power series of matrix A, in which case relation (6) is equivalent to

 $\psi_{h,f} = \varphi_{h,f} + o(h^{p+1})$. Therefore, for linear systems, the effective order and order conditions are the same. [9].

The table below shows the number of equations for the effective order and order up to the order of 10:

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6 Example

In the following example, the coefficients of the explicit method are calculated with effective order 4. If for 8 trees (up to order 4) equation (10) is written:

 $\beta\alpha(t_i) = e\beta(t_i)$, $I = 1, ..., 8$, Assuming explicit method $i > j$, $a_{ij} = 0$

$$
\alpha_1 = 1 \Rightarrow \sum_{i=1}^4 b_i = 1 \text{ , } \alpha_1 = \frac{1}{2} \Rightarrow \sum_{i=1}^4 b_i \, c_i = \frac{1}{2} \text{ , } \alpha_4 = \frac{1}{6} \Rightarrow \sum_{i,j=1}^4 b_i \, a_{ij} c_j = \frac{1}{6}
$$

$$
\alpha_8 = \frac{1}{24} \Rightarrow \sum_{i,j,k=1}^4 b_i a_{ij} a_{jk} c_k = \frac{1}{24} ,
$$

\n
$$
\alpha_3 - \alpha_5 + 2\alpha_6 - \alpha_7 = \frac{1}{4} \Rightarrow \sum_{i=1}^4 b_i c_i^2 - \sum_{i=1}^4 b_i c_i^3 + 2 \sum_{i,j=1}^4 b_i c_i a_{ij} c_j - \sum_{i,j=1}^4 b_i a_{ij} c_j^2 = \frac{1}{4}
$$

\n
$$
\frac{1}{4} \begin{vmatrix} 1 & 1 & 1 \\ \frac{1}{6} & \frac{1}{3} & 1 \\ 0 & -1 & 1 \end{vmatrix}
$$

\n
$$
\frac{1}{4} \begin{vmatrix} 1 & 1 & 1 \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \\ 0 & -1 & 1 \end{vmatrix}
$$

7 Discussion

This article discusses the concept of effective order in relation to methods. In these methods, a suitable ground has been created to reduce the calculations according to the concept of effective order. Future studies on non-explicit methods such as SIRK which is defined based on the duplication of specific values of the coefficient matrix and generalization of effective order using ESIRK, DSIRK methods and DESI are expressed [11,12].

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