Improved Runge-Kutta Methods for Solving Ordinary Differential Equations
(Penambahbaikan Kaedah Runge-Kutta untuk Menyelesaikan Persamaan Pembezaan Biasa)

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ABSTRACT

In this article we proposed three explicit Improved Runge-Kutta (IRK) methods for solving first-order ordinary differential equations. These methods are two-step in nature and require lower number of stages compared to the classical Runge-Kutta method. Therefore the new scheme is computationally more efficient at achieving the same order of local accuracy. The order conditions of the new methods are obtained up to order five using Taylor series expansion and the third and fourth order methods with different stages are derived based on the order conditions. The free parameters are obtained through minimization of the error norm. Convergence of the method is proven and the stability regions are presented. To illustrate the efficiency of the method a number of problems are solved and numerical results showed that the method is more efficient compared with the existing Runge-Kutta method.

Keywords: Convergence and stability region; improved Runge-Kutta methods; order conditions; ordinary differential equations; two-step methods

ABSTRAK

Dalam artikel ini kami mencadangkan tiga kaedah Runge-Kutta tak tersirat penambahbaikan untuk menyelesaikan persamaan pembezaan peringkat pertama. Kaedah ini adalah dalam bentuk dua langkah dan memerlukan bilangan tahap yang kurang berbanding kaedah Runge-Kutta klasik. Maka kaedah yang baru ini adalah lebih cekap bagi mencapai peringkat kejituan setempat yang sama. Syarat peringkat untuk kaedah ini hingga peringkat kelima diterbitkan menggunakan kembangan siri Taylor dan kaedah peringkat ketiga dan keempat dengan tahap yang berbeza diterbitkan berdasarkan syarat peringkat tersebut. Parameter bebasnya diperoleh melalui norma ralat yang diminimumkan. Penumpuan kaedah ini dibuktikan dan kestabilannya dipersembahkan. Untuk menunjukkan kecekapan kaedah ini, beberapa masalah diselesaikan dan keputusan berangka menunjukkan kaedah ini lebih cekap berbanding kaedah Runge-Kutta sedia ada.

Kata kunci: Kaedah dua langkah; penambahbaikan kaedah Runge-Kutta; penumpuan dan rantau kestabilan; persamaan pembezaan biasa; syarat peringkat

INTRODUCTION

Consider the numerical solution of the initial value problem for the system of ordinary differential equation:

$$y'(x) = f(x, y(x)), \qquad x \in [x_0, X],$$
$$y(x_0) = y_0. \tag{1}$$

One of the most common methods for solving numerically (1) is Runge-Kutta (RK) method. Most efforts to increase the order of RK method have been accomplished by increasing the number of Taylor's series terms used and thus the number of function evaluations. The RK method of order has a local error over the step size h of $O(h^{p+1})$. Many authors have attempted to increase the efficiency of RK methods by trying to lower the number of function evaluations required. As a result, Goeken and Johnson (2000) proposed a class of Runge-Kutta method with higher derivatives approximations for the third and fourth-order method. Xinyuan (2003) presented a class of Runge-Kutta formulae of order three and four with reduced evaluations of function. Phohomsiri and Udwadia (2004) constructed the accelerated Runge-Kutta integration schemes for the third-order method using two functions evaluation per step. Udwadia and Farahani (2008) developed the higher orders accelerated Runge-Kutta methods. However most of the methods presented are obtained for the autonomous system while the Improved Runge-Kutta methods (IRK) can be used for autonomous as well as non-autonomous systems. Rabiei and Ismail (2011) constructed the third-order Improved Runge-Kutta method for solving ordinary differential equation without minimization of the error norm. The IRK methods arise from the classical RK methods, can also be considered as a special class of two-step methods. That is, the approximate solution y_{n+1} is calculated using the values of y_n and y_{n-1}. The IRK method introduces the new terms of k_{-i}, which are calculated using $k_i, (i > 2)$ from the previous step. The scheme proposed herein has a lower number of function evaluations than the RK methods.

GENERAL FORM OF IRK METHOD

The proposed IRK method in this paper with s-stage for solving (1) has the form:

$$y_{n+1} = (1-\alpha)y_n + \alpha y_{n-1}$$
$$+ h\left(b_1 k_1 - b_{-1}k_{-1} + \sum_{i=2}^{s} b_i(k_i - k_{-i})\right), \qquad (2)$$

For $0 \le \alpha \le 1$, $1 \le n \le N-1$, where

$$k_1 = f(x_n, y_n),$$

$$k_{-1} = f(x_{n-1}, y_{n-1}),$$

$$k_i = f(x_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij}k_j), \ 2 \le i \le s.$$

$$k_{-i} = f(x_{n-1} + c_i h, y_{n-1} + h\sum_{j=1}^{i-1} a_{ij}k_{-j}), \ 2 \le i \le s.$$

for $c_2 \ldots c_s \in [0, 1]$ and f depends on both x and y while k_i and k_{-i} depend on the values of k_j and k_{-i} for $j = 1, \ldots, i-1$. Here s is the number of function evaluations performed at each step and increases with the order of local accuracy of the IRK method. In each step we only need to evaluate the values of $k_1, k_2, \ldots$, while $k_{-1}, k_{-2}, \ldots$ are calculated from the previous step. The accelerated Runge-Kutta method by Udwadia and Farahani (2008) is derived purposely for solving autonomous first order ODEs where the stage or function evaluation involved is of the form $k_i = f(y(x_n + ha_{i-1}k_{i-1}))$ where k_{i-1} is a function of y only and the term involved only k_{i-1}. There are two improvements done here, the first one is the function f is not autonomous, thus the method is not specific for $y' = f(y(x))$, but it can be used for solving both the autonomous equations as well as the more general differential equations $y' = f(x,y(x))$. The second improvement is that the internal stages k_i and k_{-i} contain more k values which are defined as $\sum_{j=1}^{i-1} a_{ij}k_j$, for $i = 2, \ldots, s$, compared to the Accelerated Runge-Kutta method in which their methods contain only one k value. This additional k values aimed to make the methods more accurate. Note that IRK method is not self-starting therefore a one-step method must provide the approximate solution of y_1 at the first step. The one-step method must be of appropriate order to ensure that the difference $y_1 - y(x_1)$ is order of p or higher. In this paper, without loss of generality we derived the method with $\alpha = 0$, so the explicit IRK method can be represented as follows:

$$y_{n+1} = y_n + h(b_1 k_1 - b_{-1}k_{-1} + \sum_{i=2}^{s} b_i(k_i - k_{-i})),$$
$$\text{for } 1 \le n \le N-1, \qquad (3)$$

where:

$$k_1 = f(x_n, y_n),$$

$$k_{-1} = f(x_{n-1}, y_{n-1}),$$

$$k_i = f(x_n + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij}k_j), \qquad 2 \le i \le s,$$

$$k_{-i} = f(x_{n-1} + c_i h, y_{n-1} + h\sum_{j=1}^{i-1} a_{ij}k_{-j}), \ 2 \le i \le s.$$

It is convenient to represent (3) by Table 1.

TABLE 1. Table of coefficients for explicit IRK method ($\alpha = 0$)

0					
c_2	a_{21}				
c_3	a_{31}	a_{32}			
.	.	.	.		
.	.	.	.		
.	.	.	.		
c_s	a_{s1}	a_{s2}	$\ldots$	a_{ss-1}	
b_{-1}	b_1	b_2	$\ldots$	b_{s-1}	b_s

ORDER CONDITIONS

Third order method with two-stage: For $s = 2$, the general form of the method is given by,

$$y_{n+1} = y_n + h(b_1 k_1 - b_{-1}k_{-1} + b_2(k_2 - k_{-2})),$$

$$k_1 = f(x_n, y_n),$$

$$k_{-1} = f(x_{n-1}, y_{n-1}),$$

$$k_2 = f(x_n + c_2 h, y_n + ha_{21}k_1),$$

$$k_{-2} = f(x_{n-1} + c_2 h, y_{n-1} + ha_{21}k_{-1}). \qquad (4)$$

where $0 \le c_2 \le 1$. In the derivation of the method we will use $c_i = \sum_{j}^{i-1} a_{ij}$, which is called the row sum condition of RK method, so here we have $c_2 = a_{21}$. Consider (1) we have:

$$y' = f(x, y), \ y'' = f_x + ff_y,$$

$$y''' = f_{xx} + 2f_{xy} + f_{yy}f^2 + f_y(f_x + ff_y). \qquad (5)$$

The values of $y'(x)$, $y''(x)$, $\ldots$ are obtained by substituting $x = x_n$. The Taylor's series expansion of $y(x_n + h)$ up to $O(h^4)$ is given by:

$$y_{n+1} = y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y''(x_n)$$
$$\frac{h^3}{3!}y'''(x_n) + O(h^4). \qquad (6)$$

Substituting (5) into (6) we have

$$y_{n+1} = y_n + fh + \frac{h^2}{h}(f_x + ff_y)$$

$$+ \frac{h^3}{6} \ (f_{xx} + 2f_{xy}f + f_{yy}f^2 + f_y f_x + f_y^2 f)$$

$$+ O(h^4). \tag{7}$$

Define $F = f_x + ff_y$, $G = f_{xx} + 2f_{xy} + f_{yy}f^2$, thus from formulas given in (5) we have $y'' = F$, $y''' = G + f_y F$. After simplifying, (7) can be written as follows:

$$y_{n+1} - y_n = hf \ \frac{h^2}{h} + F + \frac{h^3}{6} \ (G + f_y F) + O(h^4). \tag{8}$$

By using the Taylor's series expansion of k_1, k_2, k_{-1} and k_{-2} which are used in (4) we have:

$$k_1 = f,$$

$$k_{-1} = f + hF + \frac{h^2}{h} + (G + f_y F) + O(h^3),$$

$$k_2 = f + hc_2 F + \frac{h^2}{h} \ (c_2^2 G) + O(h^3),$$

$$k_{-2} = f - h(1 - c_2) F + \frac{h^2}{h} ((1 - c_2)^2 G + (1 - 2c_2) f_y F)$$

$$+ O(h^3),$$

Substituting the above formulas into (4) we obtain:

$$y_{n+1} - y_n = h(b_1 - b_{-1}) f + h^2 (b_{-1} + b_2) F$$

$$+ \frac{h^3}{2} (-b_{-1} - (1 - 2c_2) b_2) (G + f_y F)$$

$$+ O(h^4). \tag{9}$$

By comparing (9) with (8) in terms of power of h, we obtained the following order conditions up to $O(h^4)$

First order: $\qquad b_1 - b_{-1} = 1$,

Second order: $\qquad b_{-1} + b_2 = \frac{1}{2}$,

Third order: $\qquad b_2 c_2 = \frac{5}{12}$,

Third order method with three-stage: For $s = 3$, the general form of IRK can be written as:

$$y_{n+1} = y_n + h(b_1 k_1 - b_{-1} k_{-1} + b_2(k_2 - k_{-2})$$

$$+ b_3(k_3 - k_{-3})),$$

$$k_1 = f(x_n, y_n),$$

$$k_{-1} = f(x_{n-1}, y_{n-1}),$$

$$k_2 = f(x_n + c_2 h, y_n + ha_{21} k_1),$$

$$k_{-2} = f(x_{n-1} + c_2 h, y_{n-1} + ha_{21} k_{-1}),$$

$$k_3 = f(x_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)),$$

$$k_{-3} = f(x_{n-1} + c_3 h, y_{n-1} + h(a_{31} k_{-1} + a_{32} k_{-2})). \tag{10}$$

where c_2, $c_3 \in [0, 1]$. Also we considered $c_2 = a_{21}$, $c_3 = a_{31} + a_{32}$. The Taylor's series expansion of k_3 and k_{-3} are given as follows:

$$k_3 = f + hc_3 F + \frac{h^2}{h} (c_3^2 G + 2c_2 a_{32} f_y F) + O(h^3),$$

$$k_{-3} = f - h(1 - c_3) F + \frac{h^2}{h} ((1 - c_3)^2 G$$

$$+ (-2c_3 + 2c_2 a_{32} + 1) f_y F) + O(h^3).$$

Substituting the values of k_i and k_{-i}, $i = 1, 2, 3$, into (10), we have:

$$y_{n+1} - y_n = h(b_1 - b_{-1}) f + h^2(b_{-1} + b_2 + b_3) F$$

$$+ \frac{h^3}{2} (-b_{-1} - (1 - 2c_2) b_2 - (1 - 2c_3) b_3)$$

$$(G + f_y F) + O(h^4). \tag{11}$$

Comparing (11) with (8) in terms of power of h we obtained the following order conditions up to $O(h^4)$ for the method with three function evaluations per step.

First order: $\qquad b_1 - b_{-1} = 1$,

Second order: $\qquad b_{-1} + b_2 + b_3 = \frac{1}{2}$,

Third order: $\qquad b_2 c_2 + b_3 c_3 = \frac{5}{12}$,

Using the same procedure we obtained the order conditions of the method up to order five which are presented in Table 2.

CONVERGENCE

The IRK method given in (3) can be written as:

$$\begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix} = \begin{bmatrix} I & 0 \\ I & 0 \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix} + h \begin{bmatrix} b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^{s} b_i \left(k_i - k_{-i} \right) \\ 0 \end{bmatrix} \tag{12}$$

For $1 \le n \le N - 1$, where I is an m by m identity matrix. We can write (12) as:

$$\bar{y}_{n+1} = Q\bar{y}_n + h\bar{\Phi}\left(x_n, \bar{y}_n\right) \quad 1 \le n \le N - 1, \tag{13}$$

where $\bar{y}_{n+1} = \begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix}$, $\bar{y}_n = \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix}$, Q is the $2m$ by $2m$ block matrix given by:

$$Q = \begin{bmatrix} I & 0 \\ I & 0 \end{bmatrix}, \tag{14}$$

and $\bar{\Phi}$ is define by:

$$\overline{\Phi} = \begin{bmatrix} \Phi \\ 0 \end{bmatrix} = \begin{bmatrix} b_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^{s} b_i \left(k_i - k_{-i} \right) \\ 0 \end{bmatrix}. \tag{15}$$

TABLE 2. Order conditions of IRK method up to order five

Order of Method	Order Conditions
First order	$b_1 - b_{-1} = 1,$
Second order	$b_{-1} + \sum_i b_i = \dfrac{1}{2},$
Third order	$\sum_i b_i c_i = \dfrac{5}{12},$
	$\sum_i b_i c_i^2 = \dfrac{1}{3},$
Fourth order	$\sum_{i,j} b_i a_{ij} c_i = \dfrac{1}{6},$
	$\sum_i b_i c_i^3 = \dfrac{31}{120},$
Fifth order	$\sum_{i,j} b_i c_i a_{ij} c_j = \dfrac{31}{240},$
	$\sum_{i,j} b_i a_{ij} c_j^2 = \dfrac{31}{360},$
	$\sum_{i,j,k} b_i a_{ij} a_{jk} c_k = \dfrac{31}{720}.$

We defined $y(x_n)$ as the true solution and y_n is the approximate solution so we can write $y(x_0) = y_0$ and $y(x_1) = y_1 + \varepsilon_0$, for $\varepsilon_0 > 0$. In general we have:

$$\begin{bmatrix} y(x_{n+1}) \\ y(x_n) \end{bmatrix} = \begin{bmatrix} I & 0 \\ I & 0 \end{bmatrix} \begin{bmatrix} y(x_n) \\ y(x_{n-1}) \end{bmatrix}$$
$$+ h \left[h_1 k_1 - b_{-1} k_{-1} + \sum_{i=2}^{s} b_i \left(k_i - k_{-i} \right) \right]$$
$$+ h \begin{bmatrix} \varepsilon_n \\ 0 \end{bmatrix},$$

for $1 \le n \le N - 1$, which can be written as:

$$\overline{y}(x_{n+1}) = Q\overline{y}(x_n) + h\overline{\Phi}\left(x_n, \overline{y}(x_n) \right) + h\overline{\varepsilon}_n,$$
$$1 \le n \le N - 1, \tag{16}$$

where $\overline{\varepsilon}_n = \begin{bmatrix} \varepsilon_n \\ 0 \end{bmatrix}$. To prove the convergence of the method, we used the following lemma and theorems to find the bound for $\| y(x_n) - y_n \|_\infty$ while $\| y(x_n) - y_n \|_\infty \to 0$ as $h \to 0$, here $y(x_n)$ is the true solution of (1). In order to do this, we

will assume that IRK method is stable and that as h tends to zero, $\| y(x_1) - y_1 \|_\infty$ tends to zero, where x_0 is the initial value and $x_1 = x_0 + h$. Note that throughout the stability and convergence analysis, all norms denote the infinity norm $\| \cdot \|_\infty \equiv \| \cdot \|$.

Lemma 1 : For any $(x_n, y(x_n))$, (x_n, y_n) in the region D defined by

$$D = \{(x, y) \mid x \in [x_0, X], -\infty < y < \infty\}.$$

If f is a Lipschitz continuous function such that, $\| f(x_n, y(x_n)) - f(x_n, y_n) \| \le L \| y(x_n) - y_n \|$, then $\overline{\Phi}$ is a Lipschitz continuous function, and $\| \overline{\Phi}(x_n, y(x_n)) - \overline{\Phi}(x_n, y_n) \| \le \hat{L} \| y(x_n) - y_n \|$, where $L, \hat{L}$ are constants.

Proof. First, we will show by induction that

$$\left\| k_j \left(x_n, y(x_n) \right) - k_j \left(x_n, y_n \right) \right\| \le \gamma_j \left\| y(x_n) - y_n \right\|,$$
$$1 \le j \le s, \tag{17}$$

where γ_j are constant. For $j = 1$ we have:

$$\left\| k_1 \left(x_n, y(x_n) \right) - k_1 \left(x_n, y_n \right) \right\| = \left\| f \left(x_n, y(x_n) \right) - f \left(x_n, y_n \right) \right\|,$$
$$\le L \left\| y(x_n) - y_n \right\|,$$

We set $\gamma_j = L$. Assuming inequality (17) is true for $j = i - 1$, we have:

$$\left\| k_i \left(x_n, y(x_n) \right) - k_i \left(x_n, y_n \right) \right\|$$
$$= \left\| f \left(x_n + c_i h y(x_n) + \sum_{j=1}^{i-1} a_{ij} k_j \right) - f \left(x_n + c_i h, y_n + \sum_{j=1}^{i-1} a_{ij} k_j \right) \right\|$$
$$\le L \left\| y(x_n) - y_n + h \sum_{j=1}^{i-1} a_{ij} \left(k_j \left(x_n, y(x_n) \right) - k_j \left(x_n, y_n \right) \right) \right\|$$
$$\le L \left(\left\| y(x_n) - y_n \right\| + h \sum_{j=1}^{i-1} \left| a_{ij} \right| \left\| \left(k_j \left(x_n, y(x_n) \right) - k_j \left(x_n, y_n \right) \right) \right\| \right)$$
$$\le L \left(\left\| y(x_n) - y_n \right\| + h \sum_{j=1}^{i-1} \left| a_{ij} \right| \gamma_{i-1} \left\| y(x_n) - y_n \right\| \right)$$
$$= L \left(1 + h\gamma_{i-1} \sum_{j=1}^{i-1} \left| a_{ij} \right| \right) \left\| y(x_n) - y_n \right\|,$$

where $\gamma_i = L \left(1 + h\gamma_{i-1} \sum_{j=1}^{i-1} \left| a_{ij} \right| \right)$. Hence, inequality (17) holds for $j = i$ and, therefore, it holds for $1 \le j \le s$. Similarly we can show that:

$$\left\| k_{-j} \left(x_{n-1}, y(x_{n-1}) \right) - k_{-j} \left(x_{n-1}, y_{n-1} \right) \right\| \le \gamma_j \left\| y(x_{n-1}) - y_{n-1} \right\| \tag{18}$$

for $1 \le j \le s$. Function Φ can be written as

$$\Phi = b_1 k_1 - b_{-1} k_{-1} + (k_i - k_{-i})$$

$$= \sum_{i=1}^{s} b_i k_i - \sum_{i=1}^{s} b_{-i} k_{-i} \quad \text{where } b_{-i} = b_i, 2 \le i \le s$$

$$= \Phi_1 - \Phi_{-1}.$$

Using inequality (17), we can write

$$\left\| \Phi_1 \left(x_n, y(x_n) \right) - \Phi_1 \left(x_n, y_n \right) \right\|$$

$$= \left\| \sum_{j=1}^{s} b_j k_j \left(x_n, y(x_n) \right) - \sum_{j=1}^{s} b_j k_j \left(x_n, y_n \right) \right\|$$

$$\le \sum_{j=1}^{s} |b_j| \left\| k_j \left(x_n, y(x_n) \right) - k_j \left(x_n, y_n \right) \right\|$$

$$\le \left(\sum_{j=1}^{s} |b_j| \gamma_j \right) \left\| y(x_n) - y_n \right\|.$$

Similarly, using inequality (18) we can write

$$\left\| \Phi_{-1} \left(x_{n-1}, y(x_{-1}) \right) - \Phi_{-1} \left(x_{n-1}, y_{n-1} \right) \right\|$$

$$\le \left(\sum_{j=1}^{s} |b_{-j}| \gamma_j \right) \left\| y(x_{n-1}) - y_{n-1} \right\|.$$

Since $\left\| \bar{\Phi} \left(x_n, \bar{y}(x_n) \right) - \bar{\Phi} \left(x_n, \bar{y}_n \right) \right\|$

$$= \left\| \Phi \left(x_n, y(x_n) \right) - \Phi \left(x_n, y_n \right) \right\|.$$

we have:

$$\left\| \Phi \left(x_n, y(x_n) \right) - \Phi \left(x_n, y_n \right) \right\|$$

$$= \left\| \Phi_1 \left(x_n, y(x_n) \right) - \Phi_{-1} \left(x_{n-1}, y(x_{n-1}) \right) \right.$$

$$\left. - \left(\Phi_1 \left(x_n, y_n \right) - \Phi_{-1} \left(x_{n-1}, y_{n-1} \right) \right) \right\|$$

$$\le \left\| \Phi_1 \left(x_n, y(x_n) \right) - \Phi_1 \left(x_n, y_n \right) \right\|$$

$$+ \left\| \Phi_{-1} \left(x_{n-1}, y(x_{n-1}) \right) - \Phi_{-1} \left(x_{n-1}, y_{n-1} \right) \right\|$$

$$\le \left(\sum_{j=1}^{s} |b_j| \gamma_j \right) \left\| y(x_n) - y_n \right\| + \left(\sum_{j=1}^{s} |b_{-j}| \gamma_j \right)$$

$$\left\| y(x_{n-1}) - y_{n-1} \right\|.$$

Because

$$\left\| \bar{y}(x_n) - \bar{y}_n \right\| = \max \left(\left\| y(x_n) - y_n \right\|, \left\| y(x_{n-1}) - y_{n-1} \right\| \right).$$

we have:

$$\left\| y(x_n) - y_n \right\| \le \left\| \bar{y}(x_n) - \bar{y}_n \right\|,$$

$$\left\| y(x_{n-1}) - y_{n-1} \right\| \le \left\| \bar{y}(x_n) - \bar{y}_n \right\|.$$

Therefore:

$$\left\| \bar{\Phi} \left(\bar{x}_n, \bar{y}(x_n) \right) - \bar{\Phi} \left(\bar{x}_n, \bar{y}_n \right) \right\|$$

$$\le \left(\sum_{j=1}^{s} |b_j| \gamma_j + \sum_{j=1}^{s} |b_{-j}| \gamma_j \right) \left\| \bar{y}(x_n) - \bar{y}_n \right\|$$

$$= \hat{L} \left\| \bar{y}(x_n) - \bar{y}_n \right\|,$$

where $\hat{L} = \sum_{j=1}^{s} \left(|b_j| + |b_{-j}| \right) \gamma_j$. Thus, Lemma 1 is proven.

Theorem 1: *Suppose that a IRK method of order p is used to solve (1), and that f is Lipschitz continuous function, the method is stable and*

$$\left\| y(x_n) - y_n \right\| \le$$

$$M \max \left(\max_{1 \le m \le n} \left\| y(x_1) - y_1 \right\|, \max \left\| \bar{\varepsilon}_m \right\| \right), \ 2 \le n \le N,$$

where $M = 2 e^{\hat{L}(x_n - x_1)} \max \left(1, x_n - x_1 \right).$

Proof: Subtracting (16) from (13) we have

$$\bar{y}(x_{n+1}) - \bar{y}_{n+1} = Q \left(\bar{y}(x_n) - \bar{y}_n \right) + \bar{\Phi} \left(x_n, y(\bar{x}_n) \right)$$

$$- \bar{\Phi} \left(x_n, \bar{y}_n \right) + h \bar{\varepsilon}_n,$$

For $1 \le n \le N - 1$. Taking the infinity norm and using the Lipschits condition on $\bar{\Phi}$ (Lemma 1), we can write

$$\left\| \bar{y}(x_{n+1}) - \bar{y}_{n+1} \right\| \le \|Q\| \left\| \bar{y}(x_n) - \bar{y}_n \right\|$$

$$+ h \hat{L} \left\| \bar{y}(x_n) - \bar{y}_n \right\| + h \left\| \bar{\varepsilon}_n \right\|. \tag{19}$$

From (14) we have $\|Q\| = 1$ after some simplification we can write (19) as follows:

$$\left\| \bar{y}(x_{n+1}) - \bar{y}_{n+1} \right\| \le \left(1 + h \hat{L} \right) \left\| \bar{y}(x_n) - \bar{y}_n \right\|$$

$$+ h \left\| \bar{\varepsilon}_n \right\| \quad 1 \le n \le N - 1. \tag{20}$$

In the following, we will use the inequality $1 \le 1 \le u \le e^u$ for $u \ge 0$ which follows from the expression $e^u = 1 + u + \frac{1}{2} u^2 + \dots$. Now, for $2 \le n \le N$, we can write (20) as follows:

$$\left\| \bar{y}(x_{n+1}) - \bar{y}_{n+1} \right\| \le e^{\hat{L}h} \left\| \bar{y}(x_n) - \bar{y}_n \right\| + h \left\| \bar{\varepsilon}_n \right\|$$

$$\le e^{\hat{L}h} \left(e^{h\hat{L}} \left\| \bar{y}(x_{n-1}) - \bar{y}_{n-1} \right\| + h \left\| \bar{\varepsilon}_{n-1} \right\| \right) + h \left\| \bar{\varepsilon}_n \right\|$$

$$= e^{\hat{L}2h} \left\| \bar{y}(x_{n-1}) - \bar{y}_{n-1} \right\| + h \left(e^{\hat{L}h} \left\| \bar{\varepsilon}_{n-1} \right\| + \left\| \bar{\varepsilon}_n \right\| \right)$$

$$\le e^{\hat{L}nh} \left\| \bar{y}(x_1) - \bar{y}_1 \right\| + h \sum_{m=1}^{n} e^{\hat{L}(n-m)h} \left\| \bar{\varepsilon}_m \right\|.$$

Since $x_{n+1} - x_1 = nh$ and $x_{n+1} - x_{m+1} = (n-m)h$, we have:

$$\left\| \bar{y}(x_{n+1}) - \bar{y}_{n+1} \right\| \le e^{\hat{L}(x_{n+1} - x_1)} \left\| \bar{y}(x_1) - \bar{y}_1 \right\|$$

$$+ h \sum_{m=1}^{n} e^{\hat{L}(x_{n+1} - x_{m+1})} \left\| \bar{\varepsilon}_m \right\|.$$

So we have:

$$\left\| \bar{y}(x_{n+1}) - \bar{y}_n \right\| \le e^{\hat{L}(x_n - x_1)} \left\| \bar{y}(x_1) - \bar{y}_1 \right\|$$

$$+ h \sum_{m=1}^{n-1} e^{\hat{L}(x_n - x_{m+1})} \left\| \bar{\varepsilon}_m \right\|. \tag{21}$$

Since for $1 \le m \le n - 1$, $\|\bar{\varepsilon}_m\| \le \max\|\bar{\varepsilon}_m\|$,

$$e^{\hat{L}(x_n - x_{m+1})} \le e^{\hat{L}\max(x_n - x_{m+1})} = e^{\hat{L}(x_n - x_2)}$$

Now, we can write (21) as follows:

$$\|\bar{y}(x_n) - \bar{y}_n\|$$

$$\le e^{\hat{L}(x_n - x_1)}\|\bar{y}(x_1) - \bar{y}_1\| + h(n-1)e^{\hat{L}(x_n - x_2)}\max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|$$

$$\le e^{\hat{L}(x_n - x_1)}\|\bar{y}(x_1) - \bar{y}_1\| + h(n-1)e^{\hat{L}(x_n - x_1)}\max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|$$

$$= e^{\hat{L}(x_n - x_1)}\|\bar{y}(x_1) - \bar{y}_1\| + (x_n - x_1)e^{\hat{L}(x_n - x_1)}\max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|$$

$$\le e^{\hat{L}(x_n - x_1)}\|\bar{y}(x_1) - \bar{y}_1\| + (x_n - x_1)\max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|$$

$$\le e^{\hat{L}(x_n - x_1)}\max(1, x_n - x_1)\left(\|\bar{y}(x_1) - \bar{y}_1\| + \max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|\right)$$

$$\le 2e^{\hat{L}(x_n - x_1)}\max_{1 \le m \le n-1}\|1, x_n - x_1\|$$

$$\max\left(\|\bar{y}(x_1) - \bar{y}_1\|, \max_{1 \le m \le n-1}\|\bar{\varepsilon}_m\|\right). \tag{22}$$

Since $\|y(x_n) - y_n\| \le \|\bar{y}(x_n) - \bar{y}_n\|$, and $\|\bar{\varepsilon}_m\| = \|\varepsilon_m\|$, from (22) we have:

$$\|y(x_n) - y_n\| \le M \max\left(\|y(x_1) - y_1\|, \max_{1 \le m \le n-1}\|\varepsilon_m\|\right),$$

$$2 \le n \le N, \tag{23}$$

where $M = 2e^{\hat{L}(x_n - x_1)}\max(1, x_n - x_1)$. Therefore, Theorem 1 is proven.

Theorem 2: *Consider the* IRK *method of order p is used to solve (1) where f is a sufficiently smooth Lipschitz continuous function, if the approximate solution* y_1 *at* x_1 *is accurate to* $O(h^{q+1})$, *the method is convergent to order min (p, q), and*

$$\|y(x_n) - y_n\| \le M \max\left(O(h^{q+1}), O(h^{p+1})\right),$$

$$2 \le n \le N,$$

where $M = 2e^{\hat{L}(x_n - x_1)}\max(1, x_n - x_1)$.

Proof: For IRK method of order p, $\varepsilon_m = O(h^{p+1})$, for $1 \le m \le n - 1$. The approximate solution y_1 at x_1 which is required by the IRK method is provided by a one-step method such as Runge-Kutta method. If y_1 is accurate of order q, that is, $\|y(x_1) - y_1\| = O(h^{q+1})$, using inequality (23) we have:

$$\|y(x_n) - y_n\| \le M \max\left(O(h^{q+1}), O(h^{p+1})\right),$$

$$2 \le n \le N,$$

where $M = 2e^{\hat{L}(x_n - x_1)}\max(1, x_n - x_1)$. In particular, $\|y(x_n) - y_n\| \to 0$ as $h \to 0$ and Theorem 2 is proven.

DERIVATION OF THE METHODS

Using the order conditions in Table 2, we derived the IRK methods of orders $p = 3$ and $p = 4$. To determine the free parameters of the third and fourth order methods we minimized the error norm for the methods of order 4 and 5, respectively. Hence, the third order method (IRK3) with two stages ($p = 3$, $s = 2$) and fourth order method with three stages $p = 4$, $s = 3$) are obtained. Then, by satisfying as many equations as possible, for the fifth order method, we obtain the optimized fourth order method with 4-stages ($p = 4$, $s = 4$) which is denoted by IRK4-4 method. The coefficients of methods IRK3, IRK4 and IRK4-4 methods are presented in Table 3. In the last section, to illustrate the efficiency of the methods we compared the numerical results with Butcher's Runge-Kutta methods of order 2, 3 and 4 which are denoted as RK2, RK3, and RK4 methods (Butcher 2008).

STABILITY

To find the stability region, the method is applied to the test problem $y' = \lambda y$. Here, for $s = 2$ we have

$$y' = \lambda y,$$

$$k_1 = \lambda y_n, \qquad k_{-1} = \lambda y_{n-1},$$

$$k_2 = \lambda(1 + \lambda h a_{21})y_n, \quad k_{-2} = \lambda(1 + \lambda h a_{21})y_{n-1}.$$

Substituting all the above values into (4) we have:

$$y_{n+1} = \left(1 + \bar{h}\left(b_1 + b_2\left(1 + \bar{h}a_{21}\right)\right)\right)y_n$$
$$- \left(b_{-1} + b_2\left(1 + \bar{h}a_{21}\right)\right)y_{n-1}, \tag{24}$$

where $\bar{h} = \lambda h$. Substituting $y_{n+1} = \zeta^2$, $y_n = \zeta$, the following stability polynomial is obtained for the method of order three (IRK3):

$$\rho(\zeta, \bar{h}) = \zeta^2 - \left(\frac{5}{12}\bar{h}^2 + \frac{3}{2}\bar{h} + 1\right)\zeta + \frac{5}{12}\bar{h}^2 + \frac{\bar{h}}{2}. \tag{25}$$

Using the same procedure, the stability polynomial for fourth order method (IRK4) is given by:

$$\rho(\zeta, \bar{h}) = \zeta^2 - \left(\frac{1}{6}\bar{h}^3 + \frac{5}{12}\bar{h}^2 + \frac{3}{2}\bar{h} + 1\right)\zeta$$
$$+ \frac{1}{6}\bar{h}^3 + \frac{5}{12}\bar{h}^2 + \frac{\bar{h}}{2}, \tag{26}$$

and the stability polynomial for the optimized fourth order method (IRK4-4) is:

$$\rho(\zeta, \bar{h}) = \zeta^2 - \left(\frac{31}{720}\bar{h}^4 + \frac{1}{6}\bar{h}^3 + \frac{5}{12}\bar{h}^2 + \frac{3}{2}\bar{h} + 1\right)\zeta$$
$$+ \frac{31}{720}\bar{h}^4 + \frac{1}{6}\bar{h}^3 + \frac{5}{12}\bar{h}^2 + \frac{\bar{h}}{2}. \tag{27}$$

TABLE 3. Coefficients of IRK3, IRK4 and IRK4-4 methods

IRK3:

$$\begin{array}{c|cc} 0 & & \\ \dfrac{1}{2} & \dfrac{1}{2} & \\ \hline -\dfrac{1}{3} & \dfrac{2}{3} & \dfrac{5}{6} \end{array}$$

IRK4:

$$\begin{array}{c|ccc} 0 & & & \\ \dfrac{31}{60} & \dfrac{31}{60} & & \\ \dfrac{62}{85} & \dfrac{7502}{24565} & \dfrac{10416}{24565} & \\ \hline -\dfrac{157}{23064} & \dfrac{23221}{23064} & -\dfrac{1800}{6727} & \end{array}$$

IRK4-4:

$$\begin{array}{c|ccccc} 0 & & & & & \\ \dfrac{1}{5} & \dfrac{1}{5} & & & & \\ \dfrac{3}{5} & 0 & \dfrac{3}{5} & & & \\ \dfrac{4}{5} & \dfrac{2}{15} & \dfrac{4}{25} & \dfrac{38}{75} & & \\ \hline \dfrac{122825}{161448} & \dfrac{19}{288} & \dfrac{307}{288} & -\dfrac{25}{144} & \dfrac{25}{144} & \dfrac{125}{288} \end{array}$$

Stability region of the methods is the set of values of $\bar{h}$ such that all the roots of stability polynomial are inside the unit circle. Here, the stability region of IRK3, IRK4 and IRK4-4 methods are plotted in Figures 1 and 2 and found to be slightly smaller then the stability region of the existing RK methods.
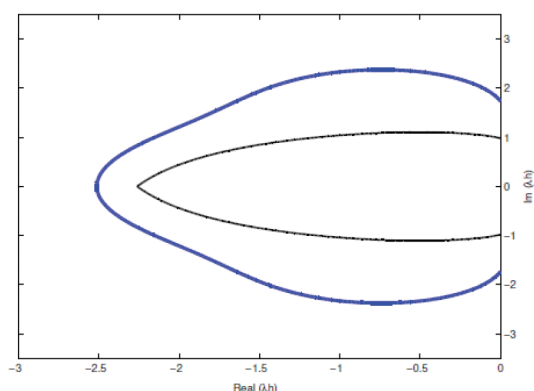

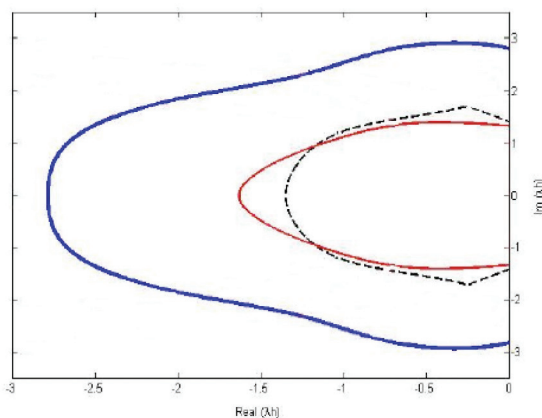FIGURE 1. Stability region of IRK3 (thin line) and RK3 (thick line) for $\bar{h} = \lambda h$

FIGURE 2. Stability region of IRK4 (thin line), IRK4-4 (thin dash line) and RK4 (thick line) for $\bar{h} = \lambda h$

NUMERICAL EXAMPLES

In this section, we tested a standard set of initial value problems to show the efficiency and accuracy of the proposed methods. The exact solution $y(x)$ is used to estimate the global error as well as to approximate the starting values of y_1 at the first step x_1. The following problems are solved for $x \in [0, 10]$.

Problem 1: $y' = \dfrac{xy}{1+x^2}, \quad y(0) = 1,$

Exact solution: $y(x) = \dfrac{1}{\sqrt{1+x^2}}.$

Source: Udwadia and Farahani (2008)

Problem 2: (an oscillatory problem)
$$y' = y\cos(x), \quad y(0) = 1,$$

Exact solution: $y(x) = e^{\sin(x)}.$
Source: Hull et al. (1982)

Problem 3: (1-body gravitational problem with eccentricity $e = 0$)
$$y_1'' = -y_1\left(y_1^2 + y_2^2\right)^{-\frac{3}{2}} \quad y_1(0) = 1, \quad y_1'(0) = 0,$$
$$y_2'' = -y_2\left(y_1^2 + y_2^2\right)^{-\frac{3}{2}} \quad y_2(0) = 0, \quad y_2'(0) = 1,$$

Exact solution: $y_1(x) = \cos(x), y_2(x) = \sin(x).$
Source: Hull et al. (1982)

The number of function evaluations versus the log(maximum global error) for the tested problems are shown in Figures 3-5.

DISCUSSION AND CONCLUSION

From Figures 3-5, we observe that IRK3 with the same number stages is more accurate compared with RK2 , IRK4 with three stages gives smaller error than RK3 also IRK4-4
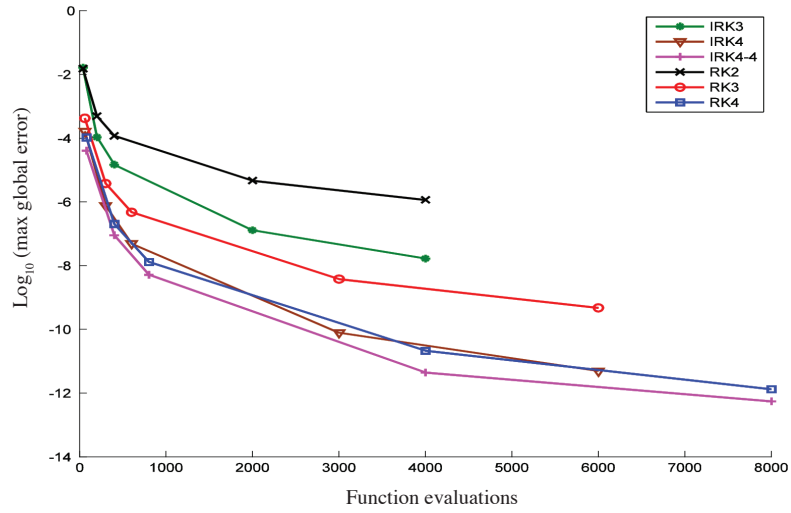
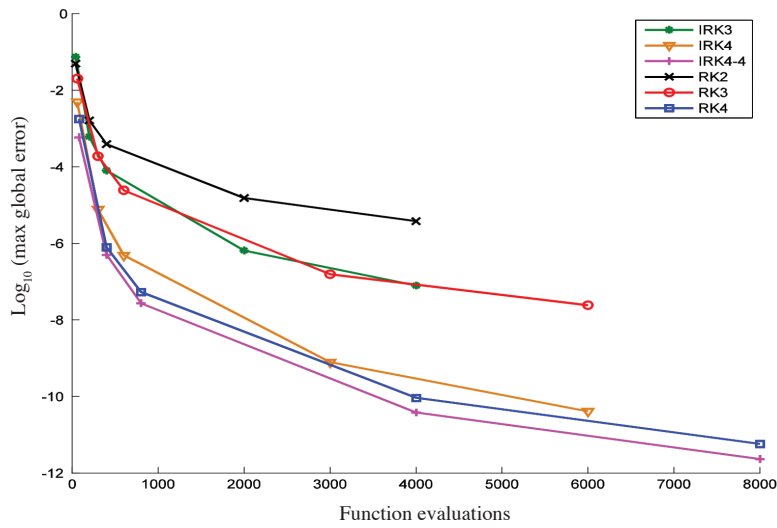FIGURE 3. Maximum global error versus number of function evaluations for problem 1

FIGURE 4. Maximum global error versus number of function evaluations for problem 2
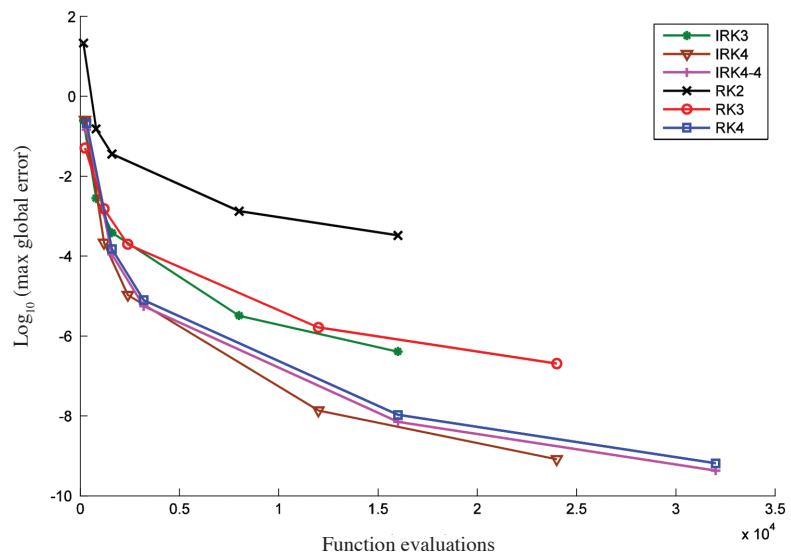

FIGURE 5. Maximum global error versus number of function evaluations for problem 3

with the same number of stages compared with RK4 is more accurate. Therefore, for all the problems the new methods produced better accuracy for the same number of function evaluations compared to the existing methods.

In this paper, the order conditions of the IRK method up to order five are derived. Based on these order conditions, we obtained IRK methods of order three and four with different stages. Convergence and stability region of the proposed methods are given. From the numerical results, we observed that for the same order of error, IRK methods with less number of stages require less number of function evaluations which leads to less computational time for approximating numerical solutions of problems compared with the existing RK methods. Therefore, we can conclude that IRK methods are computationally more efficient compared with the existing RK methods.

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