

Theoretical Analysis of Symmetric Runge-Kutta Methods

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ABSTRACT

This article give the theoretical analysis for some symmetric Runge-Kutta methods such as the 2-stage Gauss, 3-stage Gauss, 3-stage Lobatto IIIA and 4-stage Lobatto IIIA methods. The theoretical analysis on the asymptotic error expansions by the 2-stage Gauss (G2) and 3-stage Lobatto IIIA (L4) methods are studied in detailed for the Prothero-Robinson (PR) problem. For the 3-stage Gauss (G3) and 4-stage Lobatto IIIA (L4) methods, the behavior of these methods are studied numerical and theoretically for PR problem. It is observed that G3 and L4 gives oscillatory error behavior when applied to the PR problem. However, these numerical results are shown to be improved by the symmetrizer.

Keywords: Asymptotic error expansions, symmetric, smoothing, symmetrizer, extrapolation.

1. Introduction

Consider a system of an ordinary differential equation with the initial value,

$$y' = f(x, y), \quad y(x_0) = y_0, \quad (1)$$

Any Runge-Kutta (RK) methods can be used to solve problem (1). IMR and ITR methods are lower order implicit RK methods of order-2. They are symmetric RK methods. Although these two popular methods have been used widely, there are limitations due to the lower order. These methods are restricted in solving linear and nonlinear problems. These method are advantages when are used with extrapolation due the asymptotic error expansions that are in even powers (Chan, 1993, Gorgey, 2012) but however they are proven to be not stable especially the ITR (Zlatev et al., 2017)). Another example of symmetric RK methods are the 2-stage (G2) and 3-stage Gauss (G3) methods and 3-stage (L3) and 4-stage Lobatto (L4) IIIA methods (Butcher, 2016).

For Runge-Kutta methods, the asymptotic errors expansion is given by

$$y_n(x) = y(x) + \tau_1(x)h^p + \tau_2(x)h^{p+1} + \dots + \tau_{p+k}(x)h^{p+k} + O(h^{(p+k)}), \quad (2)$$

for $k = 1, 2, \dots$ where the coefficients $\tau_i(x_n)$ are independent of h .

If the method is symmetric, (2) has an asymptotic errors expansion of h in even powers.

$$y_n(x) = y(x) + \tau_1(x)h^p + \tau_2(x)h^{p+2} + \dots + \tau_{p+k}(x)h^{p+2k} + O(h^{(p+2k)}), \quad (3)$$

for $k = 1, 2, \dots$

To understand the derivation of the asymptotic error expansion, consider applying the RK methods to the following test problem known as the Prothero Robinson problem (Prothero and Robinson, 1974).

$$y' = \lambda(y - g(x)) + g'(x), \quad (4)$$

with $y(0) = 1$ where $g(x) = e^{-x}$ is a smooth function. Exact solution is given by $y(x) = g(x)$. λ is any number in the range $[-1 : -10^n]$ where $n = 1, 2, 3, \dots$. As n increases the problem become stiff. Only implicit RK methods are suitable in solving stiff problems.

Table 1: Order-2 of IMR and ITR

<p>IMR:</p> $Y = y_{n-1} + \frac{h}{2} f\left(x_{n-1} + \frac{h}{2}, Y\right),$ $y_n = y_{n-1} + hf\left(x_{n-1} + \frac{h}{2}, Y\right).$	<p>ITR:</p> $Y_1 = y_{n-1},$ $Y_2 = y_{n-1} + \frac{h}{2} hf\left(x_{n-1}, Y_1\right) + \frac{h}{2} f\left(x_{n-1} + h, Y_2\right),$ $y_n = Y_2.$
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Any implicit Runge-Kutta (RK) methods can be used to solve problem (4). Runge-Kutta method is defined by formulas (5a) and (5b)

$$Y_i = y_{n-1} + h \sum_{j=1}^s a_{ij} f\left(x_{n-1} + c_j h, Y_j\right), i = 1, 2, \dots, s. \tag{5a}$$

$$y_n = y_{n-1} + h \sum_{j=1}^s b_j f\left(x_{n-1} + c_j h, Y_j\right), j = 1, 2, \dots, s, \tag{5b}$$

where Y_i represent the internal stage values and y_n represent the update of y at the n^{th} step. Examples of order-2 RK methods are the implicit midpoint rule (IMR) and implicit trapezoidal rule (ITR) as given in Table 1.

Both IMR and ITR are also symmetric, Butcher (2016). The symmetric methods are special type of RK methods because when they are applied with extrapolation technique this makes the order of the method increase by two at a time, Chan (1993), Chan and Gorgey (2013).

The asymptotic errors expansion for IMR and ITR when applied to Prothero-Robinson (PR) problem can be shown to have even powers of h (Gorgey, 2012).

For IMR, the asymptotic error expansion is given by

$$e_n^M = (R^n - e^{-nh}) \left(\frac{1}{12} \left(\frac{1 + 3\lambda}{1 + \lambda} \right) h^2 + \frac{7}{2880} \left(\frac{1 + 6\lambda + \frac{75}{7}\lambda^2}{(1 + \lambda)^2} \right) h^4 \right) + (R^n - e^{-nh}) \left(\frac{31}{483840} \left(\frac{1 + 9\lambda + \frac{969}{31}\lambda^2 + \frac{1281}{31}\lambda^3}{(1 + \lambda)^3} \right) \right) h^6 + O(h^8), \tag{6}$$

The asymptotic error expansion by the ITR is given by

$$\begin{aligned}
 e_n^T = & - (R^n - e^{-nh}) \left(\frac{1}{6} \left(\frac{1}{1+\lambda} \right) h^2 - \frac{1}{360} \left(\frac{1+6\lambda}{(1+\lambda)^2} \right) \right) h^4 \\
 & - (R^n - e^{-nh}) \left(\frac{1}{15210} \left(\frac{1+9\lambda+\frac{51}{2}\lambda^2}{(1+\lambda)^3} \right) \right) h^6 + O(h^8). \quad (7)
 \end{aligned}$$

From the asymptotic error expansion (6) shows that when λ is large, the coefficient blow up for h^2 but not for the equation (7). R^n for both IMR and ITR is the stability function such that $R(h\lambda) = \frac{h\lambda}{1+\frac{2}{h\lambda}}$.

In this article, the derivations of the asymptotic error expansion is given for the 2-stage Gauss and 3-stage Lobatto IIIA.

Example 1.1. 2-stage Gauss (G2) and 3-stage Lobatto IIIA (L3)

Applying G2 to the Prothero-Robinson problem gives the simplified version of the internal stages as

$$\begin{aligned}
 Y_1 = & \frac{1 - \left(\frac{1}{4} + \frac{\sqrt{3}}{6} \right) z + \frac{\sqrt{3}}{24} z^2}{\left(1 - \frac{z}{4} \right) \left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} y_{n-1} - \frac{\frac{h}{4} (\lambda + 1) \left(1 - \frac{7z}{12} + \frac{z^2}{12} \right)}{\left(1 - \frac{z}{4} \right) \left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} - \frac{\sqrt{3}}{6} \right) h} \\
 & - \frac{h(\lambda + 1) \left(\frac{1}{4} - \frac{\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} + \frac{\sqrt{3}}{6} \right) h}, \\
 Y_2 = & \frac{1 + \frac{\sqrt{3}}{6} z}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} y_{n-1} - \frac{h(\lambda + 1) \left(\frac{1}{4} + \frac{\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} - \frac{\sqrt{3}}{6} \right) h} \\
 & - \frac{\frac{h}{4} (\lambda + 1) \left(1 - \frac{z}{3} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} + \frac{\sqrt{3}}{6} \right) h}.
 \end{aligned}$$

In the case of higher order methods, internal stage values play an important role especially when deriving symmetrizer (refer to Section 2) or known as the smoothing for IMR and ITR (Chan and Gorgey, 2011).

It can be easily verified that the update for G2 is given by

$$\begin{aligned}
 y_n &= y_{n-1} + \frac{h}{2}Y_1 + \frac{h}{2}Y_2, \\
 y_n &= y_{n-1} + \frac{h}{2} \left(\lambda Y_1 - (\lambda + 1)e^{-x_{n-1} - \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h} \right) \\
 &\quad + \frac{h}{2} \left(\lambda Y_2 - (\lambda + 1)e^{-x_{n-1} - \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h} \right). \tag{8}
 \end{aligned}$$

Simplifying by substituting the y_{n-1}, Y_1 and Y_2 yields

$$\begin{aligned}
 &= \left(\frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} + \frac{z^2}{12}} \right) y_{n-1} - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h} \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h}, \\
 &= R(z)y_{n-1} + \varphi_{n-1}^1 + \varphi_{n-1}^2, \tag{9}
 \end{aligned}$$

where

$$\begin{aligned}
 R(z) &= \frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} + \frac{z^2}{12}}, \quad \varphi_{n-1}^1 = -\frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h}, \quad \text{and} \\
 \varphi_{n-1}^2 &= -\frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h}.
 \end{aligned}$$

Iterating from step n to step 0, gives

$$\begin{aligned}
 y_n &= Ry_{n-1} + \varphi_{n-1}^1 + \varphi_{n-1}^2, \\
 &= R(Ry_{n-2} + \varphi_{n-2}^1 + \varphi_{n-2}^2) + \varphi_{n-1}^1 + \varphi_{n-1}^2, \\
 &= R^2y_{n-2} + (\varphi_{n-1}^1 + R\varphi_{n-2}^1) + (\varphi_{n-1}^2 + R\varphi_{n-2}^2), \\
 &\quad \vdots \\
 &= R^n y_0 + (\varphi_{n-1}^1 + R\varphi_{n-2}^1 + \dots + R^{n-1}\varphi_0^1) + (\varphi_{n-1}^2 + R\varphi_{n-2}^2 + \dots + R^{n-1}\varphi_0^2), \\
 &= R^n y_0 - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h} \left(R^{n-1} + R^{n-2}e^{-h} + \dots + e^{(n-1)h} \right) \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6} \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h} \left(R^{n-1} + R^{n-2}e^{-h} + \dots + e^{(n-1)h} \right).
 \end{aligned}$$

$$\begin{aligned}
 y_n &= R^n y_0 - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6}\right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right)} e^{-(n-1)h - \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h} \left(1 + Re^h + \dots + R^{n-1}e^{(n-1)h}\right) \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6}\right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right)} e^{-(n-1)h - \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h} \left(1 + Re^h + \dots + R^{n-1}e^{(n-1)h}\right), \\
 y_n &= R^n y_0 - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6}\right) e^{-(n-1)h - \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h}}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right)} \left(\frac{1 - R^n e^{nh}}{1 - Re^h}\right) \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6}\right) e^{-(n-1)h - \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h}}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right)} \left(\frac{1 - R^n e^{nh}}{1 - Re^h}\right), \\
 &= R^n y_0 - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6}\right) (R^n - e^{-nh})}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right) e^{\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h} (R - e^{-h})} \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6}\right) (R^n - e^{-nh})}{\left(1 - \frac{z}{2} + \frac{z^2}{12}\right) e^{\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h} (R - e^{-h})},
 \end{aligned}$$

Since $R(z) = \frac{1 + \frac{z}{2} + \frac{z^2}{12}}{1 - \frac{z}{2} + \frac{z^2}{12}}$ and $y_0 = 1$, we have

$$\begin{aligned}
 y_n &= R^n - \frac{\frac{h}{2}(\lambda + 1) \left(1 + \frac{z\sqrt{3}}{6}\right) (R^n - e^{-nh}) e^{\frac{\sqrt{3}}{6}h}}{\left(e^{\frac{h}{2}} - e^{-\frac{h}{2}}\right) + \frac{z}{2} \left(e^{\frac{h}{2}} + e^{-\frac{h}{2}}\right) + \frac{z^2}{12} \left(e^{\frac{h}{2}} - e^{-\frac{h}{2}}\right)} \\
 &\quad - \frac{\frac{h}{2}(\lambda + 1) \left(1 - \frac{z\sqrt{3}}{6}\right) (R^n - e^{-nh}) e^{-\frac{\sqrt{3}}{6}h}}{\left(e^{\frac{h}{2}} - e^{-\frac{h}{2}}\right) + \frac{z}{2} \left(e^{\frac{h}{2}} + e^{-\frac{h}{2}}\right) + \frac{z^2}{12} \left(e^{\frac{h}{2}} - e^{-\frac{h}{2}}\right)}, \\
 &= R^n - \frac{h(\lambda + 1) \left(\cosh\left(\frac{\sqrt{3}}{6}h\right) + \frac{z\sqrt{3}}{6} \sinh\left(\frac{\sqrt{3}}{6}h\right)\right)}{2 \left(1 + \frac{z^2}{12}\right) \sinh\left(\frac{h}{2}\right) + z \cosh\left(\frac{h}{2}\right)} (R^n - e^{-nh}).
 \end{aligned}$$

Hence, the numerical solution is given by

$$y_n = R^n - \frac{h(\lambda + 1) \left(\cosh\left(\frac{\sqrt{3}}{6}h\right) + \frac{h\lambda\sqrt{3}}{6} \sinh\left(\frac{\sqrt{3}}{6}h\right)\right)}{2 \left(1 + \frac{h^2\lambda^2}{12}\right) \sinh\left(\frac{h}{2}\right) + h\lambda \cosh\left(\frac{h}{2}\right)} (R^n - e^{-nh}), \quad (10)$$

since $z = h\lambda$.

The global error $e_n = y_n - e^{-nh}$ at x_n is therefore given by

$$e_n = (R^n - e^{-nh}) \left(1 - \frac{h(\lambda + 1) \left(\cosh\left(\frac{\sqrt{3}}{6}h\right) + \frac{h\lambda\sqrt{3}}{6} \sinh\left(\frac{\sqrt{3}}{6}h\right) \right)}{2 \left(1 + \frac{h^2\lambda^2}{12} \right) \sinh\left(\frac{h}{2}\right) + h\lambda \cosh\left(\frac{h}{2}\right)} \right). \quad (11)$$

Hence, the asymptotic error expansion is given by

$$\begin{aligned} e_n &= (R^n - e^{-nh}) \left(\frac{1}{4320} \left(\frac{1 + 5\lambda + 10\lambda^2}{(1 + \lambda)} \right) h^4 \right) \\ &\quad - (R^n - e^{-nh}) \left(\frac{1}{136080} \left(\frac{1 + 7\lambda + 21\lambda^2 + \frac{105}{4}\lambda^3}{(1 + \lambda)} \right) \right) h^6 \\ &\quad + (R^n - e^{-nh}) \left(\frac{17}{87091200} w \right) h^8 + O(h^{10}), \end{aligned}$$

where

$$w = \left(\frac{1 + 10\lambda + 45\lambda^2 + \frac{1900}{17}\lambda^3 + 17\lambda^4 + \frac{1400}{17}\lambda^5}{(1 + \lambda)^2} \right).$$

Next, for L3, the update has the form of

$$y_n = R(z)y_{n-1} + \varphi_{n-1}^1 + \varphi_{n-1}^2 + \varphi_{n-1}^3,$$

where $R(z)$ is the stability function as given for the G2.

$$\varphi_{n-1}^1 = -\frac{\frac{h}{6}(\lambda + 1) \left(1 + \frac{1}{2}z \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1}}, \quad \varphi_{n-1}^2 = -\frac{\frac{2}{3}h(\lambda + 1)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - \frac{h}{2}},$$

and

$$\varphi_{n-1}^3 = -\frac{\frac{h}{6}(\lambda + 1) \left(1 - \frac{1}{2}z \right)}{\left(1 - \frac{z}{2} + \frac{z^2}{12} \right)} e^{-x_{n-1} - h}$$

Similarly, iterating from step n to step 0 and for $y_0 = 1$, gives

$$y_n = R^n - \frac{\frac{h}{6}(\lambda + 1) \left(2 \cosh\left(\frac{h}{2}\right) + h\lambda \sinh\left(\frac{h}{2}\right) + 4 \right)}{2 \left(1 + \frac{h^2\lambda^2}{12} \right) \sinh\left(\frac{h}{2}\right) + h\lambda \cosh\left(\frac{h}{2}\right)} (R^n - e^{-nh})$$

Thus, the global error for L3 is given by

$$e_n = (R^n - e^{-nh}) \left(1 - \frac{\frac{h}{6}(\lambda + 1) \left(2 \cosh\left(\frac{h}{2}\right) + h\lambda \sinh\left(\frac{h}{2}\right) + 4 \right)}{2 \left(1 + \frac{h^2\lambda^2}{12} \right) \sinh\left(\frac{h}{2}\right) + h\lambda \cosh\left(\frac{h}{2}\right)} \right).$$

Hence, by the series expansion yields the asymptotic error expansion for L3 as

$$e_n = - (R^n - e^{-nh}) \left(\frac{1}{2880} \left(\frac{1 + 5\lambda}{1 + \lambda} \right) h^4 - \frac{1}{96768} \left(\frac{1 + 7\lambda + 14\lambda^2}{1 + \lambda} \right) h^6 \right) - (R^n - e^{-nh}) \left(\frac{1}{3686400} \left(\frac{(1 + \frac{15}{3}\lambda + \frac{20}{3}\lambda^2)^2}{(1 + \lambda)^2} \right) \right) h^8 + O(h^{10}).$$

This asymptotic global error expansion in even powers of h enables Richardson extrapolation to increase the order by two at a time which gives the order for both method is $O(h^6)$. Similar derivations can be derived for the 3-stage Gauss and 4-stage Lobatto IIIA methods.

Methods like Gauss such as the IMR and G3 that have odd stages, when these methods are used to solve stiff problems, the global errors show oscillatory behaviour. This is bad and can destroy the solutions.

In Figure 1, oscillations are due to the property $R(\infty) = -1$ of the stability function by the IMR and ITR.

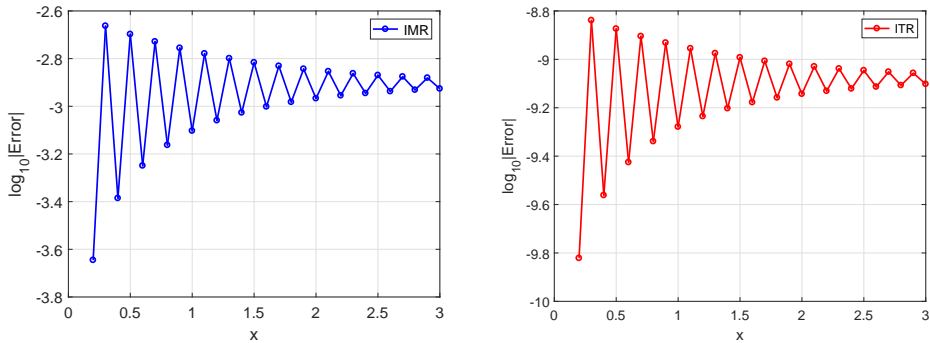


Figure 1: Error behaviour of IMR and ITR.

A similar behaviour is observed for the 3-stage method (G3) since its stability function will also tend to -1 as $z \rightarrow \infty$. Gauss methods with odd stages and Lobatto IIIA methods with even stages are expected to show similar behaviour (refer to Figure 2).

The theoretical analysis on this behaviour can be shown by expanding the global error of the G3 for the Prothero-Robinson problem.

Since G3 satisfied $B(6)$ and $C(3)$ conditions (see Butcher (2016) on simplified assumptions of the order conditions), it can be shown that the local error

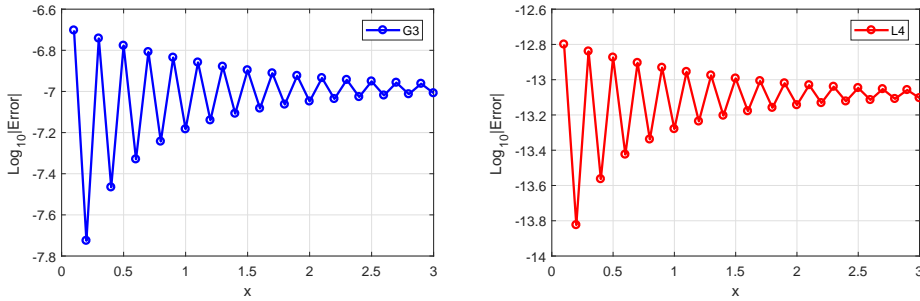


Figure 2: Error behaviour of 3-stage Gauss (G3) and 4-stage Lobatto IIIA methods (L4).

behaves like

$$\psi_i(z) = \frac{h^4}{480} \left(y^4(x_{i-1}) + hy^5(x_{i-1}) + \frac{83h^2}{600}y^6(x_{i-1}) + \frac{11h^3}{400}y^7(x_{i-1}) \right) + O(1/z),$$

as $z \rightarrow \infty$.

The local error is now depend on high derivatives such as $y^4(x), y^5(x)$ and etc that are independent of z . Now as $z \rightarrow \infty$, the global errors of G_3 is given by

$$\begin{aligned} \epsilon_1 &= \psi_1(z) \\ &= \frac{h^4}{480} \left(y^4(x_0) + hy^5(x_0) + \frac{83}{600}h^2y^6(x_0) + \frac{11}{400}h^3y^7(x_0) + O(1/z) \right) \\ &= \frac{h^4}{480} \left(1 - h + \frac{83}{600}h^2 - \frac{11}{400}h^3 + O(1/z) \right) \\ \epsilon_2 &= r\psi_1(z) + \psi_2(z) \\ &= -\frac{h^5}{480} \left(-y^5(x_0) - \frac{3}{2}hy^6(x_0) - \frac{161}{200}h^2y^7(x_0) + O(1/z) \right) \\ &= -\frac{h^5}{480} \left(1 - \frac{3}{2}h + \frac{161}{200}h^2 + O(1/z) \right) \\ \epsilon_3 &= r^2\psi_1(z) + r\psi_2(z) + \psi_3(z) \\ &= \frac{h^4}{480} \left(y^4(x_0) + 3hy^5(x_0) + \frac{83}{600}hy^6(x_0) + 4h^2y^6(x_0) + \frac{83}{300}h^2y^7(x_0) \right. \\ &\quad \left. - \frac{8927}{1200}h^3y^7(x_0) + O(1/z) \right) \\ &= \frac{h^4}{480} \left(1 - \frac{1717}{600}h + \frac{1117}{300}h^2 + \frac{8927}{1200}h^3 + O(1/z) \right) \end{aligned}$$

$$\begin{aligned}
\epsilon_4 &= r^3\psi_1(z) + r^2\psi_2(z) + r\psi_3(z) + \psi_4(z) \\
&= -\frac{h^5}{480} \left(-y^5(x_0) + \frac{83}{600}y^6(x_0) + \frac{55717}{600}hy^6(x_0) + \frac{83}{600}hy^7(x_0) \right. \\
&\quad \left. - \frac{583}{200}h^2y^7(x_0) + O(1/z) \right) \\
&= -\frac{h^5}{480} \left(\frac{683}{600} + \frac{27817}{300}h + \frac{583}{200}h^2 + O(1/z) \right).
\end{aligned}$$

For odd and even values of n , the global error has fourth and fifth derivatives respectively. Therefore, the changes of the sign will also produces the oscillations as observed in Figure 1 and Figure 2. Similar analysis can be carried out for IMR, ITR, and L4. The behaviour are not observed for the G2 and L3 since its stability function tend to 1 as $z \rightarrow \infty$ (Chan and Gorgey, 2013).

2. Dampening the Oscillatory Solutions

Extrapolation was first studied by Gragg (1965) in the study of ODEs. Gragg was trying to solve Kepler problem using explicit midpoint rule (EMR). The numerical results show that the numerical solutions of the EMR give oscillatory solutions and when apply with extrapolation the solutions failed to converge. To overcome this problem, Gragg introduced the smoothing technique that is used to dampen the oscillations in the EMR solutions. The smoothing is achieved by simply applying the formula

$$\begin{aligned}
y_1 &= y_0 + hf(x_0, y_0), \\
y_{n+1} &= y_{n-1} + 2hf(x_n, y_n).
\end{aligned}$$

$$\widehat{y}_n(x) = \frac{1}{4}(y_{n-1} + 2y_n + y_{n+1}), \quad (12a)$$

where $x_n = x_0 + nh$.

The oscillatory behaviour is caused by the parasitic component in the numerical solution.

Gragg was also the first to prove the existence of the asymptotic error expansion for the EMR. This therefore allows for the order of accuracy to be increased by eliminating the leading error term.

For IMR and ITR methods it turned out that the smoothing formula (12a) can also be used to dampen the oscillatory behaviour arise by the global errors due to the stability Chan and Gorgey (2011) (see Figure 3). The extension of smoothing known as symmetrizer is possible for higher order symmetric methods Chan (1993),Gorgey (2012).

The symmetrizer for G3 and L4 are given by Gorgey and Chan on two different articles (see (Chan and Gorgey, 2013)) and (Gorgey and Chan, 2012)). Figure 4 shows that when the G3 and L4 are applied with symmetrizer the oscillations behaviour are dampens.

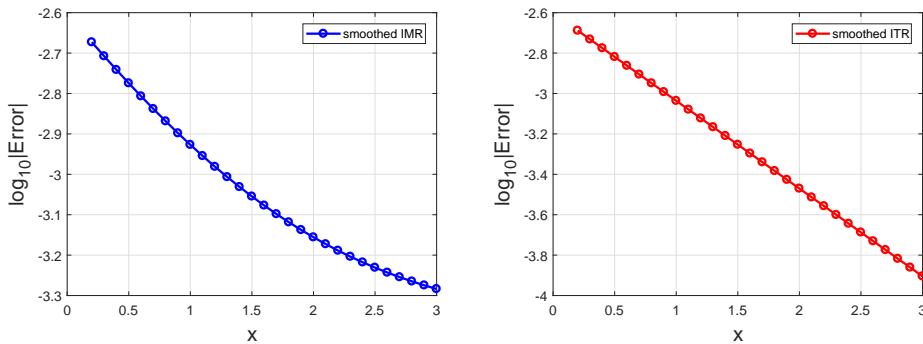


Figure 3: Error behaviour of IMR and ITR with smoothing formula.

The study of symmetric RK methods are important when using extrapolation. Extrapolation involves taking a certain linear combination of the numerical solutions of a base method applied with different stepsizes to obtain greater accuracy (Richardson, 1911).

Although the idea of extrapolation is old, many researchers are still trying to find out which mode of extrapolations is the most efficient and to avoid uncertainties many prefer to use both modes of extrapolation. For example, Faragó, Havasi and Zlatev (Faragó et al., 2010) investigated the computing time for both active and passive extrapolation compared with the Backward Euler. Their results showed that the computing done by the extrapolation for both active and passive is ten times smaller than the corresponding computing

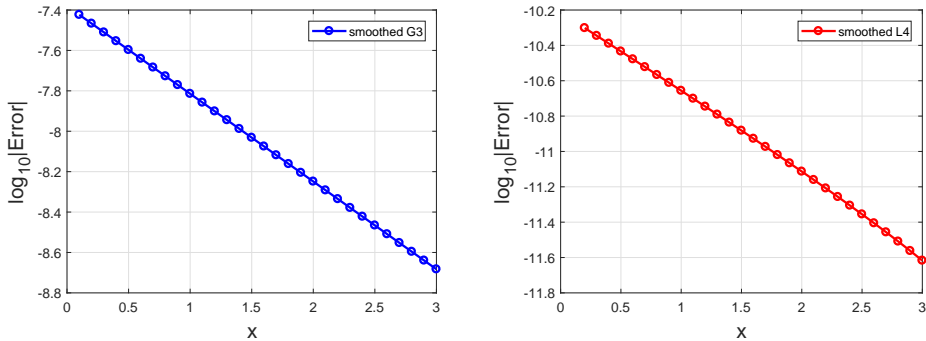


Figure 4: Error behaviour of G3 and L4 with symmetrizer.

time for the Backward Euler. Hence they concluded that regardless of active or passive modes, both modes of extrapolation are still powerful to increase the accuracy.

Several methods can be combined with extrapolation to increase the accuracy of the solutions whether in solving ordinary differential equations (ODEs), boundary value problems (BVPs) or partial differential equations (PDEs). Some numerical methods that can be used with extrapolation to solve the differential equations are fitted operator finite difference (Munyakazi and Patidar, 2008), general linear methods (Cardone et al., 2014), iterated discrete projection (Han and Wang, 2002), Runge-Kutta methods (Gorgey, 2012), Crank-Nicolson method (Gorgey, 2014), stabilized explicit Runge-Kutta methods by Vaquero and Kleefeld (2016). It has been shown that symmetric methods such as the G2, G3, L3 and L4 with symmetrizers when applied with extrapolation, the numerical solutions are observed to give greater accuracy than without symmetrizer and extrapolation (see (Chan and Gorgey, 2013) and Gorgey and Chan (2012)).

3. Conclusions

IMR, ITR, G3 and L4 are both symmetric Runge-Kutta methods. They are advantageous in solving extrapolation since the global errors have asymptotic error expansion; therefore, with extrapolation, there can be an increment of the order by 2. However, these methods are not stable especially when solving stiff Prothero Robinson test problem. The unstable behavior can be overcome by applying smoothing techniques for the IMR and ITR and symmetrizers for the G3 and L4.

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