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A New Inverse Runge–Kutta Scheme for Stiff Ordinary Differential Equation

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Abstract

The paper, discusses semi-implicit inverse Runge –Kutta Scheme for numerical solution of stiff ordinary differential equation of the form $y'=f(x,y)$, $a\le x\le b$. Its derivation adopts Taylor and binomial series expansion , while it analysis of its stability uses the well known A-stability test model equation. Both theoretical and experimental results show that the scheme is A-stable. Numerical results compared favourably with existing Euler's method.

Keywords: A-stable, Accurate, Semi-Implicit, Inverse, Local Truncation Error.

1.0 Introduction

There are problems in the field of Science, Technology and Engineering, which often lead to ODEs of the form

$$y'=f(x,y), \qquad y(x_o) = y_o, \quad a \le x \le b \tag{1.1}$$

where y depends on x. Equation (1.1) is said to be stiff if the Eigen values λ_j of the Jacobian

$$J = \frac{\partial f}{\partial x} \text{ and}$$

$$\lambda_j = U_j + iV_j,\ j=1(1)m, i = \sqrt{-1}$$

(a) $U_j < 0$; j = 1 (1)m

(b) Max (U_j)>> min (U_j), j = 1 (1) m

(c) $|U_j| << |V_j|$ for at least one value of j.

The problem associated with numerical solution of stiff systems were first discovered by [3]. Researchers have generated a lot of interest because of the difficult nature of the solution process of stiff ODEs. Other popular methods include Conventional Implicit, Semi-Implicit and Explicit Runge-Kutta Scheme. [5] introduced a rationatized Runge-Kutta Scheme of the general form.

$$y_{n+1} = \frac{y_n + \sum_{i=1}^{R} W_1 K_i}{1 + y_n \sum_{i=1}^{R} V_I H_I} \tag{1.2}$$

where

$$K_1 = hf(x_n, y_n)$$

$$K_i = hf(x_n + c_i h, y_n + \sum_{j=1}^{i} a_{ij} K_j \tag{1.3}$$

$$H_1 = hg(x_n, z_n)$$

$$H_i = hg(x_n + d_i h, \ z_n + \sum_{j=1}^{i} b_{ij} H_j) \tag{1.4}$$

$$g(x_n, z_n) = Z_n^2 \ f(x_n, y_n) = -\frac{1}{y_n^2} f(x_n, y_n) \tag{1.5}$$

Although the method is suitable, accurate and stable, it is bedeviled by the difficult nature of the function evaluation of f and g.

The method we are considering in this work is of the form

$$y_{n+1} = \frac{y_n}{1 + y_n \sum_{i=1}^{R} W_i K_i} \tag{1.6}$$

where,

$$H_1 = hg(x_n + d_i h, Z_n + \sum_{j=1}^{i} b_{ij} H_j) \tag{1.7}$$

with

$$g(x_n, z_n) = -Z_n^2 f(x_n, y_n), \qquad Z_n = 1/y_n \tag{1.8}$$

and

$$d_i = \sum_{j=1}^{R} b_{ij} \tag{1.9}$$

and it is called Inverse R-stage Runge-Kutta Scheme. This method was classified into Explicit, Semi-Implicit and Implicit. [1] proposed the Explicit one and two stage Inverse R-K scheme. In this paper, we consider the case Semi-Implicit of R = 1 for numerical solution of stiff initial values problems in ODEs.

2.0 Derivation of the Scheme

Now setting R = 1 in equation (1.6), then the one – stage semi-implicit inverse R – K scheme is of the form

$$y_{n+1} = \frac{y_n}{1 + y_n V_1 H_1} \tag{2.1}$$

where

$$H_1 = hg(x_n + d_1 h, \; z_n + b_{11} H_1) \tag{2.2}$$

with

$$g(x_n, z_n) = -Z_n^2 f(x_n, y_n) \tag{2.3}$$

with constraint

with constraint

$$d_1 = b_{11} \tag{2.4}$$

The parameters V_1, d_1, and b_{11} are to be determined from the system of non-linear equations generated by adopting the steps below.

(1) Obtain the Taylor and binomial series expansion of H_1 about point (x_n, y_n) for $i = 1(1)R$.

(2) Insert the series expansion into (2.1)

(3) Compare the final expansion with Taylor series expansion .

Recall that one-stage semi-implicit inverse Runge-Kutta scheme of order two is of the form

$$y_{n+1} = \frac{y_n}{1 + y_n V_1 H_1} \qquad (2.5)$$

The Taylor series expansion of y_{n+1} gives

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2!} y''_n + \frac{h^3}{3!} y'''_n + 0h^4 \qquad (2.6)$$

We know that

$$y'_n = f(x_n, y_n) = f_n$$

$$y''_n = f_x + f_n f_y = Df_n$$

$$y'''_n = f_{xx} + 2 f_n f_{xy} + f_n^2 f_{yy} + f_y (f_x + f_n f_y) - D^2 f_n + f_y Df_n \qquad (2.7)$$

Substitute (2.7) into (2.6), yields

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2} Df_n + \frac{h^3}{6}\left(D^2 f_n + f_y Df_n\right) + 0h^4 \qquad (2.8)$$

In the same way, expanding H_1 about (x_n, z_n) yield

$$H_1 = hN_1 + h^2M_1 + h^3R_1 + 0h^4 \qquad (2.9)$$

where

$$N_1 = g(x_n, z_n) = g_n$$

$$M_1 = d_1 (g_x + g_n g_z) = d_1 Dg_n$$

$$R_1\, g_z + ½\, d_1\, M_1 (g_x + g_n\, g_z) + ½\; d_1^2 M_1 \left(g_{xx} + 2 g_n g_{xz} + g_n^2 g_{zz}\right) \qquad (2.10)$$

Expressing g and its partial derivatives in terms of f and its partial derivatives to increase the comparison of the coefficients. This implies that

$$g_n = \frac{-f_n}{y_n^2}, \quad g_x = \frac{-f_x}{y_n^2}, \quad g_{xx} = \frac{-f_{xx}}{y_n^2}$$

$$g_z = \frac{-2 f_n}{y_n} + f_y, \quad g_{xz} = \frac{-2 f_n}{y_n} + f_{xy}$$

$$g_{xz} = -2f_n - y_n^2\, f_{yy}$$
$$g_{xzz} = -2f_x - 2y_n^2 f_{xyy,}$$
$$g_{zzz} = 4y_n^2 f_y + 6y_n^2 f_{yy} + y_n^4 f_{yyy} \tag{2.11}$$

Substitute (2.12) into (2.11) and (2.10) yields

$$N_1 = \frac{-f_n}{y_n^2},\ M_1 = \frac{d_1}{y_n^2}\left(Df_n + \frac{2f_n^2}{y_n}\right)$$
$$R_1 = \frac{d_1^2}{y_n^2}\left(D^2 f_n - 2\frac{f_n}{y_n}\right)\left(\frac{f_n^{\ 2}}{y_n} + f_x\right) \tag{2.12}$$

adopting (2.10) and (2.13) yields

$$y_{n+1} = y_n - y_n^2\left(hN_1 + h^2 M_1 + h^3 R_1 + 0h^4\right)$$
$$= y_n - y_n^2 V_1\left(hN_1 + h^2 M_1 + h^3 R_1 + 0h^4\right) \tag{2.13}$$

comparing the coefficient of the powers of h in (2.14) and (2.9). That is

$$-y_n^2\ V_1\ N_1 = f_n \tag{2.14}$$
$$-y_n^2\ V_1\left(\frac{-f_n}{y_n^2}\right) = f_n$$
$$V_1 f_n = f_n \Rightarrow \qquad V_1 = 1 \tag{2.15}$$
$$y_n^2\ V_1 M_1 = \frac{Df_n}{2}$$
$$y_n^2\ V_1\left(\frac{d_1}{y_n^2}\left(Df_n + \frac{2f_n^2}{y_n}\right)\right) = \frac{Df_n}{2}$$

$V_1 d_1 = ½$

But $V_1 = 1$

$$d_1 = ½ \tag{2.16}$$

From the constraints

$b_{11} = d_1 \Rightarrow \qquad b_{11} = d_1 = ½$

Then equation (2.6) becomes

$$y_{n+1} = \frac{y_n}{1 + y_n H_1} \tag{2.17}$$

where

$$H_1 = hg(x_n + ½\, h,\ Z_n + ½\, H_1) \tag{2.18}$$

3.0 Analysis of the Basic Properties

Naturally, all ODEs solvers are allergic to error. The magnitude of these errors determines the degree of accuracy of the scheme and their effect can be great. In this section of the paper, the error, convergence, consistency and stability analysis shall be discussed.

3.1. Error Analysis

Error of numerical approximate techniques for stiff ordinary differential equation arise from different cause, which can be classified into Discretization error, Truncation error, Round-off error.

Discretization error:

In numerical analysis for ODEs, discretisation error (e_{n+1}) associated with the scheme is the differences between the exact solution $y(x_{n+1})$ and the numerical solution y_{n+1} at point x_{n+1}. That is

$$e_{n+1} = y_{n+1} - y(x_{n+1}) \tag{3.1}$$

Since the numerical solution of the scheme involves iteration process, there exist propagation of error from step to step. The propagation of error grow or decay from step to step.

Round off error

Round-off errors is an error introduced as a result of the computing devices. Mathematically, it can be expressed as

$$\gamma_{n+1} = y_{n+1} - P_{n+1} \tag{3.2}$$

where y_{n+1} is the expected solution of the difference equation (2.1) while P_{n+1} the computer output at the $(n+1)^{th}$ iteration.

Truncation error

Truncation error on the other hand is the error introduced as a result of ignoring some of the higher terms of the power series of Taylor and Binomial series expansion during the derivation of the new scheme.

Mathematically it can be defined as

$$T_{n+1} = \mathrm{y}(\mathrm{x}_{\mathrm{n+1}}) - \frac{y(x_n)}{1 + y(x_n)\mathrm{V}_1 H_1} \tag{3.3}$$

where

$\mathrm{H}_1 = \mathrm{hg}(\mathrm{x_n}+\mathrm{d_1 h}, \quad \mathrm{z_n}+\mathrm{b}_{11}\, \mathrm{H}_1)$

For example, the local truncation error for the family of one-stage semi-implicit scheme of order two is

$$\mathrm{T}_{\mathrm{n+1}} = \left[\left(\mathrm{D}^2 f_n + \mathrm{f_y} Df_n\right)\left(\tfrac{1}{6} - \tfrac{1}{2}\mathrm{V}_1 d_1^2\right) - \mathrm{V}_1 d_1^2 \left(2\mathrm{f_n} y_n \left(\mathrm{Df_n} - \frac{2 f_n^2}{y_n}\right) - 2 f_y \frac{f_n}{y_n}\right) h^3 + Oh^4 \tag{3.4}$$

3.2 Convergence Property

The numerical scheme (2.1) for solution of stiff ODEs will be convergent if the numerical approximation y_{n+1} that is generated tends to the exact solution $y(x_{n+1})$ as the step size tend to zero.

That is,

$$\lim_{\substack{n \Rightarrow \infty \\ h \Rightarrow 0}} \left[y(\mathrm{x}_{\mathrm{n+1}}) - y_{n+1}\right] = 0 \tag{3.5}$$

To analysed the convergence of the proposed scheme the theorem stated below will be considered.

Theorem 1

Let $\{e_j, \mathrm{j} = 0\,(1)\mathrm{n}\}$ be the set of real numbers, it there exist finite constant R and S such that

$$\left|e_j\right| < R\left|e_{j+1}\right| + S\ , \ \mathrm{j} = 0(1)\mathrm{n}\text{ -1} \tag{3.6}$$

$$\left|e_j\right| \le \left(\frac{R^J - 1}{R - 1}\right) S + \mathrm{R}^{\mathrm{j}} / e_o / \tag{3.7}$$

Let e_{n+1} and T_{n+1} denote the discretization and truncation error generated by scheme (2.1) respectively.

Adopting binomial expansion and ignoring higher terms in (2.1) and (3.4) we obtain

$$y(x_{n+1}) = y(x_n) + h\,\Psi_2(x_n, y(x_n); h) + T_{n+1} \tag{3.8}$$

where Ψ_2 is a continous function in the domain $a \le x \le b$, $|y| < \infty$.

Apply

$$g\left(\mathrm{x_n}, z(x_n)\right) = \frac{1}{\mathrm{y}^2(x_n)}\,\mathrm{f}\left(\mathrm{x_n},\, \mathrm{y(z_n)}\right) \qquad (3.9)$$

where

$$\mathrm{h}\,\Psi_2(x_n\ \mathrm{y(x_n)};\mathrm{h}) = \mathrm{V_1}H_1 = \frac{h}{y^2(x_n)}\Psi_2\left(x_{\mathrm{n}}, y\left(x_n\right)\right) \qquad (3.10)$$

Similarly equation (2.1) yields

$$y_{n+1} = \mathrm{y_n} + \Psi_2\left(x_n, \mathrm{y_n}\ \mathrm{h}\right) \qquad (3.11)$$

Subtract (3.9) from (3.11) and adopt equation (3.2) leads to

$$e_{n+1} = e_n + h(\psi_2)(x_n, \mathrm{y(x_n)}; h) - h\psi_2(x_n, y_n)n\ ) + T_{n+1} \qquad (3.12)$$

Taking the absolute value on both sides of equation (3.13),we have

$$\left|e_{n+1}\right| \le \left|e_n\right| + ak < h\left|e_n\right| + T \qquad (3.13)$$

where

$$\mathrm{T} = \sup_{a\le x\le b} \left|\mathrm{T_{n+1}}\right| \text{ and by} \qquad (3.14)$$

Setting N = K

The inequality (3.13) become

$$\left|e_{n+1}\right| \le \left|e_n\right|\left(1 + h\ \mathrm{N}\right) + T \qquad (3.15)$$

Adopting theorem 1, expression (3.15) becomes

$$e_n \le \left(\frac{(1+hN)^n - 1}{hN}\right)T + (1+hN)^n\left|e_o\right| \qquad (3.16)$$

Since

$$(1+hN)^n = e^{nhN} = e^{N(x_{n-a})}$$

and $x_n \le b$, then $x_n - a \le b - a$

Consequently

$$e^{N(x_n - a)} < e^{n(b-a)}$$

$$|e_n| \leq \left(\frac{e^{N(b-a)}-1}{hN}\right)T + e^{N(b-a)}|e_o| \qquad (3.17)$$

$T_{n+1} = h\psi_2 (x_n + \theta h,\ y (x_n + \theta h)) - \psi (x_n, y(x_n)),\ 0 \leq \theta \leq 1$
$= h\psi_2 (x_n + \theta h,\ y (x_n + \theta h)) - \psi_2 (x_n, + \theta h, y(x_n) + \psi_1(x_n + \theta hy (x_n))$
$- \psi_1 (x_n + \theta hy(x_n)) - \psi_1 (x_n, y(x_n)),\ 0 \leq \theta \leq 1$ (3.18)

By taking the absolute value of (3.18) on both sides and considering equation (3.14) we have

$$T = hK\ |y(x_n + \theta h) - y(x_n)| - jh^2\theta, x_n \leq \in_1 \leq x_n + 1 \qquad (3.19)$$

by setting Q = j, and $Y = \sup_{a \leq x \leq b} y'(x)$ (3.20)

Therefore equation (3.20) becomes

$$T = h^2 \theta (N Y + Q) \qquad (3.21)$$

By setting (3.21) into (3.17), we have $|e_n| \leq h^2\theta\, e^{N(b-a)}(NY + Q) + e^{N(b-a)}|e_o|$ (3.22)

Assuming no error in the input data. That is when $e_o = 0$, then the limit as $h \to 0$, we obtain

$$\lim_{\substack{h \to 0 \\ n \to \infty}} |e_n| = 0 \qquad (3.23)$$

Thus establishing the convergence of the scheme (2.1).

3.3. Consistency Property

One stage scheme (2.1) is said to be consistent if

$y'_n = f(x_n, y_n)$ as h tends to zero.

That is

$$\lim_{h \to o}\left[\frac{y_{n+1} - y_n}{h}\right] = f(x_n, y_n)$$

To show the consistency of the scheme (2.1)
Recall that

$$y_{n+1} = \frac{y_n}{1 + y_n V_1 H_1} \qquad (3.24)$$

Adopting Binomial expansion and ignoring higher order terms

$$y_{n+1} = y_n - y_n^2 V_1 H_1 \qquad (3.25)$$

Subtracting y_n from both sides, we have

$$y_{n+1} - y_n = - y_n^2 V_1 H_1 \qquad (3.26)$$

But $\quad H_1 = \frac{-h}{y_n^2} f(x_n, y_n) \qquad (3.27)$

$$y_{n+1} - y_n = -y_n^2 V_1 \left(\frac{h}{y_n^2} f(x_n, y_n) \right) \qquad (3.28)$$

$$y_{n+1} - y_n = hV_1 f(x_n, y_n) \qquad (3.29)$$

Divide both sides by h and $V_1 = 1$

$$\frac{y_{n+1} - y_n}{h} = f(x_{n,} y_n) \qquad (3.30)$$

Taking the limit as h tends to zero

$$\lim_{h \to o} \left[\frac{y_{n+1} - y_n}{h} \right] = f(x_{n,} y_n) \qquad (3.31)$$

This shows that one-stage method of semi-implicit inverse R-K scheme is consistent.

3.4. Stability Property

As mentioned earlier that any error introduced at any stage of the computation which is not bounded can produced unstable numerical results. Therefore, we consider the stability analysis of the proposed semi-implicit Runge-Kutta scheme defined in (2.1) to access its suitability. To achieve this, we apply scheme (2.1) to [4] stability scalar test initial value problem

$$y' = \lambda y, \quad y(x_o) = y_o \qquad (3.32)$$

under the assumption that Re(λ)<< 0 from the scheme (2.1)

$$y_{n+1} = \frac{y_n}{1 + y_n V_1 H_1} \tag{3.33}$$

$$H_1 = hg(x_n + d_1 h, \quad z_n + b_{11} H_1), \quad Z_n = 1/y_n$$

$$H_1 = (1 + \lambda h b_{11})^{-1} e \lambda h . \frac{1}{y_n}$$

$$H_1 = \frac{\lambda h}{y_n (1 + \lambda h b_{11})} \tag{3.34}$$

$$y_{n+1} = \frac{y_n}{1 + \lambda h V_1 (1 + \lambda h b_{11})^{-1} e} \tag{3.35}$$

let p = λh, and e = 1

Then (3.36) becomes

$$y_{n+1} = \frac{y_n}{1 + pV_1 (1 + pb_{11})^{-1}} \tag{3.36}$$

$$y_{n+1} = \frac{1}{1 + pV_1 (1 + pb_{11})^{-1}} y_n \tag{3.37}$$

Hence let λ(p) = $\frac{1}{1 + pV_1 (1 + pb_{11})}$ (3.38)

Then equation (3.37) becomes

$$y_{n+1} = \mu(p) y_n \tag{3.39}$$

The equation is A-stable if $|\mu(p)| < 1$ (3.40)

with $V_1 = 1$, $b_{11} = d_1 = ½$

Equation (3.37) becomes

$$\frac{1}{1 + p(1 + \frac{1}{2} p)^{-1}} = \frac{1 + \frac{1}{2} p}{1 + \frac{3}{2} p} \tag{3.41}$$

Then equation (3.40) is satisfies

If

$$\left|\frac{1+\frac{1}{2}p}{1+\frac{3}{2}p}\right| < 1 \qquad (3.42)$$

That is if

$$-1 < \frac{1+\frac{1}{2}p}{1+\frac{3}{2}p} < 1 \qquad (3.43)$$

P < 1 implies that the scheme is A-stable. Also p > 0 implies that the scheme is P-stable. Since the values of p is from (-∞, ∞).

Numerical Computation and Results

In order to demonstrate the applicability of this scheme, some sample problem were considered.

Problem 1:

Consider initial value problem

$$y' = -1000\left(y - x^3\right) + 3x^2,\ y(o)=1 \qquad (3.44)$$

The theoretical solution

$$y(x) = x^3 - 1\ e^{-1000x} \qquad (3.45)$$

The numerical results are shown in table 1.

Problem 2

Consider the stiff system of ODEs of the form

$$Y' = AY \qquad (3.46)$$

where

$$A = \begin{bmatrix} 1.0 & -4.99 & 0 \\ 0 & -5.0 & 0 \\ 0 & 7.0 & -12.0 \end{bmatrix}$$

with initial conditions $\begin{bmatrix} 2 & 1 & 2 \end{bmatrix}$ in the theoretical interval $0 \le x \le 1$ while the theoretical solution are given as $y_1(x) = e^{-x} + e^{-5x}$

$$y_2(x) = e^{-5x}$$

$$y_3(x) = \mathrm{e}^{-5x} + e^{-12x} \qquad (3.47)$$

The results are shown in Table 2.

Discussion of Numerical Results

From the results obtained from the solution of the sample problem as shown in the table, the error obtained compare with the error obtained in the existing method show that the new scheme is very accurate.

It was observed that as the mesh size reduces the solution converges, which shows that the method is accurate, stable and convergent.

Table 1: RESULT OF ONE-STAGE SEMI-IMPLICIT INVERSE RUNGE-KUTTA SCHEME AND EULER'S SCHEME

H	YEXACT	PROPOSED ONE-STAGE SEMI-IMPLICIT R-K METHOD OF ORDER TWO Y_N	E1	EULER'S SCHEMES Y_N	E2
.10000000D+00	.36887944+00	.36940452D+00	.52508172D-03	.37603125D+00	.71518088D-02
.500000000D-01	.60665566D+00	.6066819D+00	.26309584D-04	.60689665D+00	.24098742D-03
.25000000D-01	.77881641D+00	.77881743D+00	.10234944D-05	.77882424 D+00	.78335668D-05
.12500000D-01	.88249886 D+00	.88249889D+00	.36809087D-07	.88249911 D+00	.24978363D-06
.62500000D-02	.96941331D+00	.93941331D+00	.12298566D-08	.96941331D+00	.78857242D-08
.31250000D-02	.96923326 D+00	.96923326D+00	.23411650D-09	.96923326D+00	.2476954D-09
.15625000D-02	.98449644 D+00	.98449644 D+00	.75289774D-11	.98449644D+00	.7763479D-11
.78125000D-03	.99221794 D+00	.99221794 D+00	.15305257D-09	.99221794D+00	.24280578D-12
.39062500D-03	.99610137 D+00	.99610137 D+00	.96332942D-11	.99610137D+00	.75495166D-14
.19531250D-03	.99804878 D+00	.99804878 D+00	.60418337D-12	.99804878 D+00	.22204460D-15
.97656250D-04	.99902391 D+00	.9902391 D+00	.15495538D-09	.99902391 D+00	.00000000D+00
.48828125D-04	.99951184 D+00	.99951184 D+00	.19385937D-10	.99951184 D+00	.11102230D-15
.24414063D-04	.99975589 D+00	.99975589 D+00	.24242830D-11	.99975589 D+00	.00000000D+00
.12207031D-04	.99987794 D+00	.99987794D+00	.3032109D-12	.99987794D+00	.11102230D-15

Table 2: RESULT OF ONE-STAGE SEMI-IMPLICIT RUNGE-KUTTA SCHEMES FOR SOLVING STIFF SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

		Y1	Y2	Y3
X	CONTROL STEP SIZE	E1	E2	E3
		.1980099667D+01	.9706425830D+00	.8869204674D+00
.3000000000D – 01	.3000000000D – 01	.8291942688D-09	.3281419103D-07	.8161313500D-05
		.1885147337D+01	.8379203859D+00	.4917945068D+00
.1774236000D+00	.1771470000D-01	.9577894033D-01	.3422855333D-08	.5357828618D-06
		.1791235536D+01	.7191953586D+00	.2663621637D+00
.3307246652D+00	.1046033532D-01	.11050933794D-10	.35587255336D-09	.3474808041D-07
		.1694213422D+01	6088845946D+00	.1365392880D+00
.4977858155D+00	.6176733963D-02	.1269873096D-11	.3655098446D-10	.2146555961D-08
		.1556933815D+01	.4729421983D+00	.4953161076D-01
.7512863895D+00	.3647299638D-01	.1425978891D-08	.3505060447D-07	.1010194837D-05
		.1435390902D+01	.3709037123D+00	.1867601194D-01
.9951298893D+00	.2153693963D-01	.1594313570D-09	.3316564301D-08	.4481540687D-07

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