A New Numerical Integrator for the Solution of Initial Value Problems in Ordinary Differential Equations.

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ABSTRACT

This research paper presents the development, analysis, and implementation of a new numerical integrator capable of solving first order initial value problems in ordinary differential equations. The algorithm developed is based on a local representation of the theoretical solution $y(x)$ to the initial value problem by a nonlinear interpolating function (comprising of the combination of polynomial, exponential and cyclometric functions). The integrator is further applied on sampled problems to generate numerical results. From the results obtained, the new numerical integrator can be said to be computationally reliable and ingenious.

(Keywords: numerical integrator, interpolating function, nonlinear, initial value problem, approximations)

INTRODUCTION

Most phenomena that occur nowadays in the fields of physical, chemical, biological, and management sciences, or in engineering and economics, can be modeled in the form of differential equations. It is also interesting to note that solutions to most differential equations that arise from these models cannot be easily obtained by analytical means. Therefore, approximate solutions are needed which are generated by means of numerical techniques. As reported in Mickens (1994), for arbitrary values of the system parameters at the present time, only numerical integration technique can provide accurate solution to the original differential equation. Also, for any numerical method to be convergent, it has to be a sufficiently accurate representation of the differential system (Lambert, 1991).

In this paper, we develop a new numerical integrator capable of solving equations of the form,

$$y' = f(x, y), y(x_0) = y_0 \qquad \textbf{(1)}$$

Many numerical integration schemes to generate the numerical solutions to problems of the form (1) have been proposed and developed by several authors. Most of these integrators were developed by representing the theoretical solution $y(x)$ to Equation (1) by an interpolating function (linear or nonlinear) $f(x)$.

This type of construction was first reported in Fatunla (1976). He proposed a numerical integrator which is particularly well suited to solve problems of the form (1) having oscillatory or exponential solutions. This method was based on the local representation of the theoretical solution $y(x)$ to the IVP (1) in the interval $[x_n, x_{n+1}]$ by a nonlinear polynomial interpolating function $F(x) = a_0 + a_1 x + breale^{(\rho x + \mu)}$, where $a_0, a_1 \, and \, b$ are real undetermined coefficients, while $\rho \, and \, \mu$ are complex parameters. Other schemes include those developed by Ademiluyi (1987), Ibijola (1997), Kama and Ibijola (2000), Wazwaz (2000), Ibijola and Ogunrinde (2010), Ibijola and Sunday (2010), and Ibijola, Bamisile and Sunday (2011), to mention a few.

Studies have shown that the Interpolants used by the authors above basically consist of the combination of a polynomial and exponential function. Having seen the performance of these schemes, we are motivated and challenged to investigate what happens if a nonlinear Interpolant that consists of the combination of polynomial, exponential and cyclometric (trigonometric) functions is used to derive a new numerical integrator.

We shall state without proof, the theorem that guarantees the existence and uniqueness of solution of the IVP (1).

Theorem 1 (Lambert, 1973; Fatunla, 1988)

Let $f(x, y)$ be defined and continuous for all points (x, y) in the region D defined by $\{(x, y) : a \le x \le b, -\infty < y < \infty\}$ where $a\ and\ b$ finite, and let there exist a constant L such that for every x, y, y^* such that $(x, y)\ and\ (x, y^*)$ are both in D:

$$\left| f(x,y) - f(x,y^*) \right| \le L|y - y*| \qquad \textbf{(2)}$$

Then if η is any given number, there exist a unique solution $y(x)$ of the initial value problem (1), where $y(x)$ is continuous and differentiable for all $(x, y)\ in\ D$. The inequality (2) is known as a Lipschitz condition and the constant L as a Lipschitz constant.

Definition 1 (Lambert 1991)

A Numerical Scheme or Numerical Method or Numerical Integrator (sometimes shortened to 'scheme' or 'method' or 'integrator') is a difference equation involving a number of consecutive approximations $y_{n+j},\ j = 0,1,2,...,k$ from which it will be possible to compute sequentially the sequence $\{y_n | n = 0,1,2, \ldots, N\}$. The integer k is called the step number of the scheme. If, $k = 1$, the method is called *one-step*, while if $k > 1$, the method is called a multi-step or $k - step$.

THE NEW INTERPOLANT

We develop a new Interpolant by combining polynomial, exponential and cyclometric (trigonometric) functions. Let us assume that the theoretical solution $y(x)$ to the initial value problem (1) can be locally represented in the interval, $[x_n, x_{n+1}], n \ge 0$ by the non-linear polynomial interpolating function,

$$F(x) = a_0 + a_1 x + a_2 x^2 + a_3 e^{\alpha x} + b \sin x \qquad \textbf{(3)}$$

where $a_0, a_1, a_2, a_3, b, and\ \alpha$ are undetermined coefficients. Let y_{n+1} be the numerical estimate to the theoretical solution $y(x_{n+1})$ at the point $x = x_{n+1}$ and that $f_n = f(x_n, y_n)$. Let also,

$$x_{n+1} = x_0 + (n+1)h, n = 0,1,2,... \qquad \textbf{(4)}$$

We then move forward to impose the following conditions on the new interpolating function (3);

a) That the interpolating function must coincide with the theoretical solution at $x = x_n\ and\ x = x_{n+1}$. In other words, we require that,

$$F(x_n) = a_0 + a_1 x_n + a_2 x_n^2 + a_3 e^{\alpha x_n} + b \sin x_n \qquad \textbf{(5)}$$

and

$$F(x_{n+1}) = a_0 + a_1 x_{n+1} + a_2 x_{n+1}^2 + a_3 e^{\alpha x_{n+1}} + b \sin x_{n+1} \qquad \textbf{(6)}$$

It implies that $F(x_n) = y(x_n)\ and\ F(x_{n+1}) = y(x_{n+1})$ from Equations (5) and (6), respectively.

b) We further require that the first, second, third and fourth derivatives with respect to x of the interpolating Function (3), respectively coincide with the differential equation as well as its first, second, third and fourth derivatives with respect to $x\ at\ x_n$. In other words, we require that,

$$\left.\begin{aligned} F^{'}(x_n) &= f_n \\ F^2(x_n) &= f_n^{'} \\ F^3(x_n) &= f_n^2 \\ and, & \\ F^4(x_n) &= f_n^3 \end{aligned}\right\} \qquad \textbf{(7)}$$

DERIVATION OF THE NEW NUMERICAL INTEGRATOR

If $F(x_n)\, and\, F(x_{n+1})$ coincide with $y_n\, and\, y_{n+1}$ respectively and that $F^{(i)}(x)$ denotes the ith total derivative of $f(x,y)$ with respect to x, and also adopt the Maclaurin series expansion for the exponential function, we have:

$$e^{\alpha x_n} = \sum_{r=0}^{\infty} \frac{\alpha^r x_n^r}{r!} = 1 + \alpha x_n + \frac{\alpha^2 x_n^2}{2!} + \frac{\alpha^3 x_n^3}{3!} + \dots \tag{8}$$

We now substitute the first few terms of Equation (8) into (5), this gives:

$$F(x_n) = y_n = a_0 + a_1 x_n + a_2 x_n^2 + a_3\left(1 + \alpha x_n + \frac{\alpha^2 x_n^2}{2!} + \frac{\alpha^3 x_n^3}{3!}\right) + b \sin x_n \tag{9}$$

Differentiating Equation (9) with respect to x at x_n gives:

$$F'(x_n) = a_1 + 2a_2 x_n + a_3\left(\alpha + \alpha^2 x_n + \frac{\alpha^3 x_n^2}{2}\right) + b \cos x_n = f_n \tag{10}$$

$$F^{(2)}(x_n) = 2a_2 + a_3(\alpha^2 + \alpha^3 x_n) - b \sin x_n = f_n' \tag{11}$$

$$F^{(3)}(x_n) = a_3 \alpha^3 - b \cos x_n = f_n^2 \tag{12}$$

$$F^{(4)}(x_n) = b \sin x_n = f_n^3 \tag{13}$$

From Equation (13),

$$b = \frac{f_n^3}{\sin x_n} \tag{14}$$

Substitute Equation (14) in (12), we have,

$$a_3 \alpha^3 - \left(\frac{f_n^3}{\sin x_n}\right) \cos x_n = f_n^2 \tag{15}$$

$$a_3 = \left(\frac{1}{\alpha^3}\right)(f_n^2 + f_n^3 \cot(x_n)) \tag{16}$$

Putting Equations (14) and (16) into Equation (11), we have:

$$2a_2 + \left(\frac{1}{\alpha^3}\right)(f_n^2 + f_n^3 \cot(x_n))(\alpha^2 + \alpha^3 x_n) - \left(\frac{f_n^3}{\sin x_n}\right) \sin x_n = f_n' \tag{17}$$

$$\Rightarrow a_2 = \left(\frac{1}{2}\right)\left\{ f_n' - (f_n^2 + f_n^3 \cot(x_n))\left(\frac{1}{\alpha} + x_n\right) + f_n^3 \right\} \tag{18}$$

Substituting Equations (14), (16) and (18) into Equation (10), we have:

$$a_1 + 2\left\{\left(\frac{1}{2}\right)\left[f_n' - (f_n^2 + f_n^3 \cot(x_n))\left(\frac{1}{\alpha} + x_n\right) + f_n^3 \right]\right\} x_n + \left(\frac{1}{\alpha^3}\right)(f_n^2 + f_n^3 \cot(x_n))\left(\alpha + \alpha^2 x_n + \frac{\alpha^3 x_n^2}{2}\right) + \left(\frac{f_n^3}{\sin x_n}\right) \cos x_n = f_n \tag{19}$$

$$\Rightarrow a_1 = f_n - \left[f_n' - (f_n^2 + f_n^3 \cot(x_n))\left(\frac{1}{\alpha} + x_n\right) + f_n^3 \right] x_n - (f_n^2 + f_n^3 \cot(x_n))\left(\frac{1}{\alpha^2} + \frac{x_n}{\alpha} + \frac{x_n^2}{2}\right) - f_n^3 \cot(x_n) \tag{20}$$

Using the assumption that $F(x_n) = y_n\, and\, F(x_{n+1}) = y_{n+1}$, we subtract Equation (5) from (6), this gives us:

$$y_{n+1} - y_n = a_1(x_{n+1} - x_n) + a_2(x_{n+1}^2 - x_n^2) + a_3(e^{\alpha x_{n+1}} - e^{\alpha x_n}) + b(\sin x_{n+1} - \sin x_n) \tag{21}$$

Using the fact that,

$$\left.\begin{aligned} &x_{n+1}-x_n=h\\ &x_{n+1}^2-x_n^2=2x_nh+h^2\\ &\sin(x_{n+1})=\sin(x_n+h)=\sin x_n\cos(h)\\ &\qquad\qquad\qquad\qquad+\cos x_n\sin(h)\end{aligned}\right\} \quad \textbf{(22)}$$

So that Equation (21) becomes:

$$\begin{aligned} y_{n+1}-y_n &= a_1h+a_2(2x_nh+h^2)+a_3e^{\alpha x_n}(e^{\alpha h}-1)\\ &\quad+b\left[(\sin x_n\cos(h)+\cos x_n\sin(h))-\sin x_n\right]\end{aligned} \quad \textbf{(23)}$$

Substituting the values of $a_1, a_2, a_3, and\ b$ in Equation (23), we have:

$$\begin{aligned} y_{n+1} &= y_n+\left\{\begin{aligned} &f_n-\left[f_n^{'}-(f_n^2+f_n^3\cot(x_n))\left(\frac{1}{\alpha}+x_n\right)+f_n^3\right]x_n\\ &-(f_n^2+f_n^3\cot(x_n))\left(\frac{1}{\alpha^2}+\frac{x_n}{\alpha}+\frac{x_n^2}{2}\right)-f_n^3\cot(x_n)\end{aligned}\right\}h\\ &\quad+\left(\frac{1}{2}\right)\left[f_n^{'}-(f_n^2+f_n^3\cot(x_n))\left(\frac{1}{\alpha}+x_n\right)+f_n^3\right](2x_nh+h^2)\\ &\quad+\left(\frac{1}{\alpha^3}\right)(f_n^2+f_n^3\cot(x_n))e^{\alpha x_n}(e^{\alpha h}-1)+\left(\frac{f_n^3}{\sin x_n}\right)\left[\begin{aligned}&(\sin x_n\cos(h)\\ &+\cos x_n\sin(h))-\sin x_n\end{aligned}\right]\end{aligned} \quad \textbf{(24)}$$

Note that,

$$\begin{aligned} &\left(\frac{f_n^3}{\sin x_n}\right)\left[(\sin x_n\cos(h)+\cos x_n\sin(h))-\sin x_n\right]\\ &\qquad=f_n^3\left[\cos(h)+\cot(x_n)\sin(h)-1\right]\end{aligned} \quad \textbf{(25)}$$

We shall now substitute the first few terms of the series expansion for $\cos(h), \sin(h),\ and\ e^{\alpha h}$ in Equation (26) into (24):

$$\left.\begin{aligned} &\cos(h)=\sum_{r=0}^{\infty}(-1)^r\left(\frac{(h)^{2r}}{(2r)!}\right)\\ &\sin(h)=\sum_{r=0}^{\infty}(-1)^r\left(\frac{(h)^{2r+1}}{(2r+1)!}\right)\\ &e^{\alpha h}=\sum_{r=0}^{\infty}\left(\frac{(\alpha h)^r}{(r)!}\right)\end{aligned}\right\} \quad \textbf{(26)}$$

$$
\begin{aligned}
y_{n+1} = y_n + h & \left\{ \begin{array}{l} f_n - \left[f_n^{'} - (f_n^2 + f_n^3 \cot(x_n)) \left(\dfrac{1}{\alpha} + x_n \right) + f_n^3 \right] x_n \\ -(f_n^2 + f_n^3 \cot(x_n)) \left(\dfrac{1}{\alpha^2} + \dfrac{x_n}{\alpha} + \dfrac{x_n^2}{2} \right) - f_n^3 \cot(x_n) \end{array} \right\} \\
& + h \left[f_n^{'} - (f_n^2 + f_n^3 \cot(x_n)) \left(\frac{1}{\alpha} + x_n \right) + f_n^3 \right] (x_n + \frac{h}{2}) \\
& + (f_n^2 + f_n^3 \cot(x_n)) e^{\alpha x_n} \left(\frac{1}{\alpha^3} \right) \left(1 + \alpha h + \frac{\alpha^2 h^2}{2!} + \frac{\alpha^3 h^3}{3!} - 1 \right) \\
& + f_n^3 \left[1 - \frac{h^2}{2!} + \frac{h^4}{4!} - \frac{h^6}{6!} - 1 + \cot(x_n) \left(h - \frac{h^3}{3!} + \frac{h^5}{5!} - \frac{h^7}{7!} \right) \right]
\end{aligned}
\qquad \textbf{(27)}
$$

Finally, we have our new numerical integrator as;

$$
y_{n+1} = y_n + h \left[\begin{array}{l} \left\{ \begin{array}{l} f_n - \left[f_n^{'} - (f_n^2 + f_n^3 \cot(x_n)) \left(\dfrac{1}{\alpha} + x_n \right) + f_n^3 \right] x_n \\ -(f_n^2 + f_n^3 \cot(x_n)) \left(\dfrac{1}{\alpha^2} + \dfrac{x_n}{\alpha} + \dfrac{x_n^2}{2} \right) - f_n^3 \cot(x_n) \end{array} \right\} \\
\qquad + \left[f_n^{'} - (f_n^2 + f_n^3 \cot(x_n)) \left(\dfrac{1}{\alpha} + x_n \right) + f_n^3 \right] (x_n + \dfrac{h}{2}) \\
\qquad + (f_n^2 + f_n^3 \cot(x_n)) e^{\alpha x_n} \left(\dfrac{1}{\alpha^2} + \dfrac{h}{(2!)(\alpha)} + \dfrac{h^2}{3!} \right) \\
\qquad + f_n^3 \left[-\dfrac{h}{2!} + \dfrac{h^3}{4!} - \dfrac{h^5}{6!} + \cot(x_n) \left(1 - \dfrac{h^2}{3!} + \dfrac{h^4}{5!} - \dfrac{h^6}{7!} \right) \right] \end{array} \right]
\qquad \textbf{(28)}
$$

NUMERICAL IMPLEMENTATION OF THE NEW INTEGRATOR

We shall now proceed to implement the new numerical integrator (28) on problems of the form (1). The implementation is carried out using FORCE 3.0 programming application language.

Problem 1 (Logistic Model):

The logistic model finds applications in various fields, among which are; neural networks, statistics, medicine, physics and so on. In Neural networks for example, the logistic model is used to introduce nonlinearity in the model and/or to clamp signals to within a specific range. In Statistics, they are used to model how the probability p of an event may be affected by one or more explanatory variables. In Medicine, they are being used to model the growth of tumors. In Chemistry, the concentration of reactants and products in autocatalytic reactions follows the logistic function. When special initial conditions are applied to the logistic model, we obtain the logistic IVP:

$$
y^{'} = y(1-y), y(0) = 0.5 \qquad \textbf{(29)}
$$

with the theoretical solution,

$$y(t) = \frac{0.5}{(0.5 + 0.5e^{-t})} \quad \textbf{(30)}$$

On the application of the new numerical integrator (28), we obtain the result shown below with step length h=0.1.

Table 1: Performance of the New Integrator (28) on $y^{'} = y(1-y), y(0) = 0.5$, h=0.1

h	Numerical Solution	Exact Solution	Error
0.100	0.52497977	0.52497917	0.00000060
0.200	0.54983515	0.54983401	0.00000113
0.300	0.57444417	0.57444251	0.00000167
0.400	0.59868979	0.59868765	0.00000215
0.500	0.62246192	0.62245935	0.00000256
0.600	0.64565927	0.64565629	0.00000298
0.700	0.66819102	0.66818780	0.00000322
0.800	0.68997794	0.68997449	0.00000346
0.900	0.71095312	0.71094948	0.00000364
1.000	0.73106223	0.73105860	0.00000364

Problem 2 (Growth Model)

Let us consider the differential equation of the form:

$$\frac{dy}{dx} = \alpha y, y(0) = 1000, t \in [0,1] \quad \textbf{(31)}$$

Equation (31) represents the rate of growth of bacteria in a colony. We shall assume that the model grows continuously and without restriction. One may ask how many bacterial are in the colony after some hours if an individual produces an average of 0.2 offspring every hour? We assume that $y(t)$ is the population size at time t. This therefore implies that (31) may be written as:

$$y' = 0.2y, y(0) = 1000, t \in [0,1] \quad \textbf{(32)}$$

with the exact solution,

$$y(t) = 1000e^{0.2t} \quad \textbf{(33)}$$

On the application of the new numerical integrator (28), we obtain the result shown below with step length h=0.1.

Table 2: Performance of the New Integrator (28) on $y' = 0.2y, y(0) = 1000, t \in [0,1]$, h=0.1

h	Numerical Solution	Exact Solution	Error
0.100	1020.20135498	1020.20135498	0.00000000
0.200	1040.81079102	1040.81079102	0.00000000
0.300	1061.83654785	1061.83654785	0.00000000
0.400	1083.28710938	1083.28710938	0.00000000
0.500	1105.17102051	1105.17102051	0.00000000
0.600	1127.49694824	1127.49682617	0.00012207
0.700	1150.27392578	1150.27380371	0.00012207
0.800	1173.51098633	1173.51086426	0.00012207
0.900	1197.21752930	1197.21728516	0.00024414
1.000	1221.40295410	1221.40270996	0.00024414

Problem 3

Consider the initial value problem,

$$y' = 4x - 2xy, (0) = 3 \quad \textbf{(34)}$$

with the theoretical solution,

$$y(x) = 2 + e^{-x^2} \quad \textbf{(35)}$$

On the application of the new numerical integrator (28), we obtain the result shown below with step length h=0.1.

Table 3: Performance of the New Integrator (28) on $y' = 4x - 2xy, (0) = 3$, h=0.1

h	Numerical Solution	Exact Solution	Error
0.100	2.97044683	2.99004984	0.01960301
0.200	2.92311978	2.96078944	0.03766966
0.300	2.86071396	2.91393113	0.05321717
0.400	2.78663635	2.85214376	0.06550741
0.500	2.70469856	2.77880073	0.07410216
0.600	2.61879468	2.69767618	0.07888150
0.700	2.53260279	2.61262655	0.08002377
0.800	2.44933867	2.52729249	0.07795382
0.900	2.37158442	2.44485807	0.07327366
1.000	2.30119967	2.36787939	0.06667972

CONCLUSION

We conclude that the numerical integrator (28) is computationally reliable going by the results obtained above, we therefore recommend it as a numerical scheme for estimating the solution to equations of the form (1).

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SUGGESTED CITATION

Sunday, J., and M.R. Odekunle. 2012. "A New numerical Integrator for the Solution of Initial Value Problems in Ordinary Differential Equations". *Pacific Journal of Science and Technology*. 13(1):221-227.

Pacific Journal of Science and Technology