An Explicit Two-step Rational Method for the Numerical Solution of First Order Initial Value Problem

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Abstract. An explicit two-step, second order rational method for the numerical solution of first order initial value problems is introduced in this paper. Existing rational multistep methods required the computations of higher derivatives from a given initial value problem. However, the new two-step rational method does not require any computation of these higher derivatives, and thus save up some computational cost. Numerical results showed that the new rational multistep method and existing rational multistep method are found to have comparable accuracy in solving first order initial value problems.

Keywords: Explicit, Two-step Rational Method, Rational Multistep Method, Finite Difference, First Order Initial Value Problems.
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INTRODUCTION

Conventional numerical methods for initial value problems (IVPs) of the form

$$y' = f(x, y),\ y(a) = \eta, \tag{1}$$

that have been widely used nowadays are those from the class of linear multistep methods and the class of linear Runge-Kutta methods. Besides methods from these two classes, there are other options such as the predictor-corrector methods, hybrid methods and extrapolation methods. On the other hand, unconventional methods for the problems in (1) are special numerical methods that are developed to solve certain types of IVPs, such as IVPs with oscillatory solutions or IVPs whose solutions possess singularities, where in most of the time, conventional methods will perform poorly. Unconventional methods might possess some outstanding features that could never be achieved by conventional methods. These features include achieving higher order of numerical accuracy with less computational cost, stronger stability properties and so on.

In this paper, we talked about unconventional methods that are based on rational functions, or better known as rational methods in the literature review. Numerical integration formulae based on rational functions were introduced by Lambert and Shaw [1], where these methods were originally used to solve problem (1) whose solution possesses singular point. However, eventually, researchers started to discover the potential of rational methods in solving even more general initial value problems such as non-stiff problems, stiff problems and problems whose solutions are known to be periodic. For excellent survey and various perspectives, see Lambert and Shaw [1], Lambert [2], Luke et al. [3], Fatunla [4, 5], van Niekerk [7, 8], Ikhile [8, 9, 10], Ramos [11], Okosun and Ademiluyi [12, 13], Teh et al. [14, 15], Yaacob et al. [16], Teh [17], Teh and Yaacob [18, 19].

Many rational methods presented in and after van Niekerk [6], required the computations of higher derivatives of (1) such as y'', y''' and so on. Reviews showed that rational method which required this kind of computations is most likely derived through the matching of its Taylor series and solving a system of simultaneous equations to obtain the unknown parameter(s). Rational methods which derived in this way could be generalized easily. However, there is another way to derive rational methods, which is through the elimination of the undetermined parameter(s). Such technique was applied in Lambert and Shaw [1], Lambert [2], Luke et al. [3] and Fatunla [4]. By using this technique, it is possible to derive rational method without derivatives higher than the first order, with careful choice of rational approximant and number of interpolation points. Therefore, computational cost is cheaper for such rational method because it does not require the computational of extra derivatives. On the other hand, generalizations for rational methods derived through elimination of undetermined parameters are usually unwieldy

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to state [1, 4]. This situation causes difficulties for theoretical analyses such as consistency, stability and convergence, to be done in a generalized manner.

In this paper, we wish to propose another alternative to derive rational method which does not require the computations of extra derivatives. On adopting the idea of Wu and Xia [20], we can approximate higher order derivatives in a rational method with their corresponding backward difference quotient. Hence, the resulting rational method will not contain any derivative higher than the first order. In the next section, we present how this alternative technique changes an existing one-step rational method to a two-step rational method. After that, we discuss the local truncation error of this two-step rational method. Finally, some tests are carried out in order to verify the validity of the new two-step rational method.

DERIVATION OF THE TWO-STEP RATIONAL METHOD VIA BACKWARD DIFFERENCE QUOTIENT

Consider the following one-step rational method given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2 y'_n y''_n}{2y'_n - hy''_n}, \tag{2}$$

where y_n and y_{n+1} are approximations to the theoretical solutions $y(x_n)$ and $y(x_{n+1})$. We note that y'_n is the approximation of the problem (1) while the approximated y''_n can be obtained by differentiating the problem (1) once.

$$y''(x)\Big|_{x=x_n} = \left.\frac{df\left(x, y(x)\right)}{dx}\right|_{x=x_n} \approx y''_n \tag{3}$$

We may also assume that $y_n = y(x_n)$, $y'_n = y'(x_n)$ and $y''_n = y''(x_n)$ by the localizing assumption that no previous truncation errors have been made. The one-step rational method in (2) is a second order method and found to be A-stable when solving the Dahlquist's test problem given by

$$y' = \lambda y,\ y(a) = y_0,\ \mathrm{Re}(\lambda) < 0. \tag{4}$$

The rational method in (2) is the most common rational method found in the literature. It was frequently reported in Lambert and Shaw [1], Lambert [2], van Niekerk [6, 7], Ikhile [8, 9] and Ramos [11].

As we can see from formula (2), it possesses a second order derivative i.e. y''_n. In order to avoid the calculation of the second order derivative in (2), we approximate y''_n with backward difference quotient given by [20]

$$y''(x_n) \approx y''_n = \frac{y'_n - y'_{n-1}}{y_n - y_{n-1}}. \tag{5}$$

Note that y_{n-1} and y'_{n-1} are the approximations of the exact solution and problem (1) at the point x_{n-1}. On substituting equation (5) into formula (2), we obtain the following rational method

$$y_{n+1} = y_n + hy'_n + \frac{h^2 y'_n \dfrac{y'_n - y'_{n-1}}{y_n - y_{n-1}}}{2y'_n - h\dfrac{y'_n - y'_{n-1}}{y_n - y_{n-1}}}. \tag{6}$$

Formula (6) is now a two-step explicit rational method due to the presence of the expressions y'_{n+1} and y_{n+1}. We rewrite formula (6) as follows

$$y_{n+2} = y_{n+1} + hy'_{n+1} + \frac{h^2 y'_{n+1} \dfrac{y'_{n+1} - y'_n}{y_{n+1} - y_n}}{2y'_{n+1} - h \dfrac{y'_{n+1} - y'_n}{y_{n+1} - y_n}}. \tag{7}$$

LOCAL TRUNCATION ERROR

For the ease to investigate the two-step explicit rational method in formula (7), we associate a difference operator L defined by

$$\begin{aligned} L\left[y(x);h\right] &= \left(y(x+2h) - y(x+h) - hy'(x+h)\right) \times \left(2y'(x+h)\left(y(x+h) - y(x)\right) - h\left(y'(x+h) - y'(x)\right)\right) \\ &\quad - h^2 y'(x+h)\left(y'(x+h) - y'(x)\right) \end{aligned} \tag{8}$$

where $y(x)$ is an arbitrary function, continuously differentiable along a finite integration interval. Expanding $y(x+2h)$, $y(x+h)$ and $y'(x+h)$ as Taylor series and collecting terms in (8) give the following results:

$$L\left[y(x);h\right] = h^3\left(-y'(x)y''(x) + y'(x)^2 - y''(x)\right) + O(h^4). \tag{9}$$

The local truncation error at x_{n+2} of formula (7) is defined to be the expression $L\left[y(x_n);h\right]$ given by equation (9), where $y(x_n)$ is the theoretical solution of problem (1) at a point x_n. Thus, the local truncation error of formula (7) denoted by the symbol LTE is then

$$\text{LTE} = h^3\left(-y'_n y''_n + (y'_n)^2 y''_n\right) + O(h^4). \tag{10}$$

where $y'_n = y'(x_n)$ and $y''_n = y''(x_n)$ by the localizing assumption. From equation (10), we immediately realized that the two-step rational method is a second order method. We note that the original method in (2) is also a second order method. Hence, we observed that order of consistency is retained even after the substitution of the backward difference quotient.

NUMERICAL EXPERIMENTS AND COMPARISONS

In this section, some test problems are used to verify the validity of the new two-step rational formula shown in equation (7). We present the maximum relative errors over the integration interval given by $\max_{0 \le n \le N}\left\{\left|y(x_n) - y_n\right|\right\}$ where N is the number of integration steps. We note that $y(x_n)$ and y_n are the theoretical solution and numerical solution of a test problem at point x_n. The numerical results generated by formula (7) are compared with the numerical results obtained from the two-step second order rational method RMM1(2,2) of Yaacob et al. [16] given by

$$y_{n+2} = y_n + \frac{2h(y'_n)^2}{y'_n - hy''_n}. \tag{11}$$

Finally, we choose the modified Euler method given by [21]

$$y_{n+1} = y_n + hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hf(x_n, y_n)\right), \tag{12}$$

as the starting method for the two-step formulae in (7) and (11).

Problem 1 (Ramos [11])

$$y'(x) = -100y(x) + 99e^{2x}, \; y(0) = 0, \; x \in [0,1]$$

The theoretical solution is given by $y(x) = 33/34\left(e^{2x} - e^{-100x}\right)$.

TABLE (1). Maximum absolute errors with respect to number of integration steps, N (*Problem 1*).

N	**Formula (7)**	**Formula (11)**
128	8.91614(-02)	7.81545(-02)
256	5.23113(-02)	1.78169(-02)

Problem 2 (Yaakub and Evans [22])

$$y''(x) + 101y'(x) + 100y(x) = 0, \; y(0) = 1.01, \; y'(0) = -2, \; x \in [0,1]$$

The theoretical solution is given by $y(x) = 0.01e^{-100x} + e^{-x}$. *Problem 2* can also be written as a system i.e.

$$y_1'(x) = y_2(x), \; y_1(0) = 1.01, \; x \in [0,1];$$
$$y_2'(x) = -100y_1(x) - 101y_2(x), \; y_2(0) = -2, \; x \in [0,1].$$

The theoretical solutions of this system are given by $y_1(x) = y(x) = 0.01e^{-100x} + e^{-x}$, $y_2(x) = y'(x) = -e^{-100x} - e^{-x}$.

TABLE (2). Maximum absolute errors with respect to number of integration steps, N (*Problem 2*).

N	**Formula (7)**	**Formula (11)**
128	9.11731(-03)	4.43877(-03)
256	3.18814(-03)	1.01548(-03)

Problem 3 (Ramos [11])

$$y'(x) = 1 + y(x)^2, \; y(0) = 1, \; x \in [0,1]$$

Problem 3 is a problem whose solution possesses singularity. The theoretical solution is $y(x) = \tan(x + \pi/4)$. From the theoretical solution, we have noticed that the solution becomes unbounded in the neighbourhood of the singularity at $x = \pi/4 \approx 0.785398163367448$.

TABLE (3). Maximum absolute errors with respect to number of integration steps, N (*Problem 3*).

N	**Formula (7)**	**Formula (11)**
16	2.55654(+02)	6.52610(+00)
32	4.20433(+09)	4.68146(+01)

CONCLUSIONS

In this paper, a two-step explicit rational method without the requirement of higher derivative was introduced. This two-step rational method was developed by replacing the second order derivative of formula (2) by its backward difference quotient shown in equation (5). Analysis showed that the new two-step rational method and its original counterpart in formula (2) possessed second order of consistency.

Results from Table 1 and Table 2 showed that the new two-step rational method in formula (7) and the RMM1(2.2) in (11) were found to have comparable accuracy in solving *Problem 1* and *Problem 2*. However, formula (7) was not suitable to solve problem whose solution possesses singularity, as indicated by the results shown in Table 3. We have notified this defect and it is probably due to the existence of the backward difference quotient in the method itself. Perhaps future studies may look into the possibility to redesign rational methods which incorporate the backward difference quotient during the process of derivation, rather than replacing higher derivatives with the quotients at the output methods. By doing so, it is possible to overcome the aforementioned defect.

REFERENCES

1. J. D. Lambert and B. Shaw, *Math. Comp.* **19**, 456-462 (1965).
2. J. D. Lambert, "Two Unconventional Classes of Methods for Stiff Systems" in *Stiff Differential Equations*, edited by R. A. Willoughby, New York: Plenum Press, 1974, pp. 171-186.
3. Y. L. Luke, W. Fair and J. Wimp, *Comput. Math. Appl.* **1**, 3-12 (1975).
4. S. O. Fatunla, *Comput. Math. Appl.* **8**, 231-239 (1982).
5. S. O. Fatunla, *Comput. Math. Appl.* **12B**, 1109-1115 (1986).
6. F. D. van Niekerk, *Comput. Math. Appl.* **13**, 367-371 (1987).
7. F. D. van Niekerk, *Comput. Math. Appl.* **16**, 1035-1039 (1988).
8. M. N. O. Ikhile, *Comput. Math. Appl.* **41**, 769-781 (2001).
9. M. N. O. Ikhile, *Comput. Math. Appl.* **44**, 545-557 (2002).
10. M. N. O. Ikhile, *Comput. Math. Appl.* **47**, 1463-1475 (2004).
11. H. Ramos, *Appl. Math. Comput.* **189**, 710-718 (2007).
12. K. O. Okosun and R. A. Ademiluyi, *Research Journal of Applied Sciences* **2**, 13-16 (2007).
13. K. O. Okosun and R. A. Ademiluyi, *Research Journal of Applied Sciences* **2**, 84-88 (2007).
14. Y. Y. Teh, N. Yaacob and N. Alias, "Numerical Comparison of Some Explicit One-step Rational Methods in Solving Initial Value Problems" in *Proceedings of the 5th Asian Mathematical Conference*, edited by S. K. Lee, School of Mathematical Sciences, Universiti Sains Malaysia, 2009.
15. Y. Y. Teh, N. Yaacob and N. Alias, *Matematika (Johor Bahru)* **27**, 59-78 (2011).
16. N. Yaacob, Y. Y. Teh, and N. Alias, *Jurnal KALAM* **3**, 26-39 (2010).
17. Y. Y. Teh, "New Rational and Pseudo-type Runge-Kutta Methods for First Order Initial Value Problems", Ph.D. Thesis, Universiti Teknologi Malaysia, 2010.
18. Y. Y. Teh and N. Yaacob, *Malays. J. Math. Sci.* 7, 31-57 (2013).
19. Y. Y. Teh and N. Yaacob, *Sains Malays.* **42**, 845-853 (2013).
20. X. Y. Wu and J. L. Xia, *Comput. Math. Appl.* **39**, 249-257 (2000).
21. J. D. Lambert, *Computational Methods in Ordinary Differential Equations*, London: John Wiley & Sons Ltd, 1973, pp. 118
22. A. R. Yaakub and D. J. Evans, *Int. J. Comput. Math.* **80**, 95-104, (2003).