Block Multistep Methods Based on Rational Approximants

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Abstract. In this study, the concept of block multistep methods based on rational approximants is introduced for the numerical solution of first order initial value problems. These numerical methods are also called rational block multistep methods. The main reason to consider block multistep methods in rational setting, is to improve the numerical accuracy and absolute stability property of existing block multistep methods that are based on polynomial approximants. For this pilot study, a 2-point explicit rational block multistep method is developed. Local truncation error and stability analysis for this new method are included as well. Numerical experimentations and results using some test problems are presented. Numerical results are satisfying in terms of numerical accuracy. Finally, future issues on the developments of rational block multistep methods are discussed.

Keywords: Rational Approximant, 2-point Explicit Rational Block Multistep Method, Initial Value Problems.
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INTRODUCTION

Numerical solutions for ordinary differential equations (ODEs) have great importance in scientific computation, as they are widely used to model the real world problems. Conventional numerical methods which have been widely used nowadays are those from the class of linear multistep methods (LMMs) and the class of Runge-Kutta methods. Besides methods from these two classes, there are other options such as the predictor-corrector methods, hybrid methods, extrapolation methods and block multistep methods (BMMs).

BMMs can be considered as a set of simultaneously applied LMMs to obtain several numerical approximations within each integration step (Sommeijer et al. [1]). For excellence surveys and various perspectives of BMMs, see, for example, Sommeijer et al.[1], Watanabe [2], Ibrahim et al.[3-4], Chollom et al.[5], Majid et al.[6-7], Mehrkanoon et al. [8], Akinfenwa et al.[9], Ehigie et al.[10], Ibijola et al.[11] and Majid and Suleiman [12]. Implicit BMMs were introduced mainly to improve the order of consistencies and stability requirements suffered by most explicit BMMs. However, extra computations are required to solve the system of nonlinear equations arise from the implementations of implicit BMMs, which are very expensive in terms of computational costs when solving large scale problems. Alternatively, some of the researchers would prefer predictor-corrector BMMs because they allow the stage-by-stage implementations without the need to solve any system of nonlinear equations. The order of consistency is determined by the order of the correctors that are usually be the implicit BMMs, while the predictors are usually be the explicit BMMs. However, the stability requirements of predictor-corrector BMMs become more restricting when the order of the methods increases, which make the numerical solution of stiff problem impossible for larger step-sizes.

Despite the shortcomings of most BMMs in terms of stability analysis, they are very useful tools in terms of solvability. Firstly, BMMs can easily be modified and extended to solve higher order initial value problems directly, as reported in Majid et al. [6-7], Ehigie et al. [10], Badmus and Yahaya [13] and Olabode [14]. Secondly, BMMs can easily be implemented on a parallel machine, as reported in Sommeijer et al.[1], Mehrkanoon et al. [8] and Chartier [15]. Thus, the potential of BMMs is obvious regardless of their stability drawbacks. In view of this, the research problem we are going to investigate is: "how can we develop BMMs which possess strong stability requirements but cheaper computational costs?" Our readings have shown that there exist some unconventional numerical methods which possess strong stability conditions but yet explicit in nature. These unconventional methods are known as rational methods because they are numerical methods based on rational functions. For excellence surveys and various perspectives, see, for example, Lambert and Shaw [16], Lambert [17], Luke et al. [18], Fatunla [19-20], van Niekerk [21-22], Ikhile [23-25], Ramos [26], Okosun and Ademiluyi [27-28], Teh et al. [29-30], Yaacob et al. [31], Teh [32], Teh and Yaacob [33-34].

Explicit rational methods are capable in solving stiff problem and problem whose solution possesses singularity but they cannot generate several numerical approximations within each integration step like BMMs. On the other hand, Adams-Moulton BMMs and backward differentiation BMMs are expensive in implementations due to the

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implicit nature of the BMMs. Moreover, all BMMs fail to solve problem whose solution possesses singularity near the singular point. By comparing the pros and cons of rational methods and BMMs, we come out with the idea to search for BMMs that are based on rational functions, or so called rational BMMs (RBMMs). We expect RBBMs to be cheaper in computational costs compare to existing implicit BMMs; possess strong stability conditions such as L-stability and able to solve stiff problems and problem whose solution possesses singularity.

In the next section, we develop a simple 2-point explicit rational block method as to explain the formulation idea of RBMM. Then, we demonstrate the calculation of principal local truncation error term and establish the absolute stability condition for the newly developed method. Some tests are carried out in order to verify the validity of the new RBMM. Finally, a conclusion is included.

FORMULATION OF 2-POINT EXPLICIT RATIONAL BLOCK METHOD

The 2-point explicit rational block method is formulated to solve the following first order initial value problem given by

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

where $f(x,y): \mathrm{R} \times \mathrm{R}^m \to \mathrm{R}^m$ and $f(x,y)$ is assumed to satisfy all the required conditions such that problem (1) possesses a unique solution. Suppose that the interval of numerical integration is $x \in [a,b] \subset \mathrm{R}$ and is divided into a series of blocks with each block containing two points as shown in Figure 1.

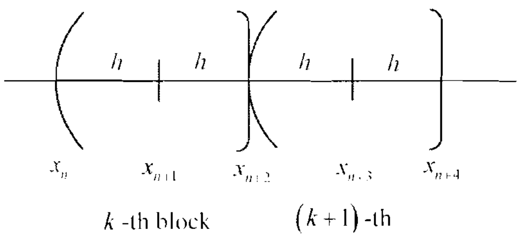

FIGURE 1. 2-point Explicit Rational Block Method

From Figure 1, we have observed that k -th block contains three points x_n, x_{n+1} and x_{n+2}, and each of these points is separated equidistantly by a constant step-size h. The next $(k+1)$ -th block also contains three points. In the k -th block, we want to use the values y_n at x_n to compute the approximation values of y_{n+1} and y_{n+2} simultaneously. In the $(k+1)$ -th block, previously computed values of y_{n+2} is used to generate the approximations values of y_{n+3} and y_{n+4}. The same computational procedure is repeated to compute the solutions for the next few blocks until the end-point i.e. $x = b$ is reached. The evaluation information from the previous step in a block could be used for other steps of the same block. The explanation provides here is nothing new and could be found in Majid et al. [7].

Along the x-axis, we consider the points x_n, x_{n+1} and x_{n+2} to be given by

$$x_n = x_0 + nh, \tag{2}$$

$$x_{n+1} = x_0 + (n+1)h, \text{ and} \tag{3}$$

$$x_{n+2} = x_0 + (n+2)h, \tag{4}$$

where h is the step-size. Let us assume that the approximate solution of (1) is locally represented in the range $[x_n, x_{n+1}]$ by the rational approximant

$$R(x)=\frac{a_0+a_1x+a_2x^2}{b_0+x}, \tag{5}$$

where a_0, a_1, a_2 and b_0 are undetermined coefficients. This rational approximant in equation (5) is required to pass through the points (x_n, y_n) and (x_{n+1}, y_{n+1}), and moreover, must assume at these points the derivatives given by $y'=f(x,y)$, $y''=f'(x,y)$ and $y'''=f''(x,y)$. Altogether, there are five equations to be satisfied i.e.

$$R(x_n)=y_n, \tag{6}$$
$$R(x_{n+1})=y_{n+1}, \tag{7}$$
$$R'(x_n)=f_n, \tag{8}$$
$$R''(x_n)=f'_n, \text{ and} \tag{9}$$
$$R'''(x_n)=f''_n, \tag{10}$$

where $f_n=f(x_n,y_n)$, $f'_n=f'(x_n,y_n)$ and $f''_n=f''(x_n,y_n)$. On using *MATHEMATICA 8.0*, the elimination of the four undetermined coefficients a_0, a_1, a_2 and b_0 from equations (6) – (10) is the one-step third order rational method proposed by Lambert and Shaw [16].

$$y_{n+1}-y_n=hf_n+\frac{h^2}{2}\frac{3(f'_n)^2}{3f'_n-hf''_n}. \tag{11}$$

Equation (11) is the formula to approximate y_{n+1} by using the information at the previous point (x_n, y_n). To approximate y_{n+2}, we have to assume that the approximate solution of (1) is locally represented in the range $[x_n, x_{n+2}]$ by the same rational approximant given in equation (5). It is crucial to retain the same rational approximant in the same block. Now, we required the rational approximant (5) to pass through the points (x_n, y_n), (x_{n+1}, y_{n+1}) and (x_{n+2}, y_{n+2}), and moreover, must assume at these points the derivative given by $y'=f(x,y)$. There are also five equations to be satisfied i.e.

$$R(x_n)=y_n, \tag{12}$$
$$R(x_{n+1})=y_{n+1}, \tag{13}$$
$$R(x_{n+2})=y_{n+2}, \tag{14}$$
$$R'(x_n)=f_n, \text{ and} \tag{15}$$
$$R'(x_{n+1})=f_{n+1}, \tag{16}$$

where $f_n=f(x_n,y_n)$ and $f_{n+1}=f(x_{n+1},y_{n+1})$. On using *MATHEMATICA 8.0*, the elimination of the four undetermined coefficients a_0, a_1, a_2 and b_0 from equations (12) – (16) is the two-step third order rational method proposed by Lambert and Shaw [16].

$$3y_{n+2}-4y_{n+1}+y_n=\frac{2h}{3}(f_n+2f_{n+1})+\frac{4h^2}{3}\frac{(f_n-f_{n+1})^2}{3(y_{n+1}-y_n)-h(f_{n+1}+2f_n)}. \tag{17}$$

Equation (17) is the formula to approximate y_{n+2} by using the information at the previous points (x_n, y_n) and (x_{n-1}, y_{n-1}). Hence, the 2-point explicit rational block method based on the rational approximant (5) consists of two formulae i.e. formulae (11) and (17).

The implementation of the 2-point explicit rational block method is rather simple: with y_n is known, compute the approximate solution y_{n+1} using formula (11); and then compute the approximate solution y_{n+2} using formula (17) with the value of y_{n+1} obtained from formula (11).

LOCAL TRUNCATION ERRORS AND STABILITY ANALYSES

Since formulae (11) and (17) are used in the same block to solve for the approximate solutions at x_{n+1} and x_{n+2}, we wish to have both formulae possess the same order of accuracy. Lambert and Shaw [16] have showed that the local truncation errors for formulae (11) and (17) are

$$\mathrm{LTE}_{(11)} = h^4 \left(\frac{1}{24} y_n^{(4)} - \frac{\left(y_n^{(3)}\right)^2}{18 y_n''} \right) + O\left(h^5\right), \tag{18}$$

and

$$\mathrm{LTE}_{(17)} = h^4 \left(\frac{1}{2} y_n^{(4)} - \frac{2}{3} \frac{\left(y_n^{(3)}\right)^2}{y_n''} \right) + O\left(h^5\right), \tag{19}$$

respectively. From the local truncation errors given in equations (18) and (19), it is easy to verify that both formulae (11) and (17) possess third order of accuracy.

To investigate the linear stability condition for formulae (11) and (17) in the same block, we need to combine both formulae and apply the Dahquist's test equation

$$y' = \lambda y,\ y(a) = y_0,\ \mathrm{Re}(\lambda) < 0, \tag{20}$$

to both formulae. With $f_{n+1} = \lambda y_{n+1}$, $f_n = \lambda y_n$, $f_n' = \lambda^2 y_n$, and $f_n'' = \lambda^3 y_n$, we can obtain the following difference equation

$$y_{n+2} = \frac{9 + 12h\lambda + 7h^2\lambda^2 + 2h^3\lambda^3}{(h\lambda - 3)^2} y_n. \tag{21}$$

On setting $h\lambda = z$, $y_{n+2} = \zeta^2$ and $y_n = \zeta^0 = 1$ in equation (21), then the stability polynomial for the 2-point explicit rational block method is

$$\zeta^2 - \frac{9 + 12z + 7z^2 + 2z^3}{(z - 3)^2} = 0. \tag{22}$$

Here, ζ can be interpreted as the roots of stability polynomial (22). By taking $z = x + iy$ in the roots of equation (22), we have plotted the region of absolute stability of the 2-point explicit rational block method in Figure 2.

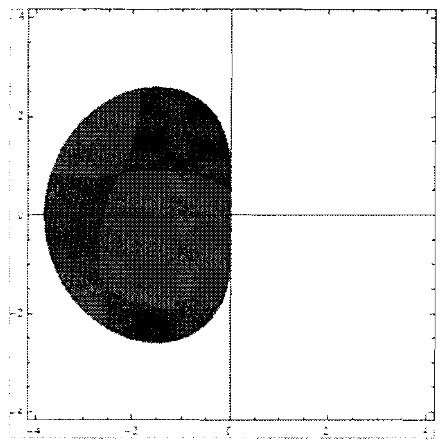

FIGURE 2. Absolute Stability Region of 2-point Explicit Rational Block Method.

The shaded region in Figure 2 is the region of absolute stability of the 2-point explicit rational block method. Hence, this shaded region can also be viewed as the 'combined' region of absolute stability of formulae (11) and (17). The shaded region is the place where the absolute value of each root of equation (22) is less than or equal to 1. From Figure 2, we can see that the region of absolute stability does not contain the whole left-hand half plane which suggests that our proposed rational block method is not A-stable.

NUMERICAL EXPERIMENTS

In this section, some test problems are used to verify the validity of the new 2-point explicit rational block method shown in formulae (11) and (17). We present the maximum absolute 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, respectively.

Problem 1

$$y'(x) = -10y(x),\, y(0) = 1,\; x \in [0,1]$$

The theoretical solution is given by $y(x) = e^{-10x}$.

TABLE (1). Maximum Absolute Errors With Respect To Number of Integration Steps, N (*Problem 1*)

N	2-point Explicit Rational Block Method
32	1.06069(-04)
64	7.39546(-06)
128	4.88814(-07)
256	3.14280(-08)

Problem 2 (Yaakub and Evans [35])

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

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	2-point Explicit Rational Block Method
32	6.26821(-03)
64	6.33658(-04)
128	4.06612(-05)
256	2.35650(-06)

Problem 3 (Ramos [26])

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

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	2-point Explicit Rational Block Method
32	1.02625(-02)
64	6.51554(-04)
128	5.14872(-05)
256	7.33577(-04)

Results from Table 1, Table 2 and Table 3 showed a consistent pattern i.e. the maximum absolute error decreases whenever the number of integration increases. This also means, whenever the step-size becomes smaller, the numerical solution also approaches the exact solution and therefore convergent.

CONCLUSIONS

In this paper, a 2-point explicit rational block method was introduced. This rational block method was able to approximate two successive solutions at the points x_{n+1} and x_{n+2} defined in the same block (see Figure 1), within every single integration step. This rational block method also contained two rational formulae, and both formulae were found to possess third order of accuracy. Figure 2 showed that the new proposed method has a finite region of absolute stability. Numerical experiments showed that the proposed rational block method generated converging numerical solution. Future study will include the numerical comparison with other existing block methods.

Finally, this is the pilot study of rational block method, and many more rational block methods will be developed in the near future, e.g. implicit rational block method, and predictor-corrector rational block method. From the rational approximant in (5), we can see that the degree of the numerator is greater than the degree of the denominator. We believed that this kind of selection yields method with finite region of absolute stability. In order to develop A-stable rational block method, we should consider a rational approximant with both numerator and denominator in equal degree. Of course, L-stable rational block method may be developed if the underlying rational approximant has the degree of denominator greater than the degree of numerator. These directions constitute a vast research dimensions to be explored in the near future.

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