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Solving Initial Value Problems with Mendeleev's Quadrature

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Abstract. This article presents the Mendeleev method to solve the initial value problems. The construction of this method using Mendeleev's quadrature is due to Pleshakov [Comp. Math. and Math. Phys., 52 (2012), 211-212.] to approximate the integral $\int_{x_i}^{x_{i+1}} f(s, Y(s))ds$. We derive the local truncation error and show the stability region of the proposed method. The computational comparisons show that Mendeleev's method is better than Euler's method, midpoint method and Heun's method.

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Keywords and Phrases: Initial value problems, Mendeleev's quadrature, Euler's method, midpoint method, Heun's method, stability region

1. Introduction

An initial value problem (IVP) is usually presented in the form

$$Y'(x) = f(x, Y(x)), \tag{1}$$

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where

$$Y(x_0) = Y_0.$$

Problem (1) can be solved by the third order Runge Kutta based on arithmatic means (classic). In the development, some authors replace the arithmatic mean with other variation means such as geometric mean [3], harmonic mean [8], heronian, root-mean-square, centroidal and contraharmonic [9]. Further improvement has been made by Ababneh and Rosita [1] which adds some weights to contraharmonic mean.

In this article, we present the Mendeleev method to solve the initial value problem (1). The presentation begins with the construction of the Mendeleev method in the second section. In the third and fourth sections, respectively, we derive the local truncation error and give the discussion of the stability of the proposed method. Furthermore, the fifth section performs the computational comparisons between the proposed method, Euler's method [2, p. 16] midpoint method [4, p. 28] Heun's method [2, p. 58] and Shampine's method [7]. A conclusion is given at the end of the discussion.

2. Mendeleev's Quadrature for Solving Initial Value Problems

Mendeleev's quadrature for computing a definite integral $\int_{x_i}^{x_{i+1}} f(x)dx$ gives two-sided approximations as follows [6]:

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{x_{i+1}-x_i}{4}\left(f(x_i)+3f\left(x_i+\frac{2}{3}(x_{i+1}-x_i)\right)\right), \tag{2}$$

and

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{x_{i+1}-x_i}{4}\left(3f\left(x_i+\frac{1}{3}(x_{i+1}-x_i)\right)+f(x_{i+1})\right). \tag{3}$$

Formulas (2) and (3) are called the left and right Mendeleev's quadratures, respectively.

Suppose that x lies in the interval $[x_0, x_0+\alpha]$, partitioned into n subintervals whose step size is $h = \frac{\alpha}{n}$, that is

$$x_i = x_0 + ih, \quad i = 0, \cdots, n.$$

Integrating both sides of (1) from x_i to x_{i+1} we obtain

$$Y(x_{i+1}) = Y(x_i) + \int_{x_i}^{x_{i+1}} f(s, Y(s))ds. \tag{4}$$

If we approximate the right-side integral of (4) with the right Mendeleev's quadrature (3), then we get

$$\int_{x_i}^{x_{i+1}} f(s, Y(s))ds = \frac{h}{4}\left(3f\left(x_i + \frac{h}{3}, Y\left(x_i + \frac{h}{3}\right)\right) + f(x_{i+1}, Y(x_{i+1}))\right), \quad (5)$$

where $h = x_{i+1} - x_i$.

By substituting (5) into the equation (4), we obtain

$$Y(x_{i+1}) = Y(x_i) + \frac{h}{4}\left(3f\left(x_i + \frac{h}{3}, Y\left(x_i + \frac{h}{3}\right)\right) + f(x_{i+1}, Y(x_{i+1}))\right). \quad (6)$$

The Taylor expansion of $Y(x_i + \frac{h}{3})$ about x_i is rewritten as

$$Y\left(x_i + \frac{h}{3}\right) \approx Y(x_i) + \frac{h}{3}Y'(x_i) = Y(x_i) + \frac{h}{3}f(x_i, Y(x_i)). \quad (7)$$

By replacing the value of $Y(x_i + \frac{h}{3})$ in (6) with approximation (7), we have

$$Y(x_{i+1}) = Y(x_i) + \frac{h}{4}\left(3f\left(x_i + \frac{h}{3}, Y(x_i) + \frac{h}{3}f(Y(x_i))\right) + f(x_{i+1}, Y(x_{i+1}))\right). \quad (8)$$

The differential equation $Y'(x) = f(x, Y(x))$ at $x = x_i$ is discretized as follows:

$$y(x_{i+1}) = y(x_i) + \frac{h}{4}\left(3f\left(x_i + \frac{h}{3}, y(x_i) + \frac{h}{3}f(y(x_i))\right) + f(x_{i+1}, y(x_{i+1}))\right), \quad (9)$$

so that we obtain the implicit Mendeleev's method to solve the initial value problem (1),

$$\left.\begin{array}{rcl} y_{i+1} &=& y_i + \frac{h}{4}(3f(x_i + \frac{h}{3}, y_i + \frac{h}{3}f(y_i)) + f(x_{i+1}, y_{i+1})), \\ y_0 &=& Y_0. \end{array}\right\} \quad (10)$$

The Taylor expansion of $Y_{(x_{i+1})}$ about $x_{i+1} = x_i$ can be written as

$$Y_(x_{i+1}) \approx Y_{(x_i)} + hY'_{(x_i)} = Y_{(x_i)} + hf(Y_{(x_i)}). \quad (11)$$

If the value of $Y_{x_{(i+1)}}$ on the right side of (8) is replaced by approximation (11), then we get the explicit Mendeleev's method

$$\left.\begin{array}{rcl} y_{i+1} &=& y_i + \frac{h}{4}(3f(x_i + \frac{h}{3}, y_i + \frac{h}{3}f(y_i)) + f(x_{(i+h)}, y_i + hf(y_i))), \\ y_0 &=& Y_0. \end{array}\right\} \quad (12)$$

Equation (12) can also be written as

$$y_{i+1} = y_i + \frac{h}{4}(3k_3 + k_2), \tag{13}$$

where

$$\begin{aligned} k_1 &= f(x_i, y_i), \\ k_2 &= f(x_i, y_i + hk_1), \\ k_3 &= f\left(x_i + \frac{h}{3}, y_i + \frac{h}{3}k_1\right). \end{aligned} \tag{14}$$

In a similar way, if we use the left Mendeleev's quadrature (2), then we get

$$\left.\begin{aligned} y_{i+1} &= y_i + \tfrac{h}{4}(f(x_i, y_i) + 3f(x_i + \tfrac{2}{3}h, y_i + \tfrac{2}{3}hf(y_i))), \\ y_0 &= Y_0. \end{aligned}\right\} \tag{15}$$

Formula (15) has been constructed by Shampine [7].

3. Local Truncation Error

Taylor expansion of $Y(x_{i+1})$ about $x_{i+1} = x_i$ can be written as

$$\begin{aligned} Y_{i+1} = Y_i + Y_i'(x_{i+1} - x_i) + \frac{1}{2}Y_i''(x_{i+1} - x_i)^2 + \frac{1}{6}Y_i'''(x_{i+1} - x_i)^3 \\ + O((x_{i+1} - x_i)^4). \end{aligned} \tag{16}$$

Suppose $f = f(Y_i)$ and $f_y = \frac{\partial f}{\partial Y}$, such that

$$Y_i' = f(Y_i) = f, \tag{17}$$

$$Y_i'' = \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial x} = f_y f, \tag{18}$$

$$Y_i''' = \left(\left(\frac{\partial^2 f}{\partial Y^2}\frac{\partial Y}{\partial x}\right)\frac{\partial Y}{\partial x} + \frac{\partial^2 Y}{\partial x^2}\frac{\partial f}{\partial Y}\right) = f^2 f_{yy} + f f_y^2. \tag{19}$$

If we substitute (17), (18), and (19) into (16), then we get

$$Y_{i+1} = Y_i + hf + \frac{1}{2}h^2 f f_y + \frac{1}{6}h^3(f^2 f_{yy} + f f_y^2) + O(h^4), \tag{20}$$

where $h = x_{i+1} - x_i$.

The Taylor expansions of the function k_2 in (14) about $y_i + hf = y_i$ and k_3 in (14) about $y_i + \frac{h}{3}f = y_i$ can be written respectively as

$$k_2 = f(y_i + hf) = f + hff_y + \frac{1}{2}h^2 f^2 f_{yy}, \tag{21}$$

and

$$k_3 = f(y_i + \frac{h}{3}f) = f + \frac{h}{3}ff_y + \frac{1}{2}\left(\frac{1}{3}\right)^2 h^2 f^2 f_{yy}. \tag{22}$$

If we substitute (21) and (22) into equation (13), then we obtain

$$y_{i+1} = y_i + hf + \frac{1}{2}h^2 ff_y + \frac{1}{6}h^3 f^2 f_{yy}. \tag{23}$$

To get the local truncation error *(LTE)* of the explicit Mendeleev's method, we calculate the difference between the numerical solution (23) and the exact solution (20)

$$LTE = Y_{i+1} - y_{i+1} = \frac{h^3}{6} ff_y. \tag{24}$$

The error formula (24) is affected by the step size h. The shorter the h, the smaller the generated error.

4. Stability Region

Looking at the differential equations (1), consider an example of the initial value problem (test problem) as follows [2, p. 128]:

$$\begin{aligned} Y'(x) &= \lambda Y(x), \quad x > 0, \\ Y(0) &= 1. \end{aligned} \tag{25}$$

The constant λ may be a complex number. The exact solution of the problem (25) is $Y(x) = e^{\lambda x}$.

If we use the explicit Mendeleev's method (12) to solve the problem (25), then we obtain

$$y_{i+1} = y_i + h\lambda y_i + \frac{1}{2}h^2\lambda^2 y_i. \tag{26}$$

By letting $h\lambda = z$, equation (26) can be written as

$$y_{i+1} = \left(1 + z + \frac{1}{2}z^2\right) y_i. \tag{27}$$

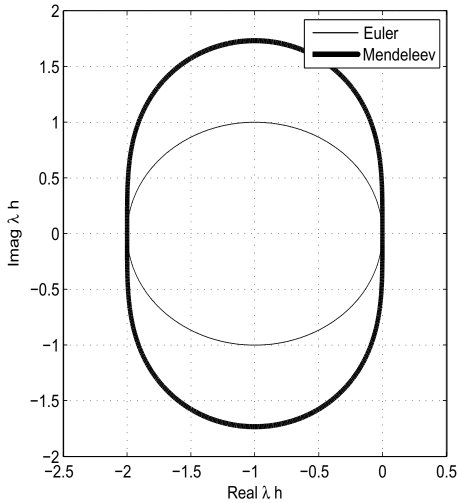

Figure 1. The stability regions of the Euler method and the explicit Mendeleev's method

Figure 1 shows that the stability region of the explicit Mendeleev's method is larger then that of the Euler method.

5. Numerical Results

In this section, we intend to compare the proposed method with other methods such as Euler's method, midpoint method, Heun's method and Shampine's method. We calculate the relative error of these examples using MATLAB v7.6 based on the number of n subintervals that varies.

Example 5.1. $Y'(x) = \frac{1}{Y(x)}, \quad 0 \leqslant x \leqslant 1, \quad Y(0) = 1$, with the exact solution $Y(x) = \sqrt{2x+1}$.

Example 5.2. $Y'(x) = \frac{1}{1+x^2} - 2(Y(x))^2, \quad 0 \leqslant x \leqslant 1, \quad Y(0) = 0$, with the exact solution $Y(x) = \frac{x}{1+x^2}$.

Example 5.3. $Y'(x) = (Y(x))^2(\ln x)^3 - 2xY(x)(\ln x)^4 + 2\ln x + 2, \quad 1 \leqslant x \leqslant 2$, $Y(1) = 0$, with the exact solution $Y(x) = 2x \ln x$.

Example 5.4. $Y'(x) = (Y(x))^2 + (2xY(x)+2)\sin^3(2x), \quad 1 \leqslant x \leqslant 2, \quad Y(1) = -1$, with the exact solution $Y(x) = -\frac{1}{x}$.

Table 1: The relative error ($\|Y_i - y_i\|_\infty$) for Example 5.1

n	Euler	Midpoint	Heun	Shampine	Mendeleev
8	0.02094	0.00081	0.00004	0.00052	0.00054
16	0.01018	0.00020	0.00000	0.00013	0.00013
32	0.00502	0.00005	0.00000	0.00003	0.00003
64	0.00249	0.00001	0.00000	0.00001	0.00001
128	0.00124	0.00000	0.00000	0.00000	0.00000

Table 2: The relative error ($\|Y_i - y_i\|_\infty$) for Example 5.2

n	Euler	Midpoint	Heun	Shampine	Mendeleev
8	0.03302	0.00182	0.00377	0.00232	0.00229
16	0.01604	0.00042	0.00087	0.00053	0.00053
32	0.00792	0.00010	0.00021	0.00013	0.00013
64	0.00394	0.00002	0.00005	0.00003	0.00003
128	0.00196	0.00001	0.00001	0.00001	0.00001

Table 3: The relative error ($\|Y_i - y_i\|_\infty$) for Example 5.3

n	Euler	Midpoint	Heun	Shampine	Mendeleev
8	0.09896	0.00045	0.00284	0.00073	0.00078
16	0.05050	0.00011	0.00068	0.00018	0.00018
32	0.02556	0.00003	0.00016	0.00004	0.00004
64	0.01286	0.00001	0.00004	0.00001	0.00001
128	0.00645	0.00000	0.00001	0.00000	0.00000

Table 4: The relative error ($\|Y_i - y_i\|_\infty$) for Example 5.4

n	Euler	Midpoint	Heun	Shampine	Mendeleev
8	0.02811	0.00158	0.00086	0.00121	0.00128
16	0.01324	0.00037	0.00017	0.00028	0.00029
32	0.00644	0.00009	0.00004	0.00007	0.00007
64	0.00318	0.00002	0.00001	0.00002	0.00002
128	0.00158	0.00001	0.00000	0.00000	0.00000

Tabel 1 shows that for Example 5.1, Heun's method is more accurate than the other methods. However, for Example 5.2, 5.3 and 5.4, the numerical results show that the relative error of the Mendeleev's method is smaller than the Euler's method, midpoint method and Heun's method.

Furthermore, the relative error is plotted againts the number of n subintervals as depicted in Figure 2.

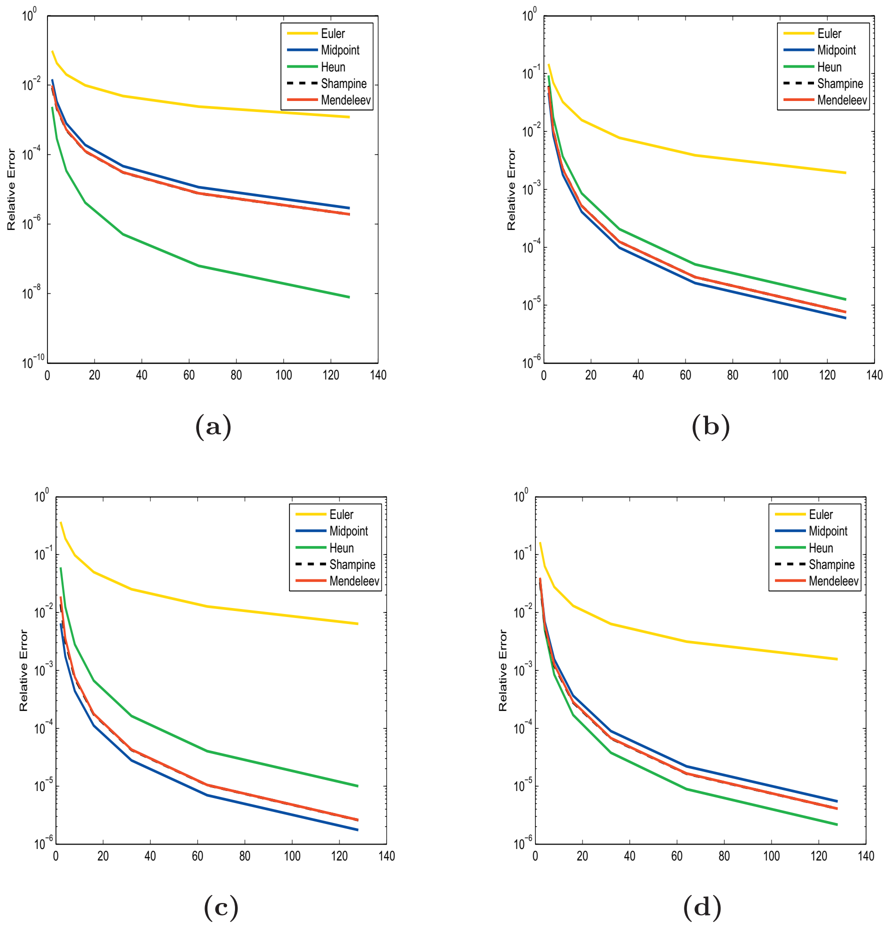

Figure 2. The relative error for IVP
(a) Example 5.1 (b) Example 5.2
(c) Example 5.3 (d) Example 5.4

6. Conclusion

Mendeleev's quadrature [6] can be used for solving initial value problems. Numerical results show that the proposed method is better than the Euler's method, midpoint method and Heun's method.

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