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An Unconditionally A-Stable Method for Initial Value Problems Based on Simpson's Rule[1]

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Abstract

In this paper we construct an algorithm to approximate the solution of the initial value problem $y'(t) = f(t, y)$ with $y(t_0) = y_0$. The method is implicit and combines the classical Simpson's rule with the Simpson's 3/8 rule to yield an unconditionally A-stable method of order 4.

Mathematics Subject Classification: 65L05

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1 Introduction

In this work we describe a numerical method based on Simpson's rule to approximate the solution of the initial value problem $y'(t) = f(t, y)$, where $f : \mathbb{R}^2 \to \mathbb{R}$ is a function of class C^1. As is well known, Simpson's rule has been used in numerical methods for the solution of initial value problems, (see [2], [3], [4], [6]). All of these methods are conditionally *A-stable*, requiring small steps for stiff problems in order to yield accurate approximations.

The method we propose in this paper combines Simpson's rule with Simpson's 3/8 rule to obtain an unconditionally *A-stable* algorithm. The procedure is not a multistep method, and differs from most one-step methods in the sense that it simultaneously yields 3 approximations of $y(t)$ at $t = t_0+h$, t_0+2h, and t_0+3h from the value $y(t_0)$. To accomplish 4th-order accuracy and *A-stability*, the algorithm solves a 3 by 3 system of algebraic equations.

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Simpson's 3/8 rule has been used in combination with Simpson's rule by Milne and Reynolds (see [3]) in order to improve the stability properties of a method proposed by Milne in [2].

2 Integration of $y'(t) = f(t, y)$ with Simpson's rule

In this section we describe how Simpson's rule and the Simpson's 3/8 rule are combined to approximate the solution of the initial value problem

$$\begin{aligned} y'(t) &= f(t, y(t)), \quad t \in [t_0, b], \\ y(t_0) &= y_0. \end{aligned} \tag{1}$$

The classical Simpson's rule approximates a definite integral of a function g as follows: let $t_0 < t_1 < t_2$ be three equally spaced points, and let $h = t_1 - t_0$. Then

$$\int_{t_0}^{t_2} g(t)dt \approx \frac{h}{3}\left[g(t_0) + 4g(t_1) + g(t_2)\right]. \tag{2}$$

Simpson's 3/8 rule approximates a definite integral of g requiring four equally spaced points: let $t_0 < t_1 < t_2 < t_3$ be equally spaced, with $h = t_1 - t_0$. The approximation takes the form

$$\int_{t_0}^{t_3} g(t)dt \approx \frac{3h}{8}\left[g(t_0) + 3g(t_1) + 3g(t_2) + g(t_3)\right]. \tag{3}$$

Both integration rules have an approximation error proportional to h^5 provided g is of class C^4 (see [7]). We now describe how this rules are used to discretize (1).

Let $t_0 < t_1 < t_2 < t_3$ be a regular partition of an interval $[t_0, t_0 + T_0]$, hence $t_k = t_0 + kh$ with $h = T_0/3$. Integrating both sides of (1) on $[t_0, t_2]$ we obtain

$$y(t_2) - y(t_0) = \int_{t_0}^{t_2} f(t, y(t))dt. \tag{4}$$

Applying Simpson's rule (2) to (4) we get the approximation

$$y(t_2) - y(t_0) \approx \frac{h}{3}\left(f(t_0, y(t_0)) + 4f(t_1, y(t_1)) + f(t_2, y(t_2))\right). \tag{5}$$

Similarly, integrating both sides of (1) on $[t_1, t_3]$ and approximating the integral with Simpson's rule we obtain

$$y(t_3) - y(t_1) \approx \frac{h}{3}\left(f(t_1, y(t_1)) + 4f(t_2, y(t_2)) + f(t_3, y(t_3))\right). \tag{6}$$

Integrating now both sides of (1) on $[t_0, t_3]$ and using Simpson's 3/8 rule to approximate the integral,

$$y(t_3) - y(t_0) \approx \frac{3h}{8}\left(f(t_0, y(t_0)) + 3f(t_1, y(t_1)) + 3f(t_2, y(t_2)) + f(t_3, y(t_3)))\right). \tag{7}$$

Given the initial value $y_0 = y(t_0)$, to obtain approximations y_1 to $y(t_1)$, y_2 to $y(t_2)$, and y_3 to $y(t_3)$, from (5)-(7) we set a system of three algebraic equations with the three unknowns y_1, y_2, y_3:

$$\begin{aligned} y_2 - y_0 &= \frac{h}{3}\left(f(t_0, y_0) + 4f(t_1, y_1) + f(t_2, y_2)\right) & (8)\\ y_3 - y_1 &= \frac{h}{3}\left(f(t_1, y_1) + 4f(t_2, y_2) + f(t_3, y_3)\right) & (9)\\ y_3 - y_0 &= \frac{3h}{8}\left(f(t_0, y_0) + 3f(t_1, y_1) + 3f(t_2, y_2) + f(t_3, y_3)\right). & (10) \end{aligned}$$

The above system of equations can be written in the form $F_h(y_1, y_2, y_3) = (0, 0, 0)$. The Jacobian matrix of F_h is given by

$$F_h' = \begin{pmatrix} -\frac{4h}{3}\frac{\partial f}{\partial y_1}(t_1, y_1) & 1 - \frac{h}{3}\frac{\partial f}{\partial y_2}(t_2, y_2) & 0 \\ -1 - \frac{h}{3}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{4h}{3}\frac{\partial f}{\partial y_2}(t_2, y_2) & 1 - \frac{h}{3}\frac{\partial f}{\partial y_3}(t_3, y_3) \\ -\frac{9h}{8}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{9h}{8}\frac{\partial f}{\partial y_2}(t_2, y_2) & 1 - \frac{3h}{8}\frac{\partial f}{\partial y_3}(t_3, y_3) \end{pmatrix}. \tag{11}$$

Hence, $F_h' = A + hB$, where

$$A = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} -\frac{4}{3}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{1}{3}\frac{\partial f}{\partial y_2}(t_2, y_2) & 0 \\ -\frac{1}{3}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{4}{3}\frac{\partial f}{\partial y_2}(t_2, y_2) & -\frac{1}{3}\frac{\partial f}{\partial y_3}(t_3, y_3) \\ -\frac{9}{8}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{9}{8}\frac{\partial f}{\partial y_2}(t_2, y_2) & -\frac{3}{8}\frac{\partial f}{\partial y_3}(t_3, y_3) \end{pmatrix}.$$

If f is of class C^1, and if $(t_1, t_2, t_3, y_1, y_2, y_3)$ is restricted to a bounded set in $\mathbb{R}^6$, there exists $\epsilon > 0$ such that if $0 < h < \epsilon$, then F_h' is invertible since A is invertible. By the inverse function theorem F_h is locally invertible. Furthermore, we have the folowing result:

Theorem 2.1 *If f is of class C^1, the system of algebraic equations (8)-(10) has a unique solution in a neighborhood of (y_0, y_0, y_0) for h sufficiently small.*

Proof

Substracting equation (9) from (10) and reordering the equations, we obtain an equivalent system of the form

$$\begin{aligned} y_1 - y_0 &= hg_1(t_0, t_1, t_2, t_3, y_0, y_1, y_2, y_3) && (12)\\ y_2 - y_0 &= hg_2(t_0, t_1, t_2, t_3, y_0, y_1, y_2, y_3) && (13)\\ y_3 - y_0 &= hg_3(t_0, t_1, t_2, t_3, y_0, y_1, y_2, y_3). && (14) \end{aligned}$$

where $g_1 = (3f(t_0, y_0)+19f(t_1, y_1)-5f(t_2, y_2)+f(t_3, y_3))/24$, $g_2 = (f(t_0, y_0)+4f(t_1, y_1)+f(t_2, y_2))/3$, and $g_3 = 3(f(t_0, y_0)+3f(t_1, y_1)+3f(t_2, y_2)+f(t_3, y_3))/8$. Here g_1, g_2 y g_3 are of class C^1 sice they are linear combinations of evaluations of f. This system of equations can be written in the form $\boldsymbol{y}-W_h(\boldsymbol{y}) = \boldsymbol{0}$, with $\boldsymbol{y} = (y_1, y_2, y_3)$. The Jacobian matrix of W_h is of the form $W_h'(\boldsymbol{y}) = hS(\boldsymbol{y})$ where

$$S(\boldsymbol{y}) = \begin{pmatrix} \frac{19}{24}\frac{\partial f}{\partial y_1}(t_1, y_1) & -\frac{5}{24}\frac{\partial f}{\partial y_2}(t_2, y_2) & \frac{1}{24}\frac{\partial f}{\partial y_3}(t_3, y_3) \\ \frac{4}{3}\frac{\partial f}{\partial y_1}(t_1, y_1) & \frac{1}{3}\frac{\partial f}{\partial y_2}(t_2, y_2) & 0 \\ \frac{9}{8}\frac{\partial f}{\partial y_1}(t_1, y_1) & \frac{9}{8}\frac{\partial f}{\partial y_2}(t_2, y_2) & \frac{3}{8}\frac{\partial f}{\partial y_3}(t_3, y_3) \end{pmatrix}.$$

Due to the continuity of $\dfrac{\partial f}{\partial y}$, the entries of S are bounded when h and $\boldsymbol{y}$ are restricted to bounded sets. When h is close to zero, the vector (t_1, t_2, t_3) is close to (t_0, t_0, t_0), and $W_h(\boldsymbol{y})$ is close to $\boldsymbol{y}_0 = (y_0, y_0, y_0)$. By continuity of W_h it can be seen that if $\overline{B}_1(\boldsymbol{y}_0)$ is the closed ball of radius 1 centered at $\boldsymbol{y}_0$, then there exists $\epsilon > 0$ such that if $0 < h < \epsilon$, then $W_h(\overline{B}_1(\boldsymbol{y}_0)) \subset \overline{B}_1(\boldsymbol{y}_0)$. Moreover, by the continuity of $\dfrac{\partial f}{\partial y}$, the Frobenius norm of $W_h'(\boldsymbol{y})$ is strictly less than 1/2 for all $\boldsymbol{y} \in \overline{B}_1(\boldsymbol{y}_0)$. Therefore W_h is a contraction map (see [5]), which implies that if $0 < h < \epsilon$ there exists $\boldsymbol{y} \in \mathbb{R}^3$ such that $W_h(\boldsymbol{y}) = \boldsymbol{y}$. It follows that there is $\boldsymbol{y} \in \mathbb{R}^3$ such that $\boldsymbol{y} - W_h(\boldsymbol{y}) = \boldsymbol{0}$. This proves that the system of equations (12)-(14) or equivalently, the system (8)-(10) has a unique solution for h sufficiently small. □

Equations (8)-(10) can be solved numerically by means of Newton's method using y_0 as an initial approximation for each of the unknowns y_1, y_2, y_3, and using finite differences to approximate the Jacobian matrix (11).

To build now approximations to $y(t)$ with $t \in [t_3, t_3 + T_1]$, one applies the previous procedure to the regular partition $t_3 < t_4 < t_5 < t_6$ using y_3 as an initail value and $h = T_1/3$ as the distance between consecutive points of the partition. It can be seen that the accuracy of this method is $O(h^4)$ when applied in an interval $[t_0, t_0 + T]$ using a regular partition with $n+1$ points, and $h = T/n$.

otra manera arbitrario; otro implícito método de (**??**) se debe resolver preguntar método numéricos

2.1 ***A-stability*** of the method

The concept of *A-stability* of a numerical method for initial value problems is useful in the numerical solution of stiff problems (see [1]). The method given by (8)-(10), to which we will refer as Simpson's 3/8, is unconditionally *A-stable* if for any step size $h > 0$ the sequence y_j produced by the algorithm when applied to the initial value problem $y'(t) = -\lambda y(t)$, $y(0) = y_0$, satisfies $y_j \to 0$ as $j \to \infty$ for any complex number λ with positive real part. The following results shows the *A-stability* of the method.

Theorem 2.2 *The Simpson's 3/8 method given by (8)-(10) is unconditionally A-stable.*

Proof

Let $h > 0$ be any step size, and let λ be any complex number with positive real part. Applying Simpson's 3/8 method to the problem $y'(t) = -\lambda y(t)$, $y(0) = y_0$, we obtain approximations y_j to $y(jh)$ satisfying:

$$y_2 - y_0 = \frac{-\lambda h}{3}\left(y_0 + 4y_1 + y_2\right) \tag{15}$$

$$y_3 - y_1 = \frac{-\lambda h}{3}\left(y_1 + 4y_2 + y_3\right) \tag{16}$$

$$y_3 - y_0 = \frac{-3\lambda h}{8}\left(y_0 + 3y_1 + 3y_2 + y_3\right). \tag{17}$$

Solving the system for y_1, y_2, y_3, and defining $z = \lambda h = x + iy$, we obtain

$$y_1 = y_0\left(\frac{-z^2 + 6z - z^3 + 12}{3z^3 + 18z + 11z^2 + 12}\right) = y_0 A_z, \tag{18}$$

$$y_2 = y_0\left(\frac{-z^2 - 6z + z^3 + 12}{3z^3 + 18z + 11z^2 + 12}\right) = y_0 B_z, \tag{19}$$

$$y_3 = y_0\left(\frac{-3z^3 + 11z^2 - 18z + 12}{3z^3 + 18z + 11z^2 + 12}\right) = y_0 C_z. \tag{20}$$

Therefore we obtain that for $j = 0, 1, 2, 3, ...,$

$$y_{3j+1} = y_0 A_z (C_z)^j, \tag{21}$$
$$y_{3j+2} = y_0 B_z (C_z)^j, \tag{22}$$
$$y_{3j+3} = y_0 (C_z)^{j+1}. \tag{23}$$

Hence the method is unconditionally *A-stable* if and only if $|C_z| < 1$ for all complex number $z = x + iy$ with positive real part. The condition $|C_z| < 1$ is equivalent to

$$\frac{r_1 + r_2}{r_3 + r_4} < 1, \tag{24}$$

where

$$r_1 = (3x^3 - 9xy^2 - 11x^2 + 11y^2 + 18x - 12)^2, \tag{25}$$
$$r_2 = (9x^2y - 3y^3 - 22xy + 18y)^2, \tag{26}$$
$$r_3 = (3x^3 - 9xy^2 + 11x^2 - 11y^2 + 18x + 12)^2, \tag{27}$$
$$r_4 = (9x^2y - 3y^3 + 22xy + 18y)^2. \tag{28}$$

A calculation shows that

$$r_1 + r_2 - r_3 - r_4 = -864x - 936x^3 - 360xy^2 - 264x^3y^2 - 132xy^4 - 132x^5,$$

which is always negative for all $y \in \mathbb{R}$ if $x > 0$. This implies that

$$0 < r_1 + r_2 < r_3 + r_4, \text{ for all } x > 0.$$

Therefore $\frac{r_1 + r_2}{r_3 + r_4} < 1$ for all $z = x + iy$ with $x > 0$. This shows that the method is unconditionally *A-stable*. □

3 Numerical experiments

To test the performance of Simpson's 3/8 algorithm (8)-(10), we have compared the method with the classical 4th-order implicit Runge-Kutta method based on the Gauss-Legendre quadratures (IRKGL4) (see [1]). We used Newton's method to solve the algebraic system of equations, and the Jacobian matrices were approximated by means of finite differences. A drawback of our algorithm is that the number of steps n is required to be of the form $n = 3m$ with m integer. In general we have observed that IRKGL4 gives approximately one more significant digit of accuracy than our algorithm when we use the same number of step size h. On the other hand, for the same number of steps, IRKGL4 requires more evaluations of the function f. When we tested both algorithms using approximately the same number of function evaluations, the accuracy of our algorithm is slightly better than IRKGL4.

Example 1. Consider the problem $y'(t) = -100y + 101e^t$, $t \in [0, 1]$, with $y(0) = 99/100$. The exact solution of this equation is $y(t) = -\frac{e^{-100t}}{1000} + e^t$. Table (1) shows the results of both algorithms when we use the same number n of steps. The step size in this case is $h = 1/n$. The accuracy of the algorithms was calculated with the relative error using the exact solution and the euclidian norm: Error $= \frac{\sqrt{\sum_{j=0}^{n} |y_j - y(jh)|^2}}{\sqrt{\sum_{j=0}^{n} |y(jh)|^2}}$.

Observe that IRKGL4 yields one more digit of accuracy than the method of Simpson's 3/8. On the other hand, the number of function evaluations (FE) is higher in IRKGL4. Table (2) shows the results of both algorithms when they use approximately the same number of function evaluations. In this case the accuracy of Simpson's 3/8 is higher than IRKGL4.

n	Error, IRKGL4	Error, Simpson's 3/8	FE, IRKGL4	FE, Simpson's 3/8
30	3.67×10^{-5}	1.61×10^{-4}	300	180
120	1.91×10^{-7}	1.76×10^{-6}	1200	480
300	4.81×10^{-9}	4.44×10^{-8}	3000	1200

Table 1: Comparison between Simpson's 3/8 method and the IRKGL4 method corresponding to Example 1. Here n is the number of steps on [0,1], FE = number of function evaluations, the error was calculated using the exact solution and the euclidian norm. In this example IRKGL4 has an error smaller than Simpson's 3/8 by approximately a factor of 10. The number of FE is higher in IRKGL4.

FE,IRKGL4	n-IRKGL4	Error, IRKGL4	FE, S3/8	n-S3/8	Error, S3/8
300	30	3.67×10^{-5}	300	25	1.03×10^{-5}
1200	120	1.91×10^{-7}	1200	100	4.44×10^{-8}
3000	300	4.81×10^{-9}	3000	250	1.1×10^{-9}

Table 2: Comparison between Simpson's 3/8 method (abbreviated in this table as S3/8) and the IRKGL4 method based on the number of function evaluations FE in Example 1. Here n-IRKGL4 is the number of steps on [0,1] for the IRKGL4 method. In this case the error in Simpson's 3/8 is smaller than in IRKGL4.

Example 2 (Taken from [7]). Consider the problem $y'(t) = -200ty^2$, $t \in [-1, 0]$, with $y(-1) = 1/101$. The exact solution of this equation is $y(t) = \frac{1}{1 + 100t^2}$. The results are presented in Tables (3) and (4).

n	Error, IRKGL4	Error, Simpson's 3/8	FE, IRKGL4	FE, Simpson's 3/8
60	2.01×10^{-5}	2.33×10^{-4}	892	486
120	1.26×10^{-6}	1.15×10^{-5}	1680	954
600	2.01×10^{-9}	1.70×10^{-8}	8384	3600

Table 3: Comparison between Simpson's 3/8 method and the IRKGL4 method corresponding to Example 2. Here n is the number of steps on [-1,0]. Again, in this example IRKGL4 has an error smaller than Simpson's 3/8 by approximately a factor of 10. The number of FE is higher in IRKGL4.

FE,IRKGL4	n-IRKGL4	Error, IRKGL4	FE, S3/8	n-S3/8	Error, S3/8
892	60	2.01×10^{-5}	882	111	1.59×10^{-5}
1680	120	1.26×10^{-6}	1674	276	3.96×10^{-7}
8384	600	2.01×10^{-9}	8268	1380	6.15×10^{-10}

Table 4: Comparison between Simpson's 3/8 method (S3/8) and the IRKGL4 method based on the number of function evaluations FE in Example 2. Here n-IRKGL4 is the number of steps on [-1,0] for the IRKGL4 method. As in Example 1, the error in Simpson's 3/8 is smaller than in IRKGL4.

4 Conclusions

We have proposed a 4th-order unconditionally A-stable method based on Simpson's rule to approximate the solution of initial value problems. The competitiveness of the method is shown by comparing it with another 4th-order unconditionally A-stable method, the implicit Runge-Kutta method based on the Gauss-Legendre quadratures (IRKGL4). Although the latter method gives approximation errors smaller than our method by a factor of 10 when they use the same number of steps, our method uses less function evaluations. Testing both algorithms in terms of function evaluations results in a smaller error of our algorithm than the on in IRKGL4. A drawback of our algorithm is that the number of steps n is required to be of the form $n = 3m$ with m integer. Numerical results for the vector form of the initial value problem will be reported in the future.

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