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Numerical Methods of Solving Stiff Ordinary Differential Equations

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Abstract

This paper describes the stiff differential equation where two numerical methods were employed, that is, Forward Interpolation and Asymptotic Form. Two numerical examples were considered with the use of Mathematical Software (MATLAB 2009b) to illustrate the performance of the methods. Hence, the conclusions were drawn from the tabulated results.

Keyword: Stiff, Forward Interpolation, Asymptotic form, Ordinary Differential Equation(ODE)

1.0 Introduction

In Mathematics, a stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small.

In the study of chemical genetics, electrical circuit theory, and problems of missile guidance a type of differential equation arises which is exceedingly difficult to solve by ordinary numerical procedures. A very satisfactory method of solution of these equations is obtained by making use of a forward interpolation process. This scheme has the unusual property of singling out and approximating a particular solution of the differential equation to the exclusion of the manifold of other solutions. This behaviour may be explained by a simple geometrical interpretation of the significance of the forward interpolation process [1].

The notion of the pseudo-stationary state of a stiff equation is said to be an equation representing the rate of formation of free radicals in a complex chemical reaction. That is, the free radicals are created and destroyed so rapidly compared to the time scale for the over-all reaction that to a first approximation the rate of production is equal to the rate of depletion.

To give some flexibility in computation, Backward differentiation formulae were derived [2, 3, 4]. Also, the work on Component wise Block partitioning were verify and compared [5] . Hence, algorithm has been designed to facilitate switching between the existing and this method during the integration process. The method described in the present paper provides a means for obtaining solutions to equations of this type to any degree of accuracy.

Consider the first Order Differential Equation

$$dy/_{dx} = \left[\frac{y-Q(x)}{\propto(x,y)}\right] \qquad (1)$$

Where the right hand side of this equation represents a general function of x and y which for each value of x has a root, $y = Q(x)$.

If Δx is the desired resolution of x or the interval which will be used in the numerical integration,

The equation is "stiff" if

$$\left|\frac{\propto(x,y)}{\Delta x}\right| \leq 1 \qquad (2)$$

And $Q(x)$is well behaved, that is it varies with x considerably more slowly than does $\exp^{(x/\alpha(x,Q(x)))}$

From eq(i), it appears that if $\propto (x,y)$is sufficiently small there is a solution, $y = Y(x)$, which lies close to $y = Q(x)$. To a first approximation, Y is given by $Y^{(1)}$,

$$Y^{(1)} = Q + \propto (x,Q)\frac{dQ}{dx} \qquad (3)$$

The second approximation, $Y^{(2)}$, is obtained by substituting $Y^{(1)}$ for y in $dy/_{dx}$ and in $\propto (x,y)$,

$$Y^{(2)} = Q + \propto \left(x, Y^{(1)}\right)\frac{dY^{(1)}}{dx} \qquad (4)$$

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If $\propto (x, y)$does not depend upon y, we can write down the resulting expression for Y,

$$Y = \sum_{i=0}^{\infty} \frac{D^i Q}{Dx^i} \tag{5}$$

Where $D/_{Dx}$ is the differential operator, $\propto (x)\, d/_{dx}$. whereas, the function Y(x) remain close to Q(x), every other solution deviates exponentially.

This can be seen by subtracting the differential equation for Y from equation (1). In the region about Y(x) (assuming that $\propto (x, y)$ varies slowly with y),

$$\propto \left(x, Y(x)\right) \frac{d(y-Y)}{dx} = (y - Y) \tag{6}$$

This integration gives

$$y - Y = Ce^{\left[\int \frac{dx}{\propto (x, Y(x))}\right]} \tag{7}$$

Where C is a constant of integration.

2.0 Methods of solving Stiff Ordinary Differential Equation

The numerical procedure described here can easily be extended to sets of simultaneous first order differential equations. The differential equations can also be uncoupled by introducing suitable linear combinations of the original dependent variables. Though, some of the uncoupled equations may be stiff in which case they can be integrated by the methods discussed below:

i. Forward Interpolation(FI):

Let $x_{0,} x_i .....x_n$ ...... be a set of values of x spaced a distance d_n between successive points. Then, the subscript on any quantity indicates that it is evaluated at the corresponding value of x. Then, evaluate y_n from knowledge of y at the previous points, that is, $y(x)$ can be approximated locally by a straight line has the slope:

$$(y')_n = \frac{y_n - y_{n-1}}{\Delta_n} \tag{8}$$

Using eq. (8) in evaluating eq (1) at the forward point to obtains

$$(y^1)_n = \frac{y_n - y_{n-1}}{\Delta_n} = \frac{y_n - Q_n}{\propto (y_n,\ x_n)} \tag{9}$$

Thus,

$$y_n = \frac{Q_n - \alpha\ (x_n,\ y_n)}{1 - \frac{\alpha\ (x_n, y_n)}{\Delta x}} \tag{10}$$

$\propto (x, y)$ does not depend upon the value of γ, equation 10 gives an explicit solution of y_n in terms of $y_{n-1;}$ otherwise, equation (10) gives an implicit relationship between y_n and y_{n-1}.

Hence, starting from a point $(x_{0,} y_0)$, equation (10) provides a numerical solution to the differential equation, in equation (1) . Since, the slope for a stiff equation has a reasonable value (neither of $Q_{(x)}$ or $y_{(x)}$), it is clear that this numerical integration scheme limits us to approximating$y_{(x)}$.

Though, it is very difficult to integrate ‘stiff’ equations by ordinary numerical methods. Small errors are rapidly magnified if the equations are integrated in the direction such that the family of solutions horn out, whereas the numerical solutions oscillate violently about Y(x) if the integration is carried out in the opposite direction.

ii. Asymptotic form:

If $\propto (x, y)$ is a function only of x, the procedure in numerical form leads to an approximate of y.

That is,

$$Q_n = y_n - \propto (x_n)\, (dy/dx)_n \tag{11}$$

Eq2: 10 can be rewritten in the form.

$$y_n - Y_n = -\left(\frac{\frac{\propto (x_n)}{\Delta x}}{1 - \frac{\propto (x_n)}{\Delta x}}\right)[y_{n-1} - Y_{n-1} + e] \tag{12}$$

Where

$$e = -Y_n + Y_{n-1} + \Delta x \left(\frac{dY}{dx}\right)_n \tag{13}$$

Expanding Y and $\frac{dY}{dx}$ in Taylor series about the point, x_{n-1}, it follows that

$$e = \frac{1}{2}(\Delta x)^2 \left(\frac{d^2 Y}{dx^2}\right)_{n-1} + \frac{1}{3}(\Delta x)^3 \left(\frac{d^3 Y}{dx^3}\right)_{n-1} + \cdots \tag{14}$$

The smaller the intervals, Δx, the smaller the error.

The error in the asymptote of the series may be reduced by using a three point formula for $\left(\frac{dy}{dx}\right)_n$ in which y is fit to a quadratic passing through $y_{n,}\ y_{n-1}\ and\ y_{n-2}$. Since the slope is evaluated at x_n, the same sort of forward interpolation is used as in the linear approximation. In place of equation (10), one obtains the following relation:

$$y_n = \frac{Q_n - 2\frac{\propto(x_n, y_n)}{\Delta x} y_{n-1} + \frac{1}{2}\frac{\propto(x_n, y_n)}{\Delta x} y_{n-3}}{1 - \frac{3}{2}\frac{\propto(x_n, y_n)}{\Delta x}} \tag{15}$$

In this case the difference between y_n and Y_n is given by

$$y_n - Y_n = \left(\frac{\frac{\propto(x_n)}{\Delta n}}{1 - \frac{3}{2}\frac{\propto(x_n)}{\Delta x}}\right) \times \left[\begin{array}{c} -2(y_{n-1} - y_{n-1}) + \frac{1}{2}(y_{n-2} - y_{n-2}) - \frac{1}{3}(\Delta x)^3 \left(\frac{d^3Y}{dx^3}\right)_{n-1} \\ -\frac{1}{12}(\Delta x)^4 \left(\frac{d^4Y}{dx^4}\right)_{n-2} + \cdots \end{array}\right] \tag{16}$$

Hence, the asymptotic form is approximately

$$y = Y + \propto(x)\left[\frac{2}{9}(\Delta x) \quad \left(\frac{d^3Y}{dx^3}\right) \quad + \frac{1}{18}(\Delta x)^3 \frac{d^4Y}{dx^4} + \ \ldots\right] \tag{17}$$

A geometrical argument of y_n approximates Y_n follows the same line as for the linear case.

3.0 Numerical Examples

We consider here some selected examples for experimentation with the methods derived in this paper, that is, forward integration and asymptotic form. The experiments were carried out by the Mathematical software (MATLAB 2009b) and the results were presented in the numerical solution of the next section.

In this section, some of the test problems were given

i. $y_1' = -1002y_1 - 1000y_2; \quad y_1(0) = 1 \quad 0 \le x \le 20$

$y_2' = y_1 - y_2(1 + y_2); \quad y_2(0) = 1$

The exact solutions are:

$y_1(x) = e^{-2x} \qquad y_2(x) = e^{-x}$

ii. $y_1' = -10y_1 + 100y_2; \quad y_1(0) = 0 \quad 0 \le x \le 20$

$y_2' = -100y_1 - 10y_2; \quad y_2(0) = 1$

$y_3' = -4y_3 \quad ; \quad y_3(0) = 1$

$y_4' = -y_4 \quad ; \quad y_4(0) = 1$

$y_5' = -0.5y_5 \quad ; \quad y_5(0) = 1$

$y_6' = -0.1y_6 \quad ; \quad y_6(0) = 1$

The exact solutions are:

$$y_1(x) = e^{-10x}\sin(100x)$$
$$y_2(x) = e^{-10x}\cos(100x)$$
$$y_3(x) = e^{-4x}$$
$$y_4(x) = e^{-x}$$
$$y_5(x) = e^{-0.5x}$$
$$y_6(x) = e^{-0.1x}$$

4.0 Numerical Solutions

The numerical results for the problem tested were tabulated below:

Table 1: Numerical results for problem 1

Limit	Method	Step	Stiff equation [i ; x ; n]	Max error	Time
10^{-2}	FI	30	[1; 0.022805; 5] [2 ;0.001715; 6]	7.5033E-03	7.13E-05
	AF	28	[1; 0.022805; 5]	1.1793E-04	7.80E-05
10^{-4}	FI	50	[1; 0.013582; 8] [2 ;0.020357; 12]	3.1105E-06	8.77E-05
	AF	43	[1; 0.013582; 8]	2.8144E-06	9.61E-05

Table 2: Numerical Results of problem 2

Limit	Method	Step	Stiff equation [i ; x ; n]	Max error	Time
10^{-2}	FI	100	[1; 0.00472; 7] [2 ;0.00483; 7] [3; 2.99872; 74] [4; 7.98534; 92]	1.3725E-04	4.562E-04
	AF	92	[1; 0.00472; 7]	2.9321E-04	5.968E-04
10^{-4}	FI	452	[1; 0.00281; 15] [2 ;0.00281; 15] [3; 9.69452; 648] [4; 5.60065; 635]	8.2063E-06	2.5671E-03
	AF	43	[1; 0.00281; 15]	1.0172E-06	2.4969E-03

5.0 Conclusion

The result generally show that Jacobian matrix is smaller and hence require less number of matrix operation in order to evaluate the Jacobian Matrix.

As an illustration, consider the numerical results of the problem I for limit $= 10^{-2}$ when the first instability occurs at x = 0.022805on the 9th step only the first equation, equations in the system is treated as stiff and the second equation remains in the non-stiff subsystem and solved using forward integration then. The second equation is treated as stiff on 6th step when x = 0.022805 using asymptotic firm.

In problem list 2 for limit$= 10^{-2}$, the first and second equations are changed to stiff system. Then on the 7th step, the third equation is placed in the stiff subsystem and the forward equation at the 95th step. Equation five and six remain in non-stiff until end of the integration. The same situation happens to other problems for all limits

In conclusion, this paper demonstrated that it is favourable to use both the forward interpolation and asymptotic firm in solving and treating the system of ordinary differential equation as a stiff to all equations when compared results with the solving stiff ODEs using componentwise Block Partitioning methods[5].

6.0 References

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