THE NUMERICAL SOLUTIONS OF SYSTEMS OF STIFF ORDINARY DIFFERENTIAL EQUATIONS

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Abstract

In this paper, some numerical methods such as semi-implicit extrapolation, Picard iterative scheme, Rosenbrock and Gear's methods were used to obtain the approximate solutions of both linear and nonlinear systems of first order initial value problems of stiff ordinary differential equations. Some systems of stiff differential equations were numerically solved with these methods and the obtained results were compared with the exact solutions where feasible. The results show that the semi-implicit extrapolation method, Rosenbrock and Gear's methods are convergent, accurate and works very well for the first order system of stiff ordinary differential equations considered while the Picard iterative scheme requires the step sizes to be extremely small.
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1. Introduction

Many initial value problems involving systems of stiff ordinary differential equations do occur in different fields of engineering sciences, particularly in the studies of the chemical reactions, the turbulent flow, chaos, vibrations, network analysis, simulation problems and so on [10].
Systems of ordinary differential equations with the initial conditions are usually given in the form;

$$Y'(t) = F(t, Y), t \in [0, T] \tag{1}$$

$$Y(0) = Y_0, \tag{2}$$

with the theoretical or exact solution given in the form $Y_e(t)$ [10].
where $Y(t) = (y_1, y_2, \cdots, y_n)^T$, $F = (f_1, f_2, f_3, \cdots, f_n)^T$, $Y'(t) = (y'_1, y'_2, \cdots, y'_n)^T$ and $Y_0 = (y_{0,1}, y_{0,2}, \cdots, y_{0,n})^T$.

Stiff ordinary differential equations are physical processes whose components have disparate time scales or whose time scale is small compared to interval over which it is studied [7]. When the general solution of first order ordinary differential equations involves the sums or differences of terms of the form $a_i e^{\lambda_i(t)}, (i = 1, 2, \cdots, n)$ where $\lambda_1, \lambda_2, \cdots, \lambda_n$ are eigenvalues in case of systems of stiff ordinary differential equations usually with negative values of large or small magnitudes [3], such equations are called the systems of stiff ordinary differential equations. The stiff problems usually involve the $Re(\lambda_i) < 0$ for $(i = 1, 2, \cdots, n)$ to decay exponentially fast as the time scale increases [5].

Stiff ordinary differential equations can be solved analytically where feasible and approximate numerical solutions can also be determined. When the equations are linear, the theoretical solutions can be easily determined with all the known analytical methods of solving ordinary differential equations [6]. But in the case of the non-linear equations of stiff ordinary differential equations, the theoretical solutions may not be easily obtained except by finding their approximate solutions numerically. The difficulty that arises in attempting to obtain a numerical approximation to the solution $Y(t)$ of a stiff equation is that of its numerical stability [8]. In order to obtain the numerical solutions of such equations, it is necessary to use a step size h such that every one of the values $h_i = h\lambda_i (i = 1, 2, \cdots, s)$ where λ_i are the eigenvalues $J(x)$ or $\frac{\partial F}{\partial Y}$ (Jacobian matrix) lies within the region of stability of the numerical method [1].

Most realistic stiff equations do not have analytical solutions and so only the numerical procedures have to be used. The conventional methods like explicit Euler's method, explicit fourth order Runge Kutta method, Taylor's series, Picard iterative scheme and so on are usually restricted to a very small step size in order that the solution be stable [7]. This means that a great deal of computer time shall be required. To overcome this stability limitation on the step size, we applied the semi-implicit extrapolation method, Rosenbrock and Gear's methods to obtain the numerical solutions of some linear and nonlinear problems considered in [4]. These methods ensure that the approximate solutions to the equations decay exponentially as the number of iterations increase [3].

2. Description of the Methods

2.1 Semi-implicit extrapolation method (SIEM)

The semi-implicit extrapolation method is obtained from the combination of the semi-implicit Euler's method and the semi-implicit midpoint rule. For details on this see [2].

2.2 The Picard's Iteration Scheme (PIS)

Let us consider the initial value problem (IVP) as given in equations (1) and (2). This has a formal solution of the form;

$$Y(t) = Y_0 + \int_{t_0}^{t} f(\tau, y(\tau)) d\tau. \tag{3}$$

An iterative procedure for the Picard iterative scheme is as follows;

- guess $Y_0(t)$ (usually $Y_0(t) = Y_0$);
- compute $Y_1(t) = Y_0 + \int_{t_0}^{t} f(\tau, Y_0(\tau))d\tau$;
- compute $Y_2(t) = Y_0 + \int_{t_0}^{t} f(\tau, Y_1(\tau))d\tau$;
- and, at step n, we have compute $Y_n(t) = Y_0 + \int_{t_0}^{t} f(\tau, Y_{n-1}(\tau))d\tau$.

2.3 The Rosenbrock's method (RM)

Rosenbrock proposed to generalize the linearly implicit approach to methods using more stages so as to achieve a higher order of consistency. The crucial consideration put forth was to no longer use the iterative Newton method, but instead to derive stable formulas by working the Jacobian matrix directly into the integration formula. His idea has found widespread use and a generally accepted formula [8] for a so called s-stage Rosenbrock method given in the form:

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i \tag{4}$$

$$k_i = hf(y_n + \sum_{j=1}^{i-1} \alpha_{ij} k_j) + hJ \sum_{j=1}^{i} \gamma_{ij} k_j \tag{5}$$

where s and the formula coefficients b_i,α_{ij} and γ_{ij} are chosen to obtain a desired order of consistency and stability for stiff problems. We can take the coefficients γ_{ii} equal for all stages i.e. $\gamma_{ii} = \gamma$ for all $i = 1, 2, ..., s$.

2.4 The Gear's method (GM)

The Gear algorithm is one of the class of methods referred to as backward differentiation formulae (BDF). The generalized BDF that forms the basis for Gear's method can be expressed as follows:

$$Y_n = h\beta_0 f(Y_n, t_n) + \sum_{j=1}^{p} \alpha_j Y_{n-j} \tag{6}$$

where n is the number of iterations, h is the time step size, p is the assumed order, β_0 and α_j are scalar quantities that are functions of the order and $F(t, Y)$ is the function which describes the rate of change [3].

3. Numerical Illustrations

In this section, we shall illustrate the efficiency of these methods as a novel solver for the systems of stiff ordinary differential equations. In order to do so, four different problems were selected as test problems. In this, two problems were selected to be linear systems with two and four variables while two problems were selected to be nonlinear systems with three variables. The numerical results were presented in tabular forms and all the numerical computations and the programming were done with

Table 1: Exact solution $(x_E(t), y_E(t))$, Semi-implicit extrapolation $(x_s(t), y_s(t))$ and Picard iterative scheme $(x_p(t), y_p(t))$ with $h = 0.1$ for example 1

n	t	$x_E(t)$	$y_E(t)$	$x_s(t)$	$y_s(t)$	$x_p(t)$	$y_p(t)$
0	0	2.0	-2.0	2.0	-2.0	2.0	-2.0
1	0.1	8.187307531	4.912384519	8.191297617	4.916068511	657706.8533	657703.5786
2	0.2	6.703200460	4.021920276	6.703802283	4.022289171	0.205x10^{10}	0.205x10^{10}
3	0.3	5.488116361	3.292869817	5.488557384	3.293134476	0.640x10^{13}	0.641x10^{13}
4	0.4	4.493289641	2.695973785	4.493621074	2.696172644	0.200x10^{17}	0.200x10^{20}

Table 2: Numerical Solutions using the Rosenbrock $(x_R(t), y_R(t))$ and the Gear's $(x_G(t), y_G(t))$ methods with $h = 0.1$ for example 1

n	t	$x_R(t)$	$y_R(t)$	$x_G(t)$	$y_G(t)$
0	0.0	2.0	-2.0	2.0	-2.0
1	0.1	8.1873083592	4.9123850148	8.1873075926	4.9123845555
2	0.2	6.7032005955	4.0219203573	6.7032005661	4.0219203433
3	0.3	5.4881165092	3.2928699055	5.4881165188	3.2928699086
4	0.4	4.4932897336	2.6959738401	4.4932898217	2.6959738880

the aid of Maple 13 software [5, 6, 10].

3.1 Example 1

We consider the following linear systems of stiff ordinary differential equations of two variables of the form

$$x'(t) = 1195x(t) - 1995y(t); x(0) = 2, \tag{7}$$

$$y'(t) = 1197x(t) - 1997y(t); y(0) = -2. \tag{8}$$

The exact solution is given as

$$x(t) = 10e^{-2t} - 8e^{-800t}, \tag{9}$$

$$y(t) = 6e^{-2t} - 8e^{-800t}. \tag{10}$$

The numerical results are presented in the Tables 1 and 2 while their corresponding errors are in Tables 3 and 4.

Table 3: The associated errors for example 1 using SIEM and PIS

n	t	$\lvert x_E - x_s \rvert$	$\lvert y_E - y_s \rvert$	$\lvert x_E - x_p \rvert$	$\lvert y_E - y_p \rvert$
0	0.0	0.0	0.0	0.0	0.0
1	0.1	3.990086x10^{-3}	3.683992x10^{-3}	657698.666	657698.6662
2	0.2	6.018230x10^{-4}	3.688950x10^{-4}	2053360199	2053360199
3	0.3	4.410230x10^{-4}	2.646590x10^{-4}	6.408537852x10^{12}	6.408537882x10^{12}
4	0.4	3.314330x10^{-4}	1.988590x10^{-4}	2.000104704x10^{16}	2.000104704x10^{16}

Table 4: The associated errors for example 1 using RM and GM

n	t	$\|x_E - x_R\|$	$\|y_E - y_R\|$	$\|x_E - x_G\|$	$\|y_E - y_G\|$
0	0.0	0.0	0.0	0.0	0.0
1	0.1	8.282x10^{-7}	4.958x10^{-7}	6.160x10^{-8}	3.650x10^{-8}
2	0.2	1.355x10^{-7}	8.130x10^{-8}	1.061x10^{-7}	6.730x10^{-8}
3	0.3	1.482x10^{-7}	8.850x10^{-8}	1.578x10^{-7}	9.160x10^{-8}
4	0.4	9.260x10^{-8}	5.510x10^{-8}	1.807x10^{-7}	1.030x10^{-7}

Table 5: The associated errors for example 2 using SIEM, RM, GM and PIS

n	t	$\|x_E - x_s\|$	$\|x_E - x_R\|$	$\|x_E - x_G\|$	$\|x_E - x_p\|$
0	0.0	0.0	0.0	0.0	0.0
1	0.00001	2.9857x10^{-6}	4.60x10^{-9}	1.00x10^{-10}	1.61x10^{-4}
2	0.00002	8.5561x10^{-4}	1.31x10^{-8}	1.00x10^{-10}	7.61x10^{-4}
3	0.00003	2.4040x10^{-3}	7.70x10^{-9}	0.00	1.71x10^{-3}
4	0.00004	4.4960x10^{-3}	1.29x10^{-8}	1.00x10^{-10}	2.94x10^{-3}

3.2 Example 2

Next, we consider the equation of the form $Y' = AY$ with $h = 10^{-5}$ where A is given in matrix form as

$$A = \begin{pmatrix} -10^4 & 100 & -10 & 1 \\ 0 & -10^3 & 10 & -10 \\ 0 & 0 & -1 & 10 \\ 0 & 0 & 0 & -0.1 \end{pmatrix}, Y_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}. \tag{11}$$

The exact solution is given as;

$$x(t) = \frac{-89990090}{8999010009}e^{-0.1t} + \frac{818090}{89901009}e^{-t} + \frac{9989911}{899010090}e^{-1000t} + \frac{89071119179}{89990100090}e^{-10000t}, \tag{12}$$

$$y(t) = \frac{9100}{89991}e^{-0.1t} - \frac{910}{8991}e^{-t} + \frac{9989911}{9989001}e^{-1000t}. \tag{13}$$

$$z(t) = \frac{100}{9}e^{-0.1t} - \frac{91}{9}e^{-t} \tag{14}$$

$$p(t) = e^{-0.1t} \tag{15}$$

The numerical results are presented in the form of associated errors given in the tables 5, 6, 7 and 8.

Table 6: The associated errors for example 2 using SIEM, RM, GM and PIS

n	t	$\lvert y_E - y_s \rvert$	$\lvert y_E - y_R \rvert$	$\lvert y_E - y_G \rvert$	$\lvert y_E - y_p \rvert$
0	0.0	0.0	0.0	0.0	0.0
1	0.00001	$3.3\text{x}10^{-9}$	0.00	0.00	$1.66\text{x}10^{-7}$
2	0.00002	$9.86\text{x}10^{-6}$	0.00	0.00	$8.27\text{x}10^{-7}$
3	0.00003	$2.94\text{x}10^{-5}$	0.00	0.00	$1.97\text{x}10^{-6}$
4	0.00004	$5.83\text{x}10^{-5}$	0.00	$1.00\text{x}10^{-10}$	$3.57\text{x}10^{-6}$

Table 7: The associated errors for example 2 using SIEM, RM, GM and PIS

n	t	$\lvert z_E - z_s \rvert$	$\lvert z_E - z_R \rvert$	$\lvert z_E - z_G \rvert$	$\lvert z_E - z_p \rvert$
0	0.0	0.0	0.0	0.0	0.0
1	0.00001	0.00	$1.00\text{x}10^{-9}$	$1.00\text{x}10^{-9}$	0.00
2	0.00002	$2.00\text{x}10^{-9}$	0.00	0.00	0.00
3	0.00003	$4.00\text{x}10^{-9}$	0.00	0.00	0.00
4	0.00004	$3.00\text{x}10^{-9}$	0.00	$1.00\text{x}10^{-10}$	0.00

Table 8: The associated errors for example 2 using SIEM, RM, GM and PIS

n	t	$\lvert p_E - p_s \rvert$	$\lvert p_E - p_R \rvert$	$\lvert p_E - p_G \rvert$	$\lvert p_E - p_p \rvert$
0	0.0	0.0	0.0	0.0	0.0
1	0.00001	0.00	0.00	0.00	0.00
2	0.00002	0.00	0.00	0.00	0.00
3	0.00003	0.00	0.00	0.00	0.00
4	0.00004	0.00	0.00	0.00	0.00

Table 9: Approximate solutions of example 3 using the semi-implicit extrapolation method and Picard iterative scheme with $h = 0.1$

n	t	$x_s(t)$	$y_s(t)$	$z_s(t)$	$x_p(t)$	$y_p(t)$	$z_p(t)$
0	0.0	1.0	2.0	2.0	1.0	2.0	2.0
1	0.1	1.2299	2.5285	1.9453	2.8683	6.1564	2.1581
2	0.2	1.3778	2.8514	1.9321	8.0868	16.9563	6.3526
3	0.3	1.5238	3.1640	1.9206	20.5618	32.4489	36.4153
4	0.4	1.7097	3.5544	1.9280	15.9347	-78.6433	75.6785

Table 10: Approximate solutions of example 3 using the Rosenbrock and Gear methods with $h = 0.1$

n	t	$x_R(t)$	$y_R(t)$	$z_R(t)$	$x_G(t)$	$y_G(t)$	$z_G(t)$
0	0.0	1.0	2.0	2.0	1.0	2.0	2.0
1	0.1	2.9700	6.2913	2.2163	2.9699	6.2913	2.2163
2	0.2	8.8418	17.8938	7.8340	8.8417	17.8938	7.8340
3	0.3	18.7367	24.1205	36.6637	18.7367	24.1205	36.6637
4	0.4	11.1371	-4.4402	42.4577	11.1371	-4.4402	42.4577

3.3 Example 3

Consider the nonlinear systems of stiff ordinary differential equations of the forms;

$$x'(t) = 10y(t) - 10x(t); x(0) = 1, \tag{16}$$

$$y'(t) = 28x(t) - y(t) - x(t)z(t); y(0) = 2, \tag{17}$$

$$z'(t) = x(t)y(t) - \frac{8z(t)}{3}; z(0) = 2, \tag{18}$$

The exact solution could not be obtained because it is a nonlinear system of equations. The approximate solutions are shown in the Tables 9 and 10.

3.4 Example 4

Also, we consider the nonlinear systems of stiff ordinary differential equations of the form;

$$x'(t) = 77.27(y(t) + x(t)(1 - 8.375 \times 10^{-6}x(t) - y(t))); x(0) = 1, \tag{19}$$

$$y'(t) = \frac{1}{77.27}(z(t) - (1 + x(t))y(t)); y(0) = 2 \tag{20}$$

$$z'(t) = 0.161(x(t) - z(t)); z(0) = 2 \tag{21}$$

This system of nonlinear equation given above is called the oregonator. It is a chemical reaction between $HBrO_2$, Br^{-1} and Ce(IV)[11]. The exact solution could not be obtained because it is a nonlinear system. The numerical solutions are given in the Tables 11 and 12.

Table 11: Approximate solutions of example 4 using the semi-implicit extrapolation method and the Picard iterative scheme with $h = 0.1$

n	t	$x_S(t)$	$y_S(t)$	$z_S(t)$	$x_P(t)$	$y_P(t)$	$z_P(t)$
0	0.0	1.0	2.0	3.0	1.0	2.0	3.0
1	0.1	2.7764	1.9928	2.9648	-21.1021	1.9887	3.0303
2	0.2	2.1018	1.9886	2.9510	125.8570	2.0344	2.7042
3	0.3	1.4236	1.9845	2.9374	-895.6621	1.6938	4.7494
4	0.4	1.9495	1.9807	2.9217	3842.7000	3.6517	-9.6848

Table 12: Approximate solutions of example 4 using the Rosenbrock and Gear methods with $h = 0.1$

n	t	$x_R(t)$	$y_R(t)$	$z_R(t)$	$x_G(t)$	$y_G(t)$	$z_G(t)$
0	0.0	1.0	2.0	3.0	1.0	2.0	3.0
1	0.1	2.0026	1.9964	2.9820	2.0026	1.9964	2.9820
2	0.2	2.0070	1.9925	2.9664	2.0070	1.9925	2.9664
3	0.3	2.0110	1.9886	2.9511	2.0110	1.9886	2.9511
4	0.4	2.0150	1.9847	2.9361	2.0150	1.9847	2.9361

4. Results and Conclusion

In this paper, we have described and demonstrated the applicability of the use of the semi-implicit extrapolation method, the Rosenbrock method, the Gear's method and the Picard iterative scheme for obtaining the approximate solutions of both linear and nonlinear systems of stiff ordinary differential equations via examples. It can be observed from the Tables $3 - 8$ that the semi-implicit extrapolation method, the Rosenbrock method and the Gear's method compared favourably well with the exact solutions where feasible.

It can be concluded that the results obtained with the use semi-implicit extrapolation method, the Rosenbrock method, the Gear's method are accurate which shows high capability of the methods compare to other explicit methods like the Picard iterative method. These methods are simple, direct and accurate. They are practical methods that can easily be implemented on computers to solve any linear and nonlinear systems of stiff ordinary differential equations. These methods help the approximate solutions not to diverge from the exact solutions, they work very well and they do not require extremely small value of the step size as in the case of the Picard iterative scheme.

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