

Numerical methodologies for higher index Differential-Algebraic Equations

A . Awasthi ^a , A. Anjaly^a

Abstract— This paper focuses mainly on the numerical methodologies for solving Differential-Algebraic Equations (abbreviated as DAEs). An overview for the existing numerical techniques is presented.

Index Terms— Applications, Backward Differentiation Formula methods, Differential-Algebraic equations, Index, Index Reduction.

1 INTRODUCTION

In a system of Differential Algebraic Equations, there are algebraic constraints on the variables. DAEs are generalisations of ODEs and have much more applications. They are obtained often during the simulation of real world problems. In this paper, we analyse the numerical methods to solve the DAEs.

A demanding problem to deal with differential algebraic equations (DAEs) is the computation of initial values. For a general DAE system, the index is the minimum number of differentiations of the system, required to obtain an ODE. It is well known that, the DAEs can be difficult to solve when their index is greater than one. For higher index systems, a straight forward discretization generally does not work well. An alternative treatment is the use of index reduction methods, whose essence is the repeated differentiation of the constraint equations until a low index.

Many physical systems are naturally described by a set of DAEs. DAEs arise in the mathematical modeling of a wide variety of problems from engineering and science such as in multibody and flexible body mechanics, electrical circuit design, optimal control, incompressible fluids, molecular dynamics, chemical kinetics (quasi steady state and partial equilibrium approximations), and chemical process control. Also, the problems that lead to DAEs are found in many applications.

2 PHYSICAL EXAMPLES

2.1 Simple Pendulum

A simple example of a DAE arises from modeling the motion of a pendulum in Cartesian coordinates.

If L = length of the pendulum, g = gravitational constant, λ = lagrange multiplier, with x and y as the cartesian coordinates of an infinitesimal ball of mass 1 at the end

we obtain the following DAE

$$\begin{aligned}x'' &= \lambda x \\y'' &= \lambda y - g \\x^2 + y^2 + L^2 &= 0\end{aligned}$$

2.2 An example arising in electrical circuit simulation:

To obtain a mathematical model for the charging of a capacitor via a resistor, we associate a potential $x_i = 1, 2, 3, \dots$ with each node of the circuit, as shown in the figure -1. The voltage source increases the potential x_3 to x_1 by U .

$$\text{i.e. } x_3 - x_1 - U = 0$$

By Kirchhoff's first law, the sum of the currents vanishes at each node. Hence, assuming ideal electronic circuits, for the second node, we obtain that

$$\frac{C(x_3' - x_2') + (x_3 - x_2)}{R} = 0,$$

R = size of the resistance of the resistor

C = capacity of the capacitor. By choosing the zero potential as $x_3 = 0$, we obtain as a mathematical model, the differential-algebraic system of index one

$$x_1 - x_3 - U = 0$$

$$\frac{C(x_3' - x_2') + (x_3 - x_2)}{R} = 0$$

$$x_3 = 0$$

It is clear that this simple system can be solved for x_3 and x_1 to obtain an ODE for x_2 only, combined with algebraic equations for x_1, x_3 .

^a.Department of Mathematics,
National Institute of Technology Calicut 673601, India.

E-mail: awasthi@nitc.ac.in (A.Awasthi)
anjalyanand90@gmail.com (A.Anjaly)

3 INDEX

A key concept regarding the DAEs is their 'Index'. DAEs are classified by their index. The index of a system of Differential Algebraic equations is the minimum number of differentiations of the system which would be required to solve for y_0 uniquely in terms of y (i.e, to obtain an explicit ODE). Index can be zero or more. DAEs with index greater than one are often referred to as higher index systems. The best way to solve a higher index DAE system is to first convert it to a lower index system by carrying out differentiations analytically. Index measures the distance from a DAE to its related ODE.

4 DAE

4.1 Index zero

DAE of index zero is an ODE itself. Initially an index zero DAE is considered.

$$\frac{dy}{dx} = x + y$$

with the initial condition $y(0) = 1$.

Solution: The solution of the considered DAE is given below by Euler's method. Let x_0 and y_0 be the initial values of x and y respectively. Here $x_0=0$ and $y_0=1$. Let the stepsize $h=0.1$. Then, $x_i = x_0 + ih; i=0,1,2,\dots$

y_i is the function value at the point x_i . Using explicit Euler's method, we have

$$y_n - y_{n-1} = h[x_{n-1} + y_{n-1}]$$

$$y_n = y_{n-1} + h[x_{n-1} + y_{n-1}]$$

Considering 'n' number of iterations, the values of y_n are obtained. This method is implemented using MATLAB. The values obtained by numerical and analytical methods are given in table-1, where the numerical solutions are denoted as y_{cal} and analytical as y_{real} . Absolute error indicates the difference between exact and computed solution. For the same example, the graph of the solution computed using BDF method of order one is plotted with the exact solution. The plot is shown in figure-2.

4.2 Index one

For an index-one problem, differentiating the algebraic equation once yields an ODE. Considered test example is given.

$$\begin{bmatrix} 1 & -x \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1' \\ y_2' \end{bmatrix} + \begin{bmatrix} 1 & -(1+x) \\ 0 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 \\ \sin x \end{bmatrix}$$

along with initial values
$$\begin{bmatrix} y_1(0) \\ y_2(0) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

The exact solution is
$$\begin{bmatrix} y_1(x) \\ y_2(x) \end{bmatrix} = \begin{bmatrix} \exp(-x) + x \sin x \\ \sin x \end{bmatrix}$$

On expanding the test example and finding the derivative of y_2 and substituting both the values of y_2 and y_2' , we obtain an index zero DAE. Here, DAE of index one is reduced to index zero.

The obtained index zero DAE is:

$$y_1' - x \cos x + y_1 - (1+x) \sin x = 0$$

$$y_1' + y_1 = x \cos x + x \sin x + \sin x$$

The example is treated with BDF-1. Using the Newton Raphson method, the solution was found out. The graphs of the exact solution and the computed solution were plotted. The plot is shown in Figure-3.

4.3 Index two

Now, we consider the higher index Differential-Algebraic Equation system of index two.

$$x(t) = \sin(t) \quad \text{with consistent initial values} \quad x(0) = \sin(0)$$

$$x'(t) + y(t) = 0 \quad y(0) = -\cos(0)$$

First, this example is treated with Crank-Nicolson method, after making a small perturbation to the initial condition as follows :

$$x(0) = \sin(0) + h^3$$

$$y(0) = -\cos(0)$$

It was observed that the graph plotted with computed and exact solutions showed up fluctuations as in figure-4.

The same test example was treated using BDF method with the same perturbation in initial conditions. Here, the plots with computed and exact solutions were almost equal, without any fluctuations. Figure-5 shows the plot.

5 NON-LINEAR SYSTEM

In this regard, the following non-linear index-2 system is considered

$$y_1' - y_2 - y_1 y_3 = 0$$

$$y_2' + \left(\frac{\pi}{3}\right)^2 y_1 - y_2 y_3 = 0$$

$$-\left(\frac{\pi}{3}\right)^2 y_1^2 - y_2^2 + 1 = 0$$

with initial conditions $y_1(0) = 0, y_2(0) = 1, y_3(0) = 0$.

Applying Backward Difference Formula of order one to the system of equations and re-arranging the system, we get as follows. Here 'h' denotes the stepsize and y_i denotes the numerical solution of y at t_i .

$$y_{1(i+1)} - y_{1(i)} - h y_{2(i+1)} - h y_{1(i+1)} y_{3(i+1)} = 0$$

$$y_{2(i+1)} - y_{2(i)} + h \left(\frac{\pi}{3}\right)^2 y_{1(i+1)} - h y_{2(i+1)} y_{3(i+1)} = 0$$

$$-\left(\frac{\pi}{3}\right)^2 y_{1(i+1)}^2 - y_{2(i+1)}^2 + 1 = 0$$

The set of equations is similar to the system $AX=B$.

On solving this and comparing the numerical solution with the exact solution at different time points with $h=0.01$ is tabulated

and results are shown in table-2.

6 FIGURES AND TABLES

6.1 Figures

Figure-1 : Electrical circuit

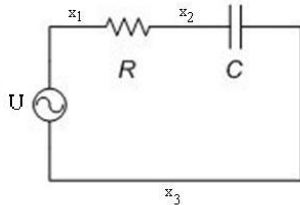


Figure-2 : Index zero DAE - Comparison of exact values and computed values using BDF

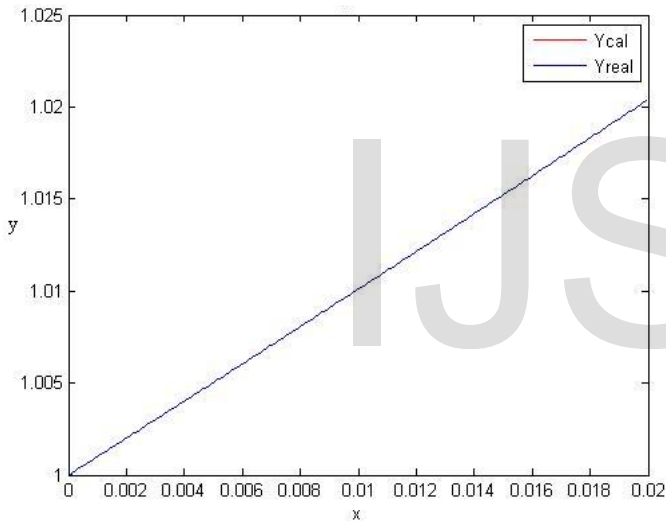


Figure-3 : Index one DAE- Comparison of exact values and computed values using BDF

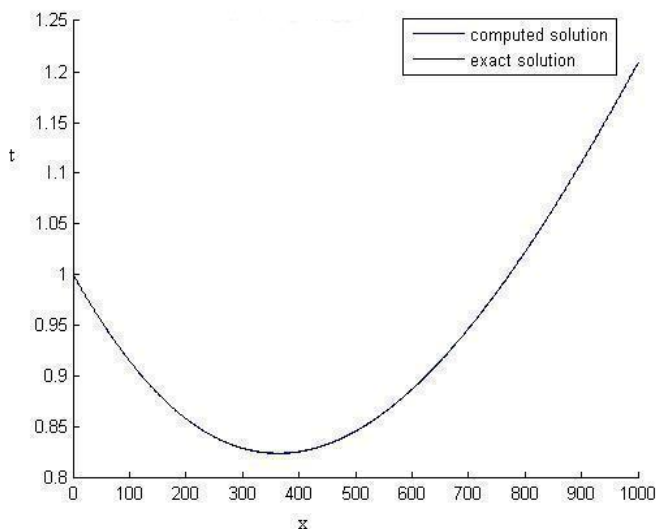
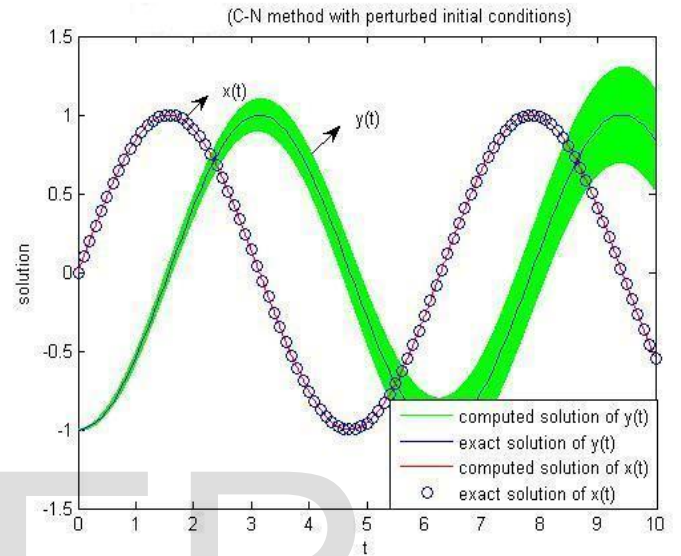
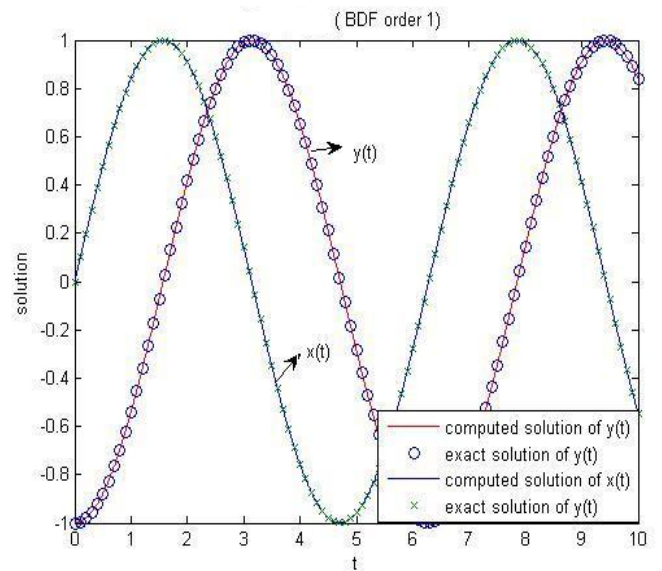


Figure- 4: Index two DAE

Figure- 5: Index2 DAE- plot : BDF with perturbed initial con



ditions



6.2 Tables

Table-1: Numerical and analytical solution of an index zero DAE

<i>Ycal</i>	<i>Yreal</i>	Absolute error (in 10 ⁻²³)
1.001001000000000	1.001001000000000	0.000000000000020
1.002004001000020	1.002004001000000	0.000000000000020
1.003009005001970	1.003009005001900	0.000000000000070
1.004016014006001	1.004016014006001	0.000000000000000
1.005025030020107	1.005025030020007	0.000000000000100
1.006036055050127	1.006036055050027	0.000000000000100
1.007049091105097	1.007049091105077	0.000000000000020
1.008064140196184	1.008064140196180	0.000000000000004
1.009081204336378	1.009081204336376	0.000000000000002

Table -2: Comparison of the Numerical solution with the exact solution at different time points with h=0.001

t	Exact solution			Computed solution			Absolute error in each component		
	<i>y</i> ₁	<i>y</i> ₂	<i>y</i> ₃	<i>y</i> ₁	<i>y</i> ₂	<i>y</i> ₃	<i>y</i> ₁	<i>y</i> ₂	<i>y</i> ₃
0.1	0.0998	0.9945	0	0.0998	0.9945	0.0005	0	0	0.0005
0.2	0.1985	0.9781	0	0.1985	0.9781	0.0005	0	0	0.0005
0.3	0.2951	0.9511	0	0.2951	0.9511	0.0005	0	0	0.0005
0.4	0.3884	0.9135	0	0.3884	0.9135	0.0005	0	0	0.0005
0.5	0.4775	0.8660	0	0.4775	0.8660	0.0005	0	0	0.0005
0.6	0.5613	0.8090	0	0.5613	0.8090	0.0005	0	0	0.0005
0.7	0.6390	0.7431	0	0.6390	0.7431	0.0005	0	0	0.0005
0.8	0.7097	0.6691	0	0.7097	0.6691	0.0005	0	0	0.0005
0.9	0.7726	0.5878	0	0.7726	0.5878	0.0005	0	0	0.0005
1.0	0.8270	0.5000	0	0.8270	0.5000	0.0005	0	0	0.0005

7 CONCLUSION

In the beginning of the work, DAE of index zero is considered. The solution of the test example was computed using BDF methods of order one, two and three respectively. Then we moved on to index one and then to index two DAEs. In all these cases, the computed solutions were found to be in good agreement with exact solutions. In order to validate the efficiency of the proposed method, various numerical experiments are done and the results of these experiments are tabulated and plotted in form of graphs. The plotted graphs reveal the fact that the computed solutions generated by BDF are almost the same as the exact solutions obtained from analytical methods. While Crank-Nicolson method showed up fluctuation between exact solution and computed solution with a small perturbation in the initial values, BDF method proved to

be stable, without any fluctuation, even with the same perturbed initial conditions. These show BDF methods are suitable for handling the system of Differential Algebraic Equations.

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