

Direct Initialisation and Solution of High-Index DAE Systems

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Abstract

Differential-algebraic equations (DAE) systems arise naturally from modelling many dynamic systems and are more difficult to handle than ordinary differential equation (ODE) systems. For instance, it is well known that difficulty arises when DAE's are solved with inconsistent initial values. Furthermore, the solution of high-index problems requires specially designed integration methods or index reduction, which are usually limited. In this work, alternatives for initialising and solving general high-index DAE systems are studied and a new algorithm for index analysis and reduction is introduced.

Keywords: High-Index; DAE systems; DAE initialisation.

1. Introduction

Differential-algebraic equations (DAE) systems arise naturally when modelling many dynamic systems. General implicit DAE system can be represented by

$$F(t, y, y') = 0 \quad (1)$$

where t is the independent variable (usually the time), $F \in \mathbb{R}^n$, y and $y' \in \mathbb{R}^n$ are the dependent variables and its derivatives with respect to t , respectively.

If (1) can be written in the *explicit* form

$$y' = f(t, y) \quad (2)$$

with the same state variables y , then (1) actually is a system of *implicit* Ordinary differential equations (ODE). In this work we are interested in problems for which such conversion is impossible or not desirable. There are several reasons to consider (1) directly (Brenan *et al.*, 1989). One of our particular interest, is when the system of equations is automatically generated by a simulation program where the models are written in an object-oriented language. In this work the process simulator EMSO (Soares and Secchi, 2003) was used to write models, develop and test methods and to obtain numerical solutions.

The basic difference between (1) and (2) is the possibility of a singular Jacobian of F with respect to y' , denoted by $\partial F / \partial y'$ or $F_{y'}$. If this is the case, the DAE cannot be rewritten as an ODE with same variables y . Then, in order to convert such DAE systems to an ODE, state transformations or derivations of the equations are needed. Usually the

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property known as *index* is used to *measure the distance* between a particular DAE and its equivalent ODE formulation. The minimum number of times that all or part of a DAE (1) must be differentiated with respect to t to determine y' as a continuous function of y and t is defined as the *differential index* ν ¹.

Obviously, accordingly to the above definition, (2) has a differential index $\nu = 0$. DAE systems with $\nu \leq 1$ and $\nu > 1$ are known as low- and high-index, respectively.

The solution of general low-index DAE systems is, in principle, no much more difficult than the solution of ODE systems but the initialisation of such systems still can pose problems (Pantelides, 1988). Furthermore, none of the currently available numerical techniques work for all high-index DAE's (Brenan *et al.*, 1989).

In this work alternatives for initialising and solving general high-index DAE systems in form (1), coming from the equation based general process simulator EMSO, are studied. Moreover, a new structural algorithm for index characterisation and reduction is presented, then the alternatives are compared when applied in typical problems.

2. Alternatives when Solving High-Index DAE Systems

Low-index DAE systems can generally be solved numerically by slightly modified ODE codes. However, for high-index systems these methods may converge poorly, they may converge to wrong solutions, or they may not converge at all (Brenan *et al.*, 1989). For these systems there are basically three general approaches:

1. Manually modify the model to obtain a lower index equivalent model;
2. Integration by specifically designed high-index solvers;
3. Apply automatic index reduction algorithms in order to obtain a lower index equivalent model.

2.1 Manual Modifications

There are some works on literature exploring how different assumptions such as equilibrium or incompressibility can affect the index of DAE systems (Lefkopoulou and Stadtherr, 1993; Gani and Cameron, 1992). Clearly such approach is not suitable for our purposes, because it is quite difficult or impossible to automate it.

2.2 Specifically Designed High-Index Solvers

As already stated, there are no method capable to handle any class of high-index DAE. Presently available numerical codes are basically modified ODE solvers (Unger *et al.*, 1995), and can be divided in two main groups:

- Solvers for high-index problems of restricted problem structure (e.g. in Hessenberg form or semi-explicit);
- Solvers for high-index problems limited for problems with index three or less.

Again, the former group of solvers is not suitable for our purposes because could be impossible to convert general DAE systems to the required stricter structure.

The last group of solvers appears to be promising for our application, mainly because problems with index higher than three are quite uncommon to appear in mathematical models of chemical processes. Representing this class of solvers, the codes PSIDE (Lioen *et al.*, 1998) and MEBDFI (Abdulla and Cash, 1999) were considered. Although no restriction in problem structure is imposed when using these codes, it is required to

¹ Other definitions of index can be found in Unger *et al.*(1994).

inform as input the *index* of each variable. In order to exemplify how the indices of the variables are determined, consider the following system of equations

$$\begin{aligned} y' &= f(t, y, z) \\ z' &= k(t, y, z, u) \\ 0 &= g(t, y) \end{aligned} \tag{3}$$

where f_z , k_u , and g_y are invertible in the neighbourhood of the solution. Then, (3) has index $\nu = 3$ and the variable y , z , and u are of index 1, 2, and 3, respectively. A more detailed description of this procedure can be found at Lioen *et al.* (1998). Should be stressed that (3) was used for demonstration purposes only and the cited codes can handle general problems as (1).

From this discussion, it is clear that in order to implant these solvers in a general process simulator a problem still remains: how to automate the determination of the index of the variables, this can be accomplished by the algorithms discussed next.

2.3 Index Analysis and Reduction

Historically, several works have addressed the problem of index characterisation and reduction, and most of these consider only the structure of the problem disregarding numerical values. From this consideration comes the property known as structural index ν_{str} which is analogue to the differential index ν but considering structural algebra.

Duff and Gear (1986) suggested a structural analysis to identify index two semi-explicit systems. Gear (1988) conceptually proposed a symbolical algorithm for index reduction, and based on this idea Bachmann *et al.* (1990) presented an algorithm for index reduction of linear systems. Unger *et al.* (1995) extended this algorithm enabling the characterisation and index reduction of general DAEs. Pantelides (1988) introduced a graph-theoretical algorithm addressing the problem of consistent initialisation of general DAEs which can be used for index reduction. The last two approaches are of similar complexity but Pantelides' algorithm is fairly well suited for an implementation in sparse matrix representation (Unger *et al.*, 1995) and therefore was preferred in this work. The basic idea of the Pantelides' algorithm is to determine minimally structurally singular (MSS) subsets of equations and then differentiate it to form an augmented system aiming at a system where no more MSS subsets can be found. In Costa Jr. *et al.* (2001) the Pantelides' algorithm was applied to index-one reduction using automatic differentiation.

2.3.1 Algorithm for index reduction

It is well known that structural analysis of DAEs is limited (see Pantelides, 1988; Unger *et al.*, 1995; and Reissig *et al.*, 2000, for further discussion on this subject). For instance, if a DAE system is structurally singular, Pantelides' approach will keep differentiating the same subset of equations ad infinitum (Pantelides, 1988). Besides this, the structural algorithm stops when an index one equivalent system is obtained and cannot reduce further the index.

In order to remove these two limitations the following modifications to the Pantelides' algorithm are suggested:

- start the search for MSS subsets with respect to all variable derivatives and not only with respect to the variable derivatives that are part of the original system;

- when a MSS subset with respect to the variable derivatives is detected, check if it is singular with respect to the entire set of variables. If this is the case then the analysis is finished because the system is structurally singular.

The first modification makes the algorithm capable to reduce the index until zero, the second checks if the system is structurally singular, avoiding infinite loop when analysing singular systems.

When the algorithm stops, the variables not covered by the association are a viable set of initial conditions. Moreover, if a Dulmage-Mendelsohn decomposition is applied to the final association, the under-constrained component consist of the entire set of valid initial conditions. Unfortunately, there is no room for presenting further details of the algorithm. Its advantages, complexity, possible implementations and underlying details will be explored in deep in a specific article to appear.

Both algorithms, Pantelides' and the proposed modifications, are implemented in the process simulator EMSO and the derivatives of the equations are obtained by a built-in symbolic differentiation code.

3. Initialising general DAE systems

It is well known that difficulty arises when DAE systems are solved with inconsistent initial values and may cause solution failures of many popular DAE solvers (Wu and White, 2001). Therefore, consistent initial values are crucial for obtaining the numerical solution. Actually, most often failures in solving a DAE system occur or have the source in initialisation, for both low- and high-index systems. Here we study an alternative approach that can be used to initialise DAE systems of any index, as follows:

- analyse the system of equations with the index analysis algorithm proposed in section 2.3.1;
- if the system is not singular, the number of dynamic degrees of freedom and the viable set of initial conditions are determined;
- if the given initial conditions are valid, solve the square system of non-linear equations (NLA) composed by the original equations, the initial conditions and the equation derivatives determined by the index analysis algorithm.

It should be noted that with this approach, the initial conditions can be general algebraic or differential equations and not just fixing the value of some variables as usual.

3.1 Initialising a Low-Index Problem

In order to compare the proposed approach for initialising low-index DAEs with usual techniques, the galvanostatic process of a thin film nickel hydroxide electrode proposed by Wu and White (2001) was considered. The model due to the authors, is an index one DAE system with two variables (y_1 and y_2) and one dynamic degree of freedom. Then, in order to initialise the system, one of the variables could be specified as initial condition and the other three (the other variable and the derivative of both) must be determined by the initialisation procedure. As any numerical technique, initialisation codes needs initial guesses for the free variables. Table 1 shows the convergence range of the initial guess of one variable when the other is given as initial condition of popular codes for solving DAE systems.

As can be seen in Table 1 the proposed method is fairly more robust. Moreover, the proposed method can initialise problems depending non-linearly on the derivatives where usual methods fail.

Table 1. Convergence range in initialising an index-one problem.

Solver	y_2 convergence range, given $y_1=0.05$ as initial condition	y_1 convergence range, given $y_2=0.38$ as initial condition
DASSL*	0.321 – 0.370	0.071 – 0.352
LIMEX*	0.318 – 0.377	0.056 – 0.418
RADAU5*	0.348 – 0.352	0.143 – 0.190
DAEIS*	-0.974 – 1.663	0.000 – 1.000
Proposed Method	-2.70 – 2.66	$-\infty - \infty$
Consistent value	0.35024	0.15513

*Data from Wu and White (2001).

3.1 Initialising High-Index Problems

The classical codes tested in previous section cannot be used to initialise high-index DAEs. On the other hand, the proposed approach was successfully used to initialise high-index problems as the classical index three pendulum model (Pantelides, 1988) or the index three batch distillation column (Logsdon and Biegler, 1993).

4. Solving high-index DAE systems

Once the initialisation step terminates successfully one can try to advance in solution. As discussed before, codes designed for high-index problems are limited to systems with index at most three and require an index analysis. To solve the problem through the reduced index equivalent system is a more general but it falls down in the well known “drift-off” effect (see Figure 1).

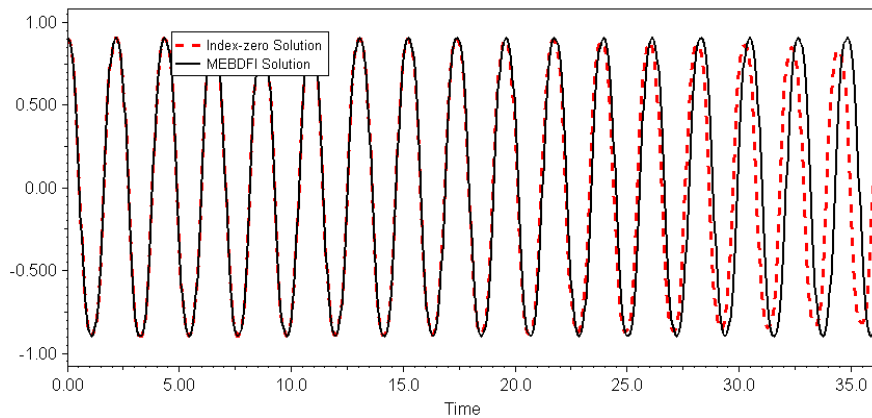


Figure 1. Numerical solution for the position of the index-three pendulum problem.

As can be seen in Figure 1, the numerical solution using an index-zero system yield acceptable results for low integration time. For long time the algebraic constraints (cable length in the pendulum problem), which are not directly considered in the index-reduced system, starts to be not respected.

5. Conclusions

Alternatives in initialising and solving general high-index DAE systems coming from the dynamic process simulator EMSO were studied. An algorithm for index analysis and reduction was introduced together with an approach for initialising both low- and high-index problems. This approach successfully initialised high-index problems and proved to be more robust than the classical codes when initialising low-index systems. For solving high-index DAE systems, currently, the better alternative is to use codes designed for high-index problems. Unfortunately, these codes can handle systems with index at most three. On the other hand, the index reduction approach can be applied to systems of any index but the solution can presents degradation. How to reduce this degradation (the “drift-off” effect) is subject of ongoing research.

References

- Abdulla T. J. and J. R. Cash, 1999, A Package for the Solution of Initial Value Problem for system of Implicit Differential Algebraic Equations, www.netlib.org/ode/mebdfi.f.
- Bachmann, R., L. Brüll, T. Mrziglod, and U. Pallaske, 1990, On Methods for Reducing the Index of Differential Algebraic Equations, *Comp. Chem. Engng*, 14, 1271-1273.
- Brenan K. E., S. L. Campbell and L. R. Petzold, 1989, Numerical Solution of Initial Value Problems in Differential-Algebraic Equations. North-Holland, New York.
- Costa Jr., E.F., R.C. Vieira, A.R. Secchi, E.C. Biscaia (2001), Automatic Structural Characterization of DAE Systems, ESCAPE-11, Kolding, Denmark, pp. 123-128.
- Duff I. S. and C. W. Gear, 1986, Computing the structural index, *SIAM J. Alg. Disc. Meth.* 7, 594-603.
- Lefkopoulos A. and M. A. Stadtherr, 1993, Index analysis of unsteady-state chemical process systems – I, *Comp. Chem. Engng* 17, 399-413.
- Lioen W. M., J.J.B. Swart and W. A van der Veen, PSIDE Users' Guide, 1998, <http://www.cwi.nl/archive/projects/PSIDE/>.
- Logsdon J. S and L. T. Biegler, 1993, Accurate Determination of Optimal Reflux Policies for the Maximum Distillate Problem in Batch Distillation, *Ind. Eng. Chem. Res.*, 32, No 4, 692-700.
- Gani R. and T. Cameron, 1992, Modelling for dynamic simulation of Chemical Processes – the index problem, *Chem. Engng Sci.* 47, 1311-1315.
- Gear C. W., 1988, Differential-algebraic equation index transformation. *SIAM J. Sci. Stat. Comput.*, 9, 39-47.
- Pantelides C. C., 1988, The consistent initialization of differential-algebraic systems, *SIAM J. Sci. Stat. Comput.* 9, 213-231.
- Reissig G., W. S. Martinson and P. Barton, 2000, Differential-Algebraic Equations of Index 1 may have an Arbitrarily High Structural Index, *SIAM J. Sci. Comput.*, 21, No 6, 1987-1990.
- Soares R. P. and A. R. Secchi, 2003, EMSO: A new Environment for Modelling, Simulation and Optimisation, ESCAPE-13, 947-952.
- Unger J., A. Kröner and W. Marquardt, 1994, Structural Analysis of Differential-Algebraic Equation Systems – Theory and Application, *Computers Chem. Engng*, 19, No 8, pp 867-882.
- Wu B., R.E. White (2001), An initialization subroutine for DAEs solvers: DAEIS, *Computers Chem. Engng*, 25, pp 301-311.