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Floating Index of Inequality Constrained DAE Systems

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Abstract

Problems of dynamic optimisation with inequality path constraints are common in industrial plants. These constraints describe conditions of the process when it operates with extreme values of the variables, based on safety and/or economics restraints. Normally, during the optimal trajectory some of the inequality constraints are activated, and those remain active during a certain period of time. This behaviour can produce a change in the differential index of the DAE system, leading to the so-called floating index phenomena (Feehery and Barton, 1998). This contribution is motivated by the high computational costs typically associated with each of the steps for the resolution of the floating index problem. The proposed new method unifies the advantages of special regularisation functions with numerical codes which integrate higher index DAE systems, avoiding the reinitialisation and index reduction steps. All the inequality constraints are described by appropriate continuous functions and the resulting DAE system can be numerically integrated directly using numerical code such as PSIDE (Lioen et al., 1998). This new procedure has been applied to two typical example: optimal control problem of index two with a state variable inequality constraint (Jacobson and Lele, 1969) and state constrained Van der Pol oscillator of index one. The main advantage of the new method is that the DAE system can be integrated continuously, preventing the restart of the numerical integration every time an inequality constraint is violated. The obtained results are identical with those obtained elsewhere encouraging new developments and extensions.

Keywords: dynamic optimisation, regularisation functions, floating index DAEs.

1. Main Text

Chemical processes models are limited by constraints that represent safety conditions, chemical or physical equilibrium or economical constraints. These constraints are generally represented by inequality equations and can be applied to control or state variables. During the dynamic simulation, the exact time when an inequality restriction is activated is normally unknown. After the constraint is activated, a new equation (or information) must be included into the mathematical model, and this equation must be satisfied until the constraint is no longer active. A possible consequence of this fact is that the differential index of the differential-algebraic equation (DAE) system representing the mathematical model of the process can change during the dynamic simulation. This behaviour characterizes the so-called floating index DAE system.
Methods of resolution of dynamic optimisation problems with inequality constraints (in the state variables) can be classified in two groups, according to the level of adopted

discretisation: total discretisation (or simultaneous approach) and partial discretisation (or sequential approach). In the first group, the dynamic system is totally discretised resulting in an algebraic system which, along with the equality and inequality constraints, is annexed to the code of non-linear programming (NLP). An advantage of this approach is the ease of manipulation of the inequality restrictions (Cuthrell and Biegler,1987 and Longsdon and Biegler,1989). However, its spectrum of application limited to a family of particularly simple and relatively small problems. For the second group, only the control variable is discretised. The resulting system of equations can be solved by techniques of dynamic programming or with non-linear programming (NLP) strategies. The main characteristic of this technique is that at each iteration of the NLP code a numerical integration of the dynamic system must be performed. Within the sequential approach, there are two different ways to handle the inequality constraints.

(a) approximate methods.
In this context, the inequalities constraints are evaluated in the neighbourhood of the feasible region by:

(i) introduction of square slack variable, converting inequality constraint to equality (Jacobson and Lele, 1969, Bryson and Ho, 1975);

(ii) measuring the degree of violation of the constraint over the entire trajectory by max operator or square max operator (Vassiliadis et al. 1994);

(iii) dislocating the limit of the constraint inside of an error defined previously - smooth approximation (Goh And Teo, 1988);

(iv) discretising the inequality constraints on a finite number of points and satisfying at the end of the segments (Chen and Vassiliadis, 2004).

(b) direct methods.
A second context consists of manipulating directly the inequalities and identifying the events (Park and Barton, 1994 and Guyou and Petzold, 2002) of activation and deactivation of the restriction. In this approach, the following steps are needed for the numerical resolution: (i) detection of activation/deactivation of constraints; (ii) index determination (and frequently index reduction); (iii) model switching; and (iv) determination of consistent initial conditions to restart integration (Feehery and Barton, 1998).

In both methods, every time an inequality constraint is reached, a new DAE system must be built, a new set of consistent initial conditions must be determined and an index reduction method must be applied in order to restart the numerical integration (Majer et al., 1995, Park and Barton, 1996, Guiyou and Petzold, 2002). The result of the activation and deactivation of the restrictions can be the change in the differential index of the system during the optimisation process and integration. The numerical effort associated to each of those steps increases the computational cost.

In this work, all the inequality constraints are described by appropriate continuous functions and the resulting DAE system can be integrated continuously. The new method allies the advantages of special regularisation functions with numerical codes that integrate higher index DAE systems, avoiding the reinitialisation and index reduction steps every time one inequality constraint is violated. This new procedure has been applied to typical example with inequality state constrained. The code PSIDE (Lioen et al., 1998) has been used for numerical integration. The obtained results are identical with obtained elsewhere encouraging new developments and extensions.

2. Numerical Example

Two examples are presented to illustrate the proposed methodology: (i) an optimal control problem with a state variable inequality constraint (Jacobson and Lele, 1969); and (ii) state constrained Van der Pol oscillator (Vassiliadis et al. 1994).

Example 1 - Optimal Control Problem with a State Variable Inequality Constraint (Index Two)

This problem was originally presented by Jacobson and Lele (1969) and consists in minimize the state variable y_3 at final time (t_{final}=1) through manipulation of control variable u(t), restricted between lower and upper bounds of -3.0 and 15, respectively. The dynamic system equations are presented in Table 1.

Table 1 – Set of Equations of Illustrative Example1.

$\frac{dy_1}{dt} = y_2$, with $y_1(0)=0$	(1)
$\frac{dy_2}{dt} = - y_2 + u$, with $y_2(0)=-1$	(2)
$\frac{dy_3}{dt} = y_1^2 + y_2^2 + 0.005u^2$, with $y_3(0)=0$	(3)
$y_2(t) - 8(t - 0.5)^2 + 0.5 \le 0$	(4)

The main idea of the proposed methodology is to smooth, during the numerical resolution, the transition between the constrained condition to the unconstrained condition. This procedure needs both: (a) the selection of the regularization function and (b) determination of the conditions that describe the feasible and infeasible region.

The use of regularization functions in the automatic initialisation of algebraic-differential systems has been proposed by Vieira and Biscaia Jr. (2000). The authors have established some criteria to guide the selection of those functions and their parameters. The chosen function for the present work is shown in Equation (5), where ξ is a parameter defined by the user (usually $0 < \xi << 1$).

$$\lambda(g,\xi) = \frac{1}{2}\cdot\left(1 - \frac{\left(\frac{g(y,t)}{\xi}\right)}{\sqrt{1+\left(\frac{g(y,t)}{\xi}\right)^2}}\right) \tag{5}$$

The determination of the set equations that describe the feasible and infeasible region is guided by an analysis of the behaviour of the inequality constraint before and after activation. In the illustrative example, the inequality is converted into a new algebraic equation with a new algebraic variable y*, which is equal to the state variable y_2 when the inequality constraint is inactive and by $8(t - 0.5)^2$ - 05 when the inequality constraint is active. In the present example, the sum of the conditions that characterize the feasible region and infeasible is represented by equation:

$$y^* = \lambda[g(y,t),\xi]\cdot y_2 + [1-\lambda[g(y,t),\xi]]\cdot[8(t-0.5)^2 - 0.5] \tag{6}$$

where g(y,t) is the inequality constraint and $\lambda[g(y,t),\xi]$ is the regularization function that presents the following property:

$$\lambda(\arg,\xi) \cong \begin{cases} 1 \ \text{para} \ \arg < 0 \\ 0 \ \text{para} \ \arg \geq 0 \end{cases} \tag{7}$$

The state variable y_2 is replaced by the new state variable y* in Equations (1) and (3). Then, the new dynamic model system is rebuilt with the Equations (1) to (3) and Equation (6). It should be pointed out that the computer code PSIDE (Lioen *et al.*, 1998) has been used to perform the numerical integration of the correspondent DAE system. This code can deal with fully implicit DAE systems of index up to 3, and its selection eliminates the need of index reduction. In this example, the index of the system is equal to 2 during the activation of the inequality constraint. The profiles obtained for the objective function and the unconstrained and constrained state variables are presented in Figures 1 and 2, respectively.

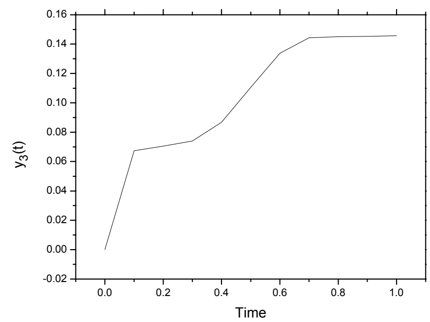

Figure 1 – Objective function profile for example 1.

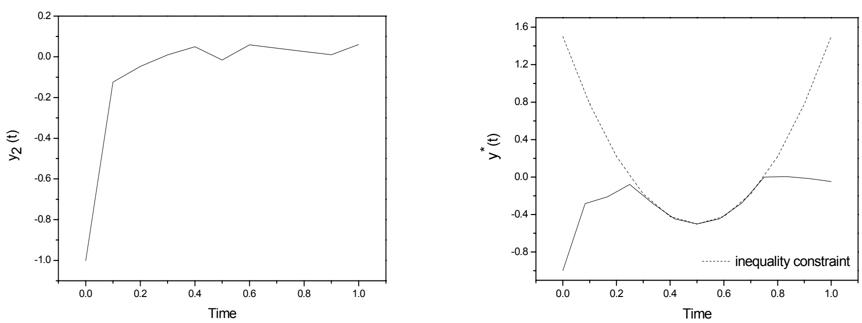

Figure 2 - Unconstrained and constrained state variables profiles in example 1.

Example 2 - State Contrainted Van der Pol Oscillator (Index One)

This problem was presented by Vassiliadis et al. (1994) and consists of minimizing the state variable y_3 at final time (t_{final}=5) through manipulation of control variable u(t), restricted between its lower and upper bounds of -0.3 and 1.0, respectively.

Table2 – Set of Equations of Illustrative Example 2.

$\frac{dy_1}{dt} = \left(1 - y_2^2\right) \cdot y_1 - y_2 + u$, with $y_1(0) = 0$	(8)
$\frac{dy_2}{dt} = y_1$, with $y_2(0) = 1$	(9)
$\frac{dy_3}{dt} = y_1^2 + y_2^2 + u^2$, with $y_3(0) = 0$	(10)
$y_1(t) \geq -0.4$	(11)

In this example, the feasible region is limited by Equation (11). When this constraint is active, the time derivative of the variable y_1 (represented by the right hand side of Equation 8) must be null, what leads to an additional constraint for the control variable. Hence, two new algebraic equations are added to the original system in order to represent the restrictions on the state variable,

$$y^* = \lambda[g(y,t),\xi] \cdot y_1 + [1 - \lambda[g(y,t),\xi]] \cdot (-0.4) \tag{12}$$

and on the control variable.

$$u^* = \lambda[g(y,t),\xi] \cdot u + [1 - \lambda[g(y,t),\xi]] \cdot \left[y_2 + 0.4 \cdot \left(1 - y_2^2\right)\right] \tag{13}$$

The results obtained for state variables are presented in the Figure 3.

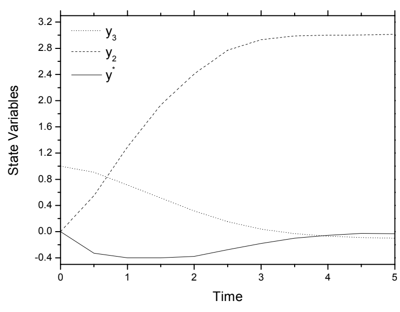

Figure 3 - State variables profiles in example 2.

3. Conclusions

In this contribution, a novel strategy for resolution of floating index DAE has been presented. In the two examples presented, the index of the DAE systems changed when the constraints became active, characterizing the floating index behaviour. The smooth switch between models via a regularisation function has been effective and suitable. Numerical results previously presented for those systems have been reproduced and the simulation effort has been greatly reduced, since the steps of reinitialization and index reduction have been completely eliminated of the simulation.

The regularization function used to change the value of the weight λ from 0 to 1 (or vice-versa) is continuous up to the first derivative. If a higher degree of continuity is required, alternative formulations have been tested by the authors. The reported function, Equation (5), has been considered the most suitable after a cost benefit analysis.

Additional examples have been studied by the authors, and the results obtained have always been encouraging, Unfortunately, due to space limitations, it has not been possible to present additional numerical results, or even to extend the discussion concerning the examples presented.

The methodology proposed in this work for handling the inequality constraints depends on the particular model being solved. However, this "taylor-made" characteristic does not compromise its utilization, due to the lack of extensive algebraic manipulation (such as differentiations) and to the simplicity of final formulation of the problem.

References

A. E. Bryson, Y-C. Ho, 1975, Applied Optimal Control, Hemisphere Publishing Corporation, Washington D. C..

C. J. Goh, K. L. Teo, 1988, Control Parameterization: A Unified Approach to Optimal Control Problems with General Constraints, Automatica, v. 24, pp. 3-18.

C. Majer, W. Marquardt, E. D. Gilles, 1995, Reinitialization of DAE's After Discontinuities, Computers and Chemical Engineering, v. 19, Suppl., pp. 507-512.

D. H. Jacobson, M. M. A. Lele, 1969, Transformation Technique for Optimal Control Problems with a State Variable Inequality Constraint, IEEE Trans. Autom. Control, v. 14, 5, pp.457-464.

J. E. Cuthrell, L. T. Biegler, 1987, On the Optimization of Differential-Algebraic Process Systems, AIChE J., v. 8, pp. 1257-1270.

J. S. Logsdon, L. T. Biegler, 1989, Accurate Solution of Differential-Algebraic Optimization Problems, Ind. Eng. Chem. Res., v. 28, pp. 1628-1639.

M. Guiyou, L. R. Petzold, 2002, Efficient Integration Over Discontinuities for Differential-Algebraic Systems, Mathematics and Computers in Simulation, v. 43, pp. 65-79.

R. C. Vieira, E. C. Biscaia Jr., 2000, Direct Methods for Consistent Initialisation of DAE Systems, Computers and Chemical Engineering, v. 25, pp. 1299-1311.

T. Park, P. I. Barton, 1996, State Event Location in Differential-Algebraic Models, ACM Transactions on Modeling and Computer Simulation, v. 6, 2, pp. 137-165.

T. W. C. C. Chen, V. S. Vassiliadis, 2004, Inequality path constraints in optimal control: a finite iteration ε-convergent scheme based on pointwise discretisation, Journal of Process Control, v. 15, pp. 353-362.

V. S. Vassiliadis, R. W. H. Sargent, C. C. Pantelides, 1994, Solution of a Class of Multistage Dynamic Optimization Problems. 1. Problems with Path Constraints, Process Design and Control by Ind. Eng. Chem. Res., v. 33, pp. 2123-2133.

W. F. Feehery, P. I. Barton, 1998, Dynamic Optimization With State Variable Path Constraints, Computers and Chemical Engineering, v. 22, 9, pp.1241-1256.

W. M. Lioen, J. J. B. De Swart, W. A. Van Der Veen, 1998, PSIDE users guide, Report MAS-R9834, CWI, Amsterdam, Holanda. URL: http://www.cwi.nl/cwi/projects/PSIDE.