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Structural forms and consistent initial values for DAEs from applications

Strukturformen und konsistente Anfangswerte für Algebro-Differentialgleichungen aus Anwendungsgebieten (englischsprachig)

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Structural forms and consistent initial values for DAEs from applications

Diana Estévez Schwarz

Abstract

One of the difficulties associated with the numerical integration of DAEs is the computation of consistent initial values. A consistent initial value has to fulfill the explicit constraints as well as the hidden constraints that may result from differentiation.

If certain structural assumptions are given, then a consistent initialization can be determined sequentially starting from a value that fulfills the explicit constraints. In a second step, a correction of this value is computed successively solving linear subproblems that involve the hidden constraints.

In this report, we summarize some of the existing results for this approach and focus on specific generalizations for DAE forms that are given in applications. On the one hand, the structure of DAEs resulting from water tube systems is discussed and analyzed with regard to consistent initialization. On the other hand, we discuss DAEs in triangular chain form with Hessenberg subsystems as well as Hessenberg DAEs that are coupled to index-1 constraints.

1 Introduction

"It is a basic tenet of numerical analysis that structure should be exploited whenever solving a problem".
G. H. Golub and C. F. van Loan in [7].

DAE structures that are given in applications should be exploited computing a consistent initialization. In order to describe these beneficial structures, we will shortly give an overview of the basic theoretical framework.

In this paper, we consider quasi-linear DAEs of the form

$$Ax'(t) + b(x(t), t) = 0 \tag{1}$$

for a constant nonregular matrix A and define Q as a projector onto $N := \ker A$, $P := I - Q$ and W_0 as a projector along $\operatorname{im} A$.

According to ODE theory, we define for DAEs:

Definition 1.1 *A vector $x_0 \in I\!R^m$ is a consistent initial value of (1), if there exists a solution of (1) that fulfills $x(t_0) = x_0$.*

In practice, we are also interested in the corresponding values of the derivatives appearing in the DAE. The following definition will characterize these values properly.

Definition 1.2 *A vector* (x_0, Py_0) *is a consistent initialization of (1) if* x_0 *is a consistent initial value and* (x_0, Py_0) *fulfills the equation*

$$APy_0 + b(x_0, t_0) = Ay_0 + b(x_0, t_0) = 0.$$

In order to simplify the notation for examples involving several variables, in the following we will use Px'_0 to denote Py_0.

Taking into account that (1) involves some algebraic equations, a consistent initial value has to fulfill precisely these algebraic equations. If higher index problems are considered, the differentiation of these algebraic equations leads to further algebraic equations, called hidden constraints, which a consistent initial value has to fulfill, too.

Notice now that all solutions of (1) lie in

$$M_0(t) := \{x \in \mathcal{D} : W_0 b(x,t) = 0\}.$$

In the index-1 case, the set of consistent initial values is given by $M_0(t)$.

For the index-2 case, the consistent initial values have to lie in a subset denoted

$$M_1(t) \subset M_0(t),$$

which is defined by the so-called hidden constraints and $M_0(t)$. For higher index cases, corresponding subsets have to be considered.

2 Consistent initialization for index-2 DAEs

With regard to Sections 3 and 4 we briefly summarize some results from [3]. Note that we considerably simplified some of the assumptions taking advantage of the structural properties of the equations that will be considered in this paper.

In the following, we assume that (1) is index-2 tractable and that sufficient smoothness is given. Moreover, for

$$S(x,t) := \{z \in I\!R^m : W_0 b'_x(x,t) z = 0\}.$$

we assume that

$$N \cap S(x,t) \qquad \text{is constant,}$$

define T as a projector onto $N \cap S(x,t)$, suppose that $TQ = QT = T$ holds, and define $U := I - T$.

Note that $N \cap S(x,t)$ describes the so-called index-2 components. Hence, Tx is determined neither by a differential equation nor by a derivative-free equation, but by inherent differentiation.

Let us further assume that

$$\text{im } (A + b'_x(x,t)Q)$$

is constant and define W_1 as a projector along im $(A + b'_x(x,t)Q)$ with $W_1 W_0 = W_1$.

Let us finally suppose that (1) has the following structure that restricts the nonlinearity

$$Ax'(t) + \tilde{b}(Ux(t),t) + \mathcal{B}(Ux(t),t)Tx(t) = 0 \tag{2}$$

for a matrix $\mathcal{B}(Ux(t),t)$, i.e., we suppose, that the $N \cap S$-component occurs only linearly.

For this specific structure it results that the hidden constraints arise only from the differentiated W_1–part of the equations, i.e., from

$$(W_1\tilde{b})'_x(Ux,t)Px' + (W_1\tilde{b})'_t(Ux,t) \quad = \quad 0. \tag{3}$$

Correspondingly, the set of consistent initial values for a DAE system of the form (2) is given by

$$\begin{aligned} M_1(t) \quad := \quad \Big\{ z : \ \exists y \quad & A(Uz,t)y + \tilde{b}(Uz,t) + \mathcal{B}(Uz,t)Tz = 0, \\ & (W_1\tilde{b})'_x(Uz,t)y + (W_1\tilde{b})'_t(Uz,t) = 0 \Big\}. \end{aligned}$$

As a consequence, consistent initial values can be computed as follows:

Theorem 2.1 *[3] Suppose that some values (x^0, Py^0) fulfilling*

$$Ay^0 + \tilde{b}(Ux^0, t_0) + \mathcal{B}(Ux^0, t)Tx^0 \quad = \quad 0$$

are given. We obtain a consistent initialization (x_0, Py_0) starting up from (x^0, Py^0) setting $Ux_0 := Ux^0$, computing the unique solution $(\hat{x}_0, P\hat{y}_0)$ of the linear system

$$\begin{aligned} A\hat{y}_0 + \mathcal{B}(Ux_0,t)T\hat{x}_0 &= 0, \\ U\hat{x}_0 &= 0, \\ (W_1\tilde{b})'_x(Ux_0,t_0)P[y^0 + \hat{y}_0] & \\ +(W_1\tilde{b})'_t(Ux_0,t_0) &= 0, \end{aligned}$$

and setting

$$\begin{aligned} x_0 &= x^0 + \hat{x}_0, \\ Py_0 &= Py^0 + P\hat{y}_0. \end{aligned}$$

Note that the above structural assumptions are more restrictive than in [3], where:

- on the one hand, $A(Ux,t)$ was allowed. This assumption was required for the conventional MNA equations.

- on the other hand, $W_1(Ux, t)$ was allowed. This assumption was required for the charge-oriented MNA equations. Thus, in the equation corresponding to (3) the projector W_1 is not differentiated in [3].

However, for the applications considered below the simplified assumptions are sufficient. Moreover, we will see that the equations from Section 3 present the special structure

$$Ax'(t) + \tilde{b}(Ux(t), t) + \mathcal{B}Tx(t) = 0, \tag{4}$$

for a constant matrix $\mathcal{B}$. This special structure was also carefully analyzed in [3] with regard to numerical consequences for the implicit Euler method and the trapezoidal rule.

3 Water tube system

In this section we focus on DAEs resulting for the water tube system problem presented in [9]. Firstly, we formulate the equations in general terms and give, secondly, some numerical results for the specific example of [9].

Note that a water tube system is represented by a set of n_{nodes} nodes, wich are connected by n_{tubes} tubes. Hence, we can consider it as a oriented graph of nodes and branches and describe it by the incidence Matrix $A \in I\!R^{n_{nodes} \times n_{tubes}}$:

$$a_{ik} := \begin{cases} +1 & \text{if branch k leaves node } i, \\ -1 & \text{if branch k enters node } i, \\ 0 & \text{if branch } k \text{ is not incident with node } i. \end{cases}$$

This incidence matrix describes the branch-node relations of the network graph. Note that in [9] the node-node incidence matrix is used instead.

In the model, every node can have inflow and outflow. We describe them by $e^{in}(t) \in I\!R^{n_{nodes}}$ and $e^{out}(t) \in I\!R^{n_{nodes}}$.

There are two kinds of nodes: buffer nodes (b-nodes), to which a buffer is attached, and normal nodes (n-nodes). Hence, we suppose

$$n_{nodes} = n_b + n_n.$$

Let us assume that the nodes are ordered in such a way that we may split the incidence matrix as follows

$$A = \begin{pmatrix} A_b \\ A_n \end{pmatrix}, \quad A_b \in I\!R^{n_b \times n_{tubes}}, \quad A_n \in I\!R^{n_n \times n_{tubes}}$$

i.e., b-nodes are described first and n-nodes subsequently.

To model the flow of the water, several quantities are considered, whereas some of them can be computed directly from others. Let $p_b \in I\!R^{n_b}$ and $p_n \in I\!R^{n_n}$ be vectors describing the pressure in the buffer and the normal nodes, respectively. According to [9], to model the flow through the tubes, $\phi \in I\!R^{n_{tubes}}$, equations of the form

$$V\phi' = A_b^T p_b + A_n^T p_n + g_1(\lambda, \phi, t)$$

are considered, whereas V is a diagonal matrix, g_1 is a nonlinear function, and the coefficients of resistance of the tubes, $\lambda \in I\!R^{n_{tubes}}$, are related to ϕ by nonlinear equations of the form

$$g_2(\lambda, \phi, t) = 0.$$

Let us analogously suppose that correspondingly ordered vectors

$$e^{in}(t) = \begin{pmatrix} e_b^{in} \\ e_n^{in} \end{pmatrix} \qquad e^{out}(t) = \begin{pmatrix} e_b^{out} \\ e_n^{out} \end{pmatrix}$$

are given. Applying Kirchhoff's Law to each node we obtain:

$$\begin{aligned} A_b\phi + e_b^{in}(t) + e_b^{out}(t) &= Cp_b', \\ A_n\phi + e_n^{in}(t) + e_n^{out}(t) &= 0, \end{aligned}$$

whereas C is a diagonal Matrix.

Summarizing, the equations present the following structure

$$V\phi' = A_b^T p_b + A_n^T p_n + g_1(\lambda, \phi, t), \tag{5}$$
$$0 = g_2(\lambda, \phi, t), \tag{6}$$
$$Cp_b' = A_b\phi + e_b^{in}(t) + e_b^{out}(t), \tag{7}$$
$$0 = A_n\phi + e_n^{in}(t) + e_n^{out}(t). \tag{8}$$

Assuming that V and C are constant regular matrices, $\frac{\partial g_2}{\partial \lambda}$ is nonsingular, and A_n has full row rank, it follows that all assumptions from Section 2 are fulfilled. For $x = (\phi, \lambda, p_b, p_n)$ the corresponding projectors read:

$$W_0 = \begin{pmatrix} 0 & & & \\ & I_{n_{tubes}} & & \\ & & 0 & \\ & & & I_{n_n} \end{pmatrix}, \qquad W_1 = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & I_{n_n} \end{pmatrix},$$

$$Q = \begin{pmatrix} 0 & & & \\ & I_{n_{tubes}} & & \\ & & 0 & \\ & & & I_{n_n} \end{pmatrix}, \qquad T = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 0 & \\ & & & I_{n_n} \end{pmatrix},$$

whereas $I_{n_{tubes}}$ and I_{n_n} denote the identity matrices of the dimension n_{tubes} and n_n (for normal nodes), respectively.

In fact, straightforward computation leads to the hidden contraints

$$0 = A_n V^{-1}\left(A_b^T p_b + A_n^T p_n + g_1(\lambda, \phi, t)\right) + e_n^{in'}(t) + e_n^{out'}(t).$$

With regard to the computation of a consistent initialization let us suppose that values

$$(\phi^0, \lambda^0)$$

that fulfill

$$\begin{aligned} 0 &= g_2(\lambda^0, \phi^0, t_0), \\ 0 &= A_n\phi^0 + e_n^{in}(t_0) + e_n^{out}(t_0), \end{aligned}$$

and some arbitrary values

$$(p_b^0, p_n^0)$$

are given and define

$$\begin{aligned}
\phi'^0 &= V^{-1}\left(A_b^T p_b^0 + A_n^T p_n^0 + g_1(\lambda^0, \phi^0, t_0)\right), \\
p_b'^0 &= C^{-1}\left(A_b \phi^0 + e_b^{in}(t_0) + e_b^{out}(t_0)\right).
\end{aligned}$$

Then, accordingly to Theorem 2.1, a consistent initalization can be determined as follows:

- First of all, set

$$\begin{aligned}
\phi_0 &:= \phi^0, \\
\lambda_0 &:= \lambda^0, \\
p_{b0} &:= p_b^0.
\end{aligned}$$

- Secondly, determine $(\hat{p}_{n_0}, \hat{\phi}'_0)$ solving

$$\begin{aligned}
V\hat{\phi}'_0 &= A_n^T \hat{p}_{n_0}, \\
0 &= A_n\left(\phi'^0 + \hat{\phi}'_0\right) + e_n^{in'}(t_0) + e_n^{out'}(t_0).
\end{aligned}$$

  Since A_n has full row rank, the solution of this system is uniquely defined.

- Finally, set

$$\begin{aligned}
p_{n0} &:= p_n^0 + \hat{p}_{n_0}, \\
\phi'_0 &:= \phi'^0 + \hat{\phi}'_0, \\
p'_{b0} &:= p_b'^0.
\end{aligned}$$

Finally, let us point out that, since p_n (the index-2 component) appears only linearly with constant coefficients, the structural properties corresponding to (4) are given for

$$\mathcal{B} = \begin{pmatrix} 0 & 0 & 0 & A_n^T \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{9}$$

Let us now focus on the example of [9]. The Matrix A reads

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & -1 & 1 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$

Due to the fact that all diagonal elements of V are supposed to be equal to v, for $\phi^{'0} = 0$ it results (considering the quadratic norm):

$$
\begin{aligned}
\hat{p}_{1_0} &= -\frac{v}{275}\left(521 \cdot e_1^{in'}(t_0) + 4 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{2_0} &= -\frac{v}{275}\left(246 \cdot e_1^{in'}(t_0) + 4 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{3_0} &= -\frac{v}{275}\left(94 \cdot e_1^{in'}(t_0) + 6 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{4_0} &= -\frac{v}{275}\left(36 \cdot e_1^{in'}(t_0) + 14 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{6_0} &= -\frac{v}{275}\left(123 \cdot e_1^{in'}(t_0) + 2 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{7_0} &= -\frac{v}{275}\left(14 \cdot e_1^{in'}(t_0) + 36 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{9_0} &= -\frac{v}{275}\left(2 \cdot e_1^{in'}(t_0) + 123 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{10_0} &= -\frac{v}{2} e_{10}^{out'}(t_0), \\
\hat{p}_{11_0} &= -\frac{v}{275}\left(4 \cdot e_1^{in'}(t_0) + 246 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{12_0} &= -\frac{v}{275}\left(6 \cdot e_1^{in'}(t_0) + 94 \cdot e_{13}^{in'}(t_0)\right), \\
\hat{p}_{13_0} &= -\frac{v}{275}\left(4 \cdot e_1^{in'}(t_0) + 521 \cdot e_{13}^{in'}(t_0)\right).
\end{aligned}
$$

Observe how the symmetry of the result reflects the symmetry of the network represented in [9].

Since in the example all values of the derivatives of the input and output functions are zero, $\hat{p}_{n_0}$ is also zero and the given value from [9] is trivially consistent.

On that account, let us consider for x^0 the numerical solution for $t_0 = 0.612E+05$ using PSIDE as described in [9]. Suppose that for $(\phi^0, \lambda^0, p_b^0)$ precisely these values are given and, in order to test our initialization approach, assume $p_n^0 = 0$. Note that the corresponding value of $\phi^{'0}$ is not zero. The consistent value for p_n results to be

$$
p_{n_0} = \hat{p}_{n_0} = 1.0e+005 \cdot \begin{pmatrix} 1.11127172445388 \\ 1.11127016244451 \\ 1.11126938591833 \\ 1.11126940383237 \\ 1.11126937696131 \\ 1.11127023410067 \\ 1.11127450541665 \\ 1.11125515888109 \\ 1.11127896524092 \\ 1.11127125287727 \\ 1.11129851077039 \end{pmatrix}.
$$

These values do not coincide exactly with the values obtained by PSIDE for $t_0 = 0.612E+05$. In fact, if also for p_n^0 the values from the numerical solution are chosen, then for consistency we still obtain a correction:

$$\hat{p}_{n_0} = \begin{pmatrix} 0.06457236291058 \\ 0.03105146480413 \\ 0.01305629910703 \\ 0.00811743250241 \\ 0.01552573239479 \\ 0.01129599829834 \\ 0.00859008476985 \\ 0.00000000001433 \\ 0.01718016952515 \\ 0.02577056230529 \\ 0.01717986154569 \end{pmatrix}.$$

Hence, the latter values precisely give us information about the 'inconsistency' of the numerical solution.

Note finally that due to (9), the results from [3] imply for the implicit Euler method and the trapezoidal rule that an error in p_n is not transferred to other components. In fact, the Euler method gives the same results starting with x^0 and x_0 and for the trapezoidal rule it holds that the results differ only in p_n.

4 DAEs in Hessenberg form with restricted nonlinearity

For index-2 DAEs in Hessenberg form the restricted nonlinearity described by (2) implies that the equations present the form

$$\begin{aligned} x_1'(t) &= \tilde{b}_1(x_1(t),t) + \mathcal{B}_1(x_1(t),t)x_2(t), & (10) \\ 0 &= \tilde{b}_2(x_1(t),t). & (11) \end{aligned}$$

Note that all structural assumptions from Section 2 are given and that it holds

$$T = Q = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \quad W_1 = W_0 = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}.$$

In this case, Theorem 2.1 implies that, if values ${x_1}^0$ fulfilling (11) are given, for computing a consistent initialization we set $x_{10} = x_1^0$ and then solve the linear system that reads:

$$\begin{aligned} y_{10} &= \tilde{b}_1(x_{10},t) + \mathcal{B}_1(x_{10},t_0)x_{20}, \\ 0 &= [\tilde{b}_2]_x'(x_{10},t_0)y_{10} + [\tilde{b}_2]_t'(x_{10},t_0), \end{aligned}$$

where (y_{10}, x_{20}) are the unknowns.

As an example, the equations used for the simulation of the dynamics of multibody systems in the index-2 formulation from [8] precisely present this structure.

Let us now focus on the generalization of this initialization approach.

Definition 4.1 *[5] Consider nonlinear Hessenberg DAEs of order r, $r \geq 2$, presenting the structure:*

$$\begin{aligned} x_1' &= B_{1,r}(x_1, x_2, ..., x_{r-1}, t)x_r + g_1(x_1, x_2, ..., x_{r-1}, t), && (12)\\ x_i' &= B_{i,i-1}(x_i, x_{i+1}, \ldots, x_{r-1}, t)x_{i-1} + g_i(x_i, ..., x_{r-1}, t), && (13)\\ 0 &= f_r(x_{r-1}, t), && (14) \end{aligned}$$

$x_1 \in I\!R^{m_1}$, $x_r \in I\!R^{m_r}$, $x_i \in I\!R^{m_i}$, $m = m_1 + ... + m_r$, $g_i \in I\!R^{m_i}$,
$B_{1,r} \in I\!R^{m_1 \times m_r}$, $B_{i,i-1} \in I\!R^{m_i \times m_{i-1}}$, $i = 2, ..., r-1$, *and*

$$\frac{\partial f_r}{\partial x_{r-1}} \cdot \frac{\partial f_{r-1}}{\partial x_{r-2}} \cdots \frac{\partial f_2}{\partial x_1} \cdot \frac{\partial f_1}{\partial x_r} \quad = \quad \frac{\partial f_r}{\partial x_{r-1}} \cdot B_{r-1,r-2} \cdots B_{2,1} \cdot B_{1,r}$$

is nonsingular. We denote this class of nonlinear systems DAEs in "Hessenberg form with restricted nonlinearity".

Recall that for DAEs in Hessenberg form the order coincides with the index and that, consequently, the computation of a consistent initialization involves $r-1$ differentiations.

Definition 4.2 *[5] To shorten denotations, we introduce successively the following abbreviations:*

$$\begin{aligned} \Omega_{r-1} &:= \left(\frac{\partial f_r}{\partial x_{r-1}}\right)\\ \Omega_{r-i} &:= \Omega_{r-i+1} B_{r-i+1,r-i} \quad \textit{for} \quad i = 2, \ldots, r-1. \end{aligned}$$

Note that this definition implies:

$$\begin{aligned} \Omega_{r-1} &:= \Omega_{r-1}(x_{r-1}, t),\\ \Omega_{r-i} &:= \Omega_{r-i}(x_{r-i+1}, \ldots, x_{r-1}, t) \quad \textit{for} \quad i = 2, \ldots, r-1. \end{aligned}$$

Define further

$$\begin{aligned} R_{r-1}(x_{r-1}, t) &:= \frac{\partial f_r}{\partial t}(\cdot),\\ R_{r-i}(x_{r-i}, \ldots, x_{r-1}, t) &:= \frac{\partial\big(\Omega_{r-i}(\cdot)x_{r-i} + \Omega_{r-i+1}(\cdot)g_{r-i+1}(\cdot) + R_{r-i+1}(\cdot)\big)}{\partial t}\\ + \sum_{j=r-i+1}^{r} & \Bigg(\frac{\partial\big(\Omega_{r-i}(\cdot)x_{r-i} + \Omega_{r-i+1}(\cdot)g_{r-i+1}(\cdot) + R_{r-i+1}(\cdot)\big)}{\partial x_j}\\ & \cdot [B_{j,j-1}(\cdot)x_{j-1} + g_j(\cdot)] \Bigg) \end{aligned}$$

for $i = 2, \ldots, r-1$ successively.

Theorem 4.3 *[5] Consider DAEs in Hessenberg form with restricted nonlinearity of order r. Suppose that a value x_{r-1}^0, that fulfills the equation*

$$0 \;=\; f_r(x_{r-1}^0, t_0),$$

and some arbitrary values $(x_1^0, \ldots, x_{r-2}^0)$ are given.
Then, we may calculate a consistent initial value $(x_{10}, \ldots, x_{r0})$ as follows:

- *Set* $x_{r-1_0} := {x_{r-1}}^0$.
- *Consider* $j = r-2, \ldots, 1$ *successively. In each step,* $x_{j+1_0}, \ldots, x_{r-1_0}$ *are supposed to be fixed from previous steps and we proceed to compute* x_{j_0} *considering the correction*

  $$\hat{x}_{j_0} := x_{j_0} - {x_j}^0.$$

  This correction $\hat{x}_{j_0}$ *with* $\|\hat{x}_{j_0}\| = \min$ *is computed by solving the possibly underdetermined linear system*

  $$\Omega_j \hat{x}_{j_0} = -\Omega_j {x_j}^0 - \Omega_{j+1}(\cdot) g_{j+1}(\cdot) - R_{j+1}(\cdot),$$

  whereas for all the values that appear in the expressions $\Omega_j(\cdot)$, $g_{j+1}(\cdot)$, *and* $R_{j+1}(\cdot)$ *we substituted the values* $(x_{j+1_0}, \ldots, x_{r-1_0})$ *calculated in the corresponding previous steps. Once the correction is determined, we simply set*

  $$x_{j_0} = {x_j}^0 + \hat{x}_{j_0}.$$

  Consequently, we obtain a value x_{j_0} *that fulfills the hidden constraint and*

  $$\left\| x_{j_0} - x_j^0 \right\| = \min.$$

- *Finally,* x_{r0} *is determined as the solution of the linear system*

  $$\Omega_1(\cdot) B_{1,r}(\cdot) x_{r0} = -\Omega_1(\cdot) g_1(\cdot) - R_1(\cdot).$$

After calculating these values, the corresponding initial values for the derivatives, $x'_{1_0}, \ldots, x'_{r-1_0}$, *may be calculated directly from the equations (12)-(14).*

In [5], the approach is illustrated for several examples of [9] in Hessenberg form. For the common index-3 formulation of the equations used for the simulation of the dynamics of multibody systems, the above stated assumptions are given and the initialization procedure coincides, in fact, with the proposal presented in [10].

5 DAEs in Hessenberg triangular chain form

With regard to yet another generalization, in the following we say that a DAE is in a (lower) Hessenberg triangular chain form of order k and with restricted nonlinearity, if it can be written as

$$\begin{array}{rcl} H_1(x_1', x_1, t) &=& 0 \\ H_2(x_2', x_1, x_2, t) &=& 0 \\ & \vdots & \\ H_k(x_k', x_1, \ldots, x_k, t) &=& 0 \end{array}$$

and the system defined by the funcion H_j is in Hessenberg form in the variable x_j with restricted nonlinearity, i.e., for $x_j = (x_{j_1}, \ldots, x_{j_{r_j}})$ it is of the Hessenberg form of order r_j, $r_j \geq 2$:

$$\begin{aligned}
x'_{j_1} &= B^j_{1,j_{r_j}}(x_1, \ldots, x_{j-1}, x_{j_1}, x_{j_2}, ..., x_{j_{r_j-1}}, t)x_{j_{r_j}} \\
&\quad + g^j_{j_1}(x_1, \ldots, x_{j-1}, x_{j_1}, x_{j_2}, ..., x_{j_{r_j-1}}, t), \\
x'_{j_i} &= B^j_{j_i,j_i-1}(x_1, \ldots, x_{j-1}, x_{j_i}, x_{j_{i+1}}, \ldots, x_{j_{r_j-1}}, t)x_{j_{i-1}} \\
&\quad + g^j_{j_i}(x_1, \ldots, x_{j-1}, x_{j_i}, ..., x_{j_{r_j-1}}, t), \\
0 &= f^j_{r_j}(x_1, \ldots, x_{j-1}, x_{j_{r_j-1}}, t),
\end{aligned}$$

$x_{j_1} \in I\!R^{m_{j_1}}$, $x_{j_{r_j}} \in I\!R^{m_{j_{r_j}}}$, $x_{j_i} \in I\!R^{m_{j_i}}$, $m_j = m_{j_1} + ... + m_{j_{r_j}}$, $g^j_{j_i} \in I\!R^{m_{j_i}}$, $B^j_{1,r_j} \in I\!R^{m_{j_1} \times m_{j_{r_j}}}$, $B^j_{j_i,j_{i-1}} \in I\!R^{m_{j_i} \times m_{j_{i-1}}}$, $j_i = j_2, ..., j_{r_j-1}$, and

$$\frac{\partial f^j_{r_j}}{\partial x_{j_{r_j-1}}} \cdot B^j_{j_{r_j-1}, j_{r_j-2}} \cdots B^j_{j_2,j_1} \cdot B^j_{j_1,j_{r_j}}$$

is nonsingular.

A consistent initialization for systems that present the above defined structure can be undertaken as follows:

- Determine a consistent initial value x_{10} as stated in Theorem 4.3 and compute all corresponding values for ${x_1}'_0$. Note that in order to determine ${x_{r_1}}'_0$ the expression

$$\begin{aligned}
\Omega^1_1(x_{1_2}, \ldots, x_{1_{r_1-1}})B^1_{1,r_1}(x_{1_1}, \ldots, x_{1_{r_1-1}}, t)x_{1_{r_1}} = \\
-\Omega^1_1(x_{1_2}, \ldots, x_{1_{r_1-1}}, t)g^1_1(x_{1_1}, \ldots, x_{1_{r_1-1}}, t) - R^1_1(x_{1_2}, \ldots, x_{1_{r_1-1}}, t)
\end{aligned}$$

  has to be differentiated and all values have to be substituted. However, this differentiation for the computation of ${x_{r_1}}'_0$ is only necessary, if x_{r_1} appears in subsequent blocks.

- Determine successive consistent values x_{j_0} ($j = 2, \ldots, k$ successively) as follows:
  - Determine a value $x^0_{j_{r_j-1}}$ that fulfills the equation

$$0 = f^j_{r_j}(x_{10}, \ldots, x_{j-1_0}, x^0_{j_{r_j-1}}, t_0)$$

    and some arbitrary values $(x^0_{j_1}, \ldots, x^0_{j_{r_j-2}})$. Set $x_{j_{r_j-1}0} = x^0_{j_{r_j-1}}$.
  - Consider $i = r_j - 2, \ldots, 1$ successively. In each step,

$$x_{10}, \ldots, x_{j-1_0}, x_{j_{i+1}0}, \ldots, x_{j_{r_j-1}0}$$

    are fixed and we proceed to compute x_{j_i0} considering the correction

$$\hat{x}_{j_{i0}} := x_{j_i0} - {x_{j_i}}^0.$$

    This correction $\hat{x}_{j_{i0}}$ with $\left\|\hat{x}_{j_{i0}}\right\| = \min$ is computed by solving a possibly underdetermined linear system analogously as described in Theorem 4.3 .

– Compute all corresponding values for ${x_j}_0'$ analogously as we did for ${x_1}_0'$. Again, the additional differentiation is only necessary, if the $x_{j_{r_j}}$-component of a block H_j appears in subsequent Hessenberg blocks.

Note that for this generalization there are two main aspects that have to be taken into account:

- The nonlinear equations

$$0 = f^j_{r_j}(x_{10}, \ldots, x_{j-10}, x^0_{j_{r_j-1}}, t_0)$$

have to be solved for each block H_j. Hence, a consistent initialization cannot be computed solving only linear subproblems unless these equations are linear.

- In each step, we may need to compute not only $P{x_j}_0'$, but ${x_j}_0'$, if the $x_{j_{r_j}}$-component of a block H_j appears in subsequent Hessenberg blocks.

We illustrate this straight-forward generalization and the specified aspects by means of a well-known example.

Consider the DAEs resulting from the exothermic reactor model (cf. [11]):

$$\begin{aligned}
C' &= K_1(C_f(t) - C) - R, && (15)\\
0 &= C - u(t), && (16)\\
T' &= K_1(T_f(t) - T) + K_2 R - K_3(T - T_C), && (17)\\
0 &= R - K_3 e^{\frac{-K_4}{T}} C, && (18)
\end{aligned}$$

whereas K_1, K_2 K_3 K_4 are constants, C_f and T_f are the feed reactant concentration and feed temperature (assumed to be known functions). The variables C and T are the corresponding quantities in the product, $u(t)$ is an input function prescibing C, R is the reaction rate per unit volume, and T_C is the temperature of the cooling medium (which can be varied).

Note that (15)-(16) presents a Hessenberg triangular chain form of order 2. For the above notation this would imply that for $x_1 = (C, R)$, (15)-(16) correspond to

$$H_1(x_1', x_1, t) = 0.$$

Since the order of H_1 is 2, consistent initial values C_0 and R_0 result as follows:
Set

$$C_0 := u(t_0)$$

and afterwards

$$R_0 := K_1(C_f(t_0) - C_0) - u'(t_0).$$

Set then

$$C_0' = u'(t_0)$$

and

$$R_0' := K_1(C_f'(t_0) - u'(t_0)) - u''(t_0).$$

Note that the last value has to be determined because R appears in equation (18).

Moreover, for $x_2 = (T, T_C)$, (17)-(18) is in Hessenberg form in the variable x_2. Hence, (17)-(18) correspond to

$$H_2(x_2', x_1, x_2, t) = 0.$$

The order from H_2 is again 2. Consistent initial values result then as follows.

To obtain T_0 solve the nonlinear equation

$$R_0 = K_3 e^{\frac{-K_4}{T_0}} C_0.$$

Afterwards, determine T_{C0} by solving the linear equation

$$\begin{aligned} 0 &= K_1(C_f'(t_0) - u'(t_0)) - u''(t_0) \\ &\quad -K_3 e^{\frac{-K_4}{T_0}} C_0 \frac{-K_4}{T_0^2} \left(K_1(T_f(t_0) - T_0) + K_2 R_0 - K_3(T_0 - T_{C0})\right) \\ &\quad -K_3 e^{\frac{-K_4}{T_0}} C_0'. \end{aligned}$$

6 DAEs in Hessenberg form with coupled index-1 constraints

In this section we consider DAEs presenting Hessenberg form with restricted nonlinearity coupled with index-1 conditions. DAEs of this type appear, for instance, in the modeling of contact problems in multibody systems dynamics.

Definition 6.1 *Consider nonlinear DAEs presenting the structure:*

$$\begin{aligned} x_1' &= B_{1,r}(x_1, x_2, ..., x_{r-1}, x_{r+1}, t)x_r + g_1(x_1, x_2, ..., x_{r-1}, x_{r+1}, t), && (19) \\ x_i' &= B_{i,i-1}(x_i, x_{i+1}, \dots, x_{r-1}, x_{r+1}, t)x_{i-1} + g_i(x_i, ..., x_{r-1}, x_{r+1}, t), && (20) \\ 0 &= f_r(x_{r-1}, x_{r+1}, t), && (21) \\ 0 &= f_{r+1}(x_{r-1}, x_{r+1}, t) && (22) \end{aligned}$$

$r \geq 2$, $x_1 \in I\!R^{m_1}$, $x_r \in I\!R^{m_r}$, $x_{r+1} \in I\!R^{m_{r+1}}$, $x_i \in I\!R^{m_i}$, $m = m_1 + ... + m_r + m_{r+1}$, $g_i \in I\!R^{m_i}$, $B_{1,r} \in I\!R^{m_1 \times m_r}$, $B_{i,i-1} \in I\!R^{m_i \times m_{i-1}}$, $i = 2, ..., r-1$, whereas

$$\frac{\partial f_r}{\partial x_{r-1}} \cdot B_{r-1,r-2} \cdots B_{2,1} \cdot B_{1,r}$$

is nonsingular and

$$\frac{\partial f_{r+1}}{\partial x_{r+1}}$$

is nonsingular.

A consistent initialization for systems that present this structure can be undertaken as follows. Suppose that values (x_{r-1}^0, x_{r+1}^0) fulfilling

$$\begin{aligned} 0 &= f_r(x_{r-1}^0, x_{r+1}^0, t_0), \\ 0 &= f_{r+1}(x_{r-1}^0, x_{r+1}^0, t_0) \end{aligned}$$

and some arbitrary values $(x_1^0, \ldots, x_{r-2}^0)$ are given.
Then, we may calculate a consistent initial value $(x_{1_0}, \ldots, x_{r0})$ as follows:

- Set

$$\begin{aligned} x_{r-1_0} &:= x_{r-1}{}^0, \\ x_{r+1_0} &:= x_{r+1}{}^0. \end{aligned}$$

- Determine x'_{r+1_0} and x_{r-2_0} solving the system

$$\begin{aligned} 0 &= [f_r]'_{x_{r+1}}(x_{r-1_0}, x_{r+1_0}, t_0)x'_{r+1_0} + \\ &\quad [f_r]'_{x_{r-1}}(x_{r-1_0}, x_{r+1_0}, t_0)\,(B_{r-1,r-2}x_{r-2_0} + g_{r-1}) + \\ &\quad [f_r]'_t(x_{r-1_0}, x_{r+1_0}, t_0) \\ 0 &= [f_{r+1}]'_{x_{r+1}}(x_{r-1_0}, x_{r+1_0}, t_0)x'_{r+1_0} + \\ &\quad [f_{r+1}]'_{x_{r-1}}(x_{r-1}^0, x_{r+1}^0, t_0)\,(B_{r-1,r-2}x_{r-2_0} + g_{r-1}) + \\ &\quad [f_{r+1}]'_t(x_{r-1_0}, x_{r+1_0}, t_0) \\ \left\| x_{r-2_0} - x_{r-2}^0 \right\| &= \min \end{aligned}$$

  for

$$\begin{aligned} B_{r-1,r-2} &= B_{r-1,r-2}(x_{r-1_0}, x_{r+1_0}, t_0), \\ g_{r-1} &= g_{r-1}(x_{r-1_0}, x_{r+1_0}, t_0). \end{aligned}$$

  At this point, we assume that this system is solvable. Later on we will see that this assumption is usual for the DAEs arising from contact problems.

- Determine successively x_{j_0} for $j = r-3, \ldots, 1$ and x_{r_0} analogously to Theorem 4.3, considering additionally x_{r+1_0} and x'_{r+1_0}.

As an example presenting these structural properties let us consider the structure of contact problems in multibody dynamics as stated in [2]. Denote

- $p \in \mathbb{R}^{n_p}$ are position coordinates,
- $p_r \in \mathbb{R}^{n_{con}}$ are the coordinates of the contact points,
- $v \in \mathbb{R}^{n_p}$ are velocities,
- $\lambda \in \mathbb{R}^{n_\lambda}$ are Lagrange multipliers, with $n_\lambda \leq n_p$,

- $M(p)$ is the positive definite mass matrix,
- $f(p, p_r, v)$ are the applied outer forces,
- $g_{con}(p, p_r)$ are the contact conditions,
- $g_{npe}(p, p_r)$ are the non-penetrating conditions,
- $G(p, p_r) := \frac{\partial g_{con}}{\partial p}(p, p_r)$ is the constraint matrix with full rank n_λ.

Moreover, due to the specific relation between the contact and the non-penetrating conditions

$$\frac{\partial g_{con}}{\partial p_r}(p, p_r) = 0 \tag{23}$$

holds (cf. [2]).

The formulation presented in [2] reads:

$$\begin{aligned} p' &= v, \\ M(p)v' &= f(p, p_r, v) - G(p, p_r)^T \lambda, \\ 0 &= g_{con}(p, p_r), \\ 0 &= g_{npe}(p, p_r). \end{aligned}$$

To recognize the structure introduced above, we prefer the following equivalent form:

$$\begin{aligned} v' &= M(p)^{-1} f(p, p_r, v) - M(p)^{-1} G(p, p_r)^T \lambda, \\ p' &= v, \\ 0 &= g_{con}(p, p_r), \\ 0 &= g_{npe}(p, p_r). \end{aligned}$$

We assume that the assumptions from Definition 6.1 are given and the index is 3. According to the approach presented above we have $r = 3$, $x_1 = v$, $x_2 = p$, $x_3 = \lambda$ and $x_4 = p_r$. A consistent initial value can be determined as follows:

- Determine values (p_0, p_{r0}) fulfilling

  $$\begin{aligned} 0 &= g_{con}(p_0, p_{r0}) \\ 0 &= g_{npe}(p_0, p_{r0}) \end{aligned}$$

  and suppose that a value v^0 is given.

- Determine (p'_{r0}, v_0) solving

  $$\begin{aligned} 0 &= [g_{con}]'_p(p_0, p_{r0})v_0 + [g_{con}]'_{p_r}(p_0, p_{r0})p'_{r_0} \\ 0 &= [g_{npe}]'_p(p_0, p_{r0})v_0 + [g_{npe}]'_{p_r}(p_0, p_{r0})p'_{r_0} \\ \left\|v_0 - v^0\right\| &= \min. \end{aligned}$$

Due to (23) and $[g_{con}]'_p = G$ this system is solvable and can be reduced to

$$\begin{aligned} 0 &= G(p_0, p_{r0})v_0 \\ \|v_0 - v^0\| &= \min \end{aligned}$$

and

$$0 = [g_{npe}]'_p(p_0, p_{r0})v_0 + [g_{npe}]'_{p_r}(p_0, p_{r0})p'_{r0}.$$

- Determine λ_0 solving the linear system

$$\begin{aligned} (G(p_0, p_{r0})M(p_0)^{-1}G(p_0, p_{r0})^T)\lambda_0 &= G(p_0, p_{r0})M(p_0)^{-1}f(p_0, p_{r0}, v_0) + \\ &\quad \tilde{G}(p_0, p_{r0}, p'_{r0}, v_0)v_0. \end{aligned}$$

  for $\tilde{G}(p, p_r, p'_r, v) := \frac{d}{dt}G(p, p_r)$.

Note that in applications often $v^0 = 0$ is chosen. In this case it suffices to set $v_0 = v^0 = 0$ and solve

$$(G(p_0, p_{r0})M(p_0)^{-1}G(p_0, p_{r0})^T)\lambda_0 = G(p_0, p_{r0})M(p_0)^{-1}f(p_0, p_{r0}, v_0)$$

to determine λ_0. The computation of p'_{r0} is not required in this case.

So far, the Lagrange multipliers were supposed to fulfill our assumptions on restricted nonlinearity. However, for advanced models that consider friction forces that depend on the constraint forces $-G(p, p_r)^T\lambda$, this property is not given since the resulting force vector may depend nonlinearly on λ, leading to systems of the form

$$\begin{aligned} p' &= v, \\ M(p)v' &= f(p, p_r, v, \lambda) - G(p, p_r)^T\lambda, \\ 0 &= g_{con}(p, p_r), \\ 0 &= g_{npe}(p, p_r). \end{aligned}$$

With regard to the solvability of these systems, it is assumed that the generalized Grübler condition

$$rank\ G(p, p_r) = rank\ G(p, p_r)M(p)^{-1}\left(\frac{\partial f}{\partial \lambda}(p, p_r, v, \lambda) - G(p, p_r)^T\right) = n_\lambda$$

is given. For systems presenting this structure the initialization procedure can be applied straight-forward. In this case, for the computation of λ_0 a nonlinear system has to be solved instead of a linear system.

Let us focus on even more general systems that have additional inner state variables that we denote by β and time-dependent outer forces, leading to equations of the form

$$\begin{aligned} p' &= v, && (24) \\ M(p)v' &= f(p, p_r, v, \lambda, \beta, t) - G(p, p_r)^T\lambda, && (25) \\ \beta' &= d(p, p_r, v, \lambda, \beta, t), && (26) \\ 0 &= g_{con}(p, p_r), && (27) \\ 0 &= g_{npe}(p, p_r). && (28) \end{aligned}$$

With regard to consistent initialization, the value of β_0 can be chosen arbitrarily. p_0, p_{r0} and v_0 are independent of the choice of β_0 and can be determined analogously as in the preceding case. However, the corresponding λ_0 will depend, in general, on the choice of β_0. In fact, if $v^0 = v_0 = 0$ is chosen, λ_0 results from

$$G(p_0, p_{r0})M(p_0)^{-1}\left[f(p_0, p_{r0}, v_0, \lambda_0, \beta_0, t_0) - G(p_0, p_{r0})^T\lambda_0)\right] = 0. \tag{29}$$

Note finally that the wheelset problem from [9] and [2] in its index-3 formulation presents the structure (24)-(28). The normal forces N, that depend on the Lagrange multipliers λ_1 and λ_2, appear in the nonlinear expressions for the creep forces $T_{1,2_{L|R}}$, i.e., f depends nonlinearly on λ. Moreover, β presents the deviation of the angular velocity and is given by an additional differential equation. In the index-2 formulation from [9], the following equations are considered:

$$\begin{aligned} p' &= v, && (30)\\ M(p)v' &= f(p, p_r, v, \lambda, \beta, t) - G(p, p_r)^T\lambda, && (31)\\ \beta' &= d(p, p_r, v, \lambda, \beta, t), && (32)\\ 0 &= G(p, p_r)v, && (33)\\ 0 &= g_{npe}(p, p_r). && (34) \end{aligned}$$

Since λ, that is now the index-2 component, remains in a nonlinear expression, the structure (2) is not given either. Consequently, also in the index-2 formulation we have to solve the nonlinear equations (29) in order to compute λ_0 with our initialization approach. Note that for the wheelset problem the dimension of (30)-(34) is 17 and the dimension of (29) is just 2.

7 Conclusion

In this paper, we give an overview of structural classes of DAEs that allow the step-by-step computation of consistent initial values. For these DAEs, a consistent initialization can be determined sequentially starting from a value that fulfills the explicit constraints. In a second step, a correction of this value is computed solving successively linear subproblems that involve the hidden constraints.

For the DAEs resulting from circuit simulation, such an approach resulted to be especially suitable and allowed a better understanding of numerical features observed in applications (see [3], [4], [6] and [1]). In the first part of this report it is shown how the results from [3] can be applied to DAEs resulting from the simulation of a water tube system.

For DAEs in Hessenberg form of arbitrary order, the approach is also feasible if certain assumptions regarding the nonlinearity are given (see [5]). The DAEs resulting from multibody dynamics precisely fulfill these conditions and the method for the consistent initialization coincides with well-understood approaches from multibody dynamics literature (see e.g. [10]).

In the second part of this report, the results from [5] are generalized for DAEs in Hessenberg triangular chain form. Afterwards, the results from [5] are also generalized for DAEs in Hessenberg form with coupled index-1 constraints. We finally point out that the restricted nonlinearity is not given for some applications and discuss how the initialization approach can be generalized if nonlinear subsystems of equations are solved.

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