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On Asymptotics in Case of Dae's

For some classes of differential-algebraic equations (dae's) $F(x', x, t) = 0$, criteria for the asymptotic stability of solutions will be given. Since dae's represent differential equations on (implicitly given) manifolds, these properties are naturally connected with the related manifolds. Moreover, it is known that the underlying ode for x might show a completely different stability behavior than the dae itself and the differential equation on the manifold, respectively. Since one cannot expect that generic finite difference methods approximate the manifold precisely without profound information on the inner structure, one is faced with changes of the stability properties of finite difference methods compared to the case of explicit differential equations. For linear time-varying dae's, this is exemplified using BDF- and IRK-methods.

1. Introduction

Implicit ordinary differential equations

$$F(x', x, t) = 0 \tag{1}$$

arise frequently in applications. So-called differential-algebraic equations (dae's) are those systems where the Jacobian $\frac{\partial}{\partial y}F(y, x, t)$ is singular for all (y, x, t) from the domain of definition of F. Examples of such systems can be found when modelling constraint mechanical multibody systems, electrical networks, and chemical processes.

The importance of solving dae's has led to a growing number of investigations concerning the numerical solution of such problems. Today, for large classes of dae's, results about the feasibility, (zero-) stability and convergence of numerical methods are known (cf. [2, 1, 3]). On the other hand, only little attention has been paid to the asymptotic behavior of the continuous solutions as well as of their numerical approximations. Mostly it is assumed that the known properties of ode methods remain valid. This assumption is backed up by some results in the index 1 case [2]. We will show that the situation is more complicated in the higher index case.

2. The index 1 case

A number of widely used notions for the characterization of asymptotic properties of integration methods for *explicit* systems relies on the complex scalar test equation

$$z' = \lambda z. \tag{2}$$

The behavior of a numerical method applied to (2) is the same if this method is applied to a linear constant coefficient system

$$x' = Ax. \tag{3}$$

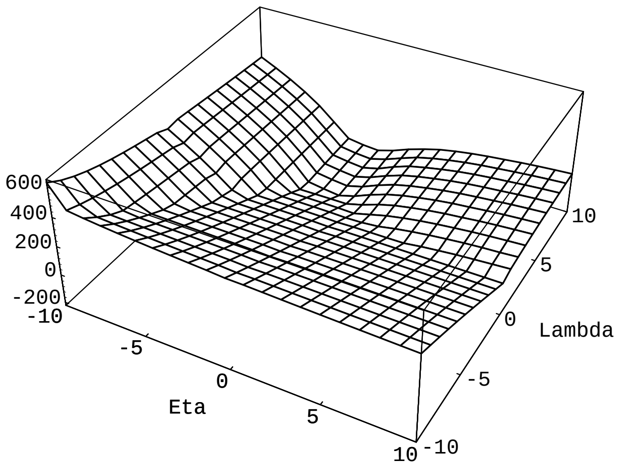
Here, the role of λ is replaced by the eigenvalues of A. The justification for restricting the consideration to (3) is given by Lyapunov's theory: The linearization of a nonlinear autonomous explicit system at a stationary point provides criteria for the asymptotic behavior of solutions. Essentially the same is true for index 1 and 2 dae's [8]. Therefore, we are led to the constant coefficient dae

$$Ax'(t) + Bx(t) = 0 \tag{4}$$

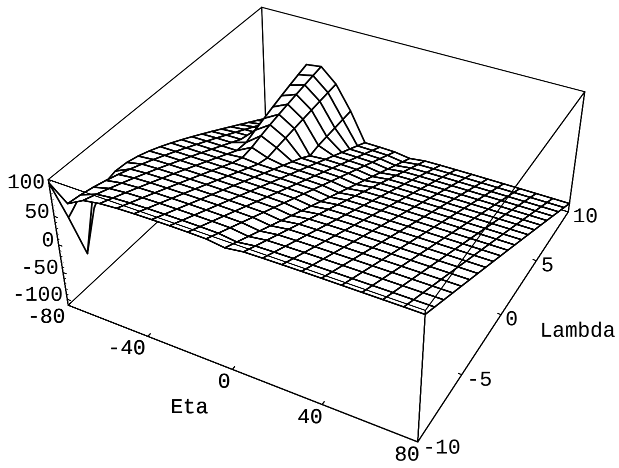
with regular matrix pencil (A, B). This equation can be transformed into the *Kronecker canonical form*

$$\begin{pmatrix} I & 0 \\ 0 & J_0 \end{pmatrix} \begin{pmatrix} y' \\ z' \end{pmatrix} + \begin{pmatrix} W & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = 0. \tag{5}$$

J_0 is a nilpotent matrix ($J_0^k = 0$ for some integer k). Since discretization and transformation to (5) commute for many methods, the numerical solution for z vanishes identically, whereas y is discretized like an explicit system. Hence, the numerical methods preserve their known asymptotic stability properties.



5-step BDF, $T = 40$, $\beta = 1$, $\lambda = -10, \ldots, +10$, $\eta = -10, \ldots, +10$, $h = 0.1$



RKM of Crouzeix, $T = 10$, $\beta = 1$, $\lambda = -10, \ldots, +10$, $\eta = -80, \ldots, +80$, $h = 0.01$

Similar results about B-stability are more difficult to obtain. It is well-known that so-called *algebraically stable* Runge-Kutta methods are B-stable [5, p. 193]. In [2, p. 129] a similar result is shown to be true for index 1 dae's (1) provided that (i) the nullspace $\mathcal{N}(\frac{\partial}{\partial y}F(y,x,t))$ of $\frac{\partial}{\partial y}F(y,x,t)$ does *not* depend on (y,x,t), and (ii) the Runge-Kutta method is a so-called IRK(DAE) (a stiffly accurate method [5, p. 45]). There are simple linear examples showing that the backward Euler method loses its B-stability if (i) is not valid. Note that the backward Euler method is also the 1-step BDF.

3. The index 2 case

Unfortunately, in the case of index 2 dae's the situation is considerably more complicated. Consider the dae

$$A(t)x'(t) + B(t)x(t) = 0, t \geq 0 \tag{6}$$

with

$$A(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, B(t) = \begin{pmatrix} \lambda & -\beta & -1 \\ \beta\eta t(1-\eta t) - \eta & \lambda & -\eta t \\ 1-\eta t & 1 & 0 \end{pmatrix},$$

where $\beta, \eta, \lambda \in \mathbb{R}$ are constants. Note that this is a so-called index 2 Hessenberg system. All solutions of (6) must fulfill the third equation of (6) together with its total derivative $(1-\eta t)x_1' + x_2' - \eta x_2 = 0$ such that

$$\begin{aligned} (1-\eta t)x_1 + x_2 &= 0 \\ \beta\eta t(1-\eta t)x_1 - \beta(1-\eta t)x_2 - x_3 &= 0. \end{aligned}$$

Eliminating the algebraic relations (6) is reduced to the scalar equation $x_1' + \lambda x_1 = 0$. If $x^0 \in \mathbb{R}^3$ is a consistent initial value at $t = 0$, the solution is

$$x(t) = \begin{pmatrix} x_1^0 e^{-\lambda t} \\ x_1^0(\eta t - 1)e^{-\lambda t} \\ x_1^0 \beta(1-\eta t)e^{-\lambda t} \end{pmatrix}.$$

Consequently, the asymptotic stability is governed by the sign of λ independently of η and β. The dae was solved using a 5-step BDF method and an algebraically stable and stiffly accurate 2-stage Runge-Kutta method introduced by Crouzeix [4, p. 207]. The figures show the logarithm of the norm of the numerical solution at the end of the interval $[0,T]$ for different values of η and λ. The analytic solution would result (almost) in a plane. Note that, for $\eta = 0$, the equation is a constant coefficient system. The results indicate that the asymptotic behavior of the numerical solution depends not only on the asymptotic stability of the inherent differential equation (controlled by λ), but also on the geometry of the problem (controlled by η).

4. Asymptotic stability

In view of the results for index 1 dae's it is sufficient to consider time-dependent linear dae's $A(t)x'(t)+B(t)x(t)=0$ for $t\in[0,\infty)$ where the nullspace $\mathcal{N}(A(t))$ of the leading coefficient matrix *does not depend on* t. For our purposes it is even sufficient to restrict ourselves to the class of *semiexplicit* systems, i.e.

$$A(t)=\begin{pmatrix} I & 0\\ 0 & 0\end{pmatrix}, B(t)=-\begin{pmatrix} B_{11}(t) & B_{12}(t)\\ B_{21}(t) & B_{22}(t)\end{pmatrix}.$$

More explicitly, the system under consideration is now

$$\begin{aligned} y' &= B_{11}y+B_{12}z\\ 0 &= B_{21}y+B_{22}z. \end{aligned} \tag{7}$$

Equation (7) is a *transferable* dae or a dae *with global index 1* if $B_{22}(t)$ is nonsingular for all $t\geq 0$. Obviously, (7) is equivalent to the system

$$\begin{aligned} y' &= (B_{11}-B_{12}B_{22}^{-1}B_{21})y\\ z &= -B_{22}^{-1}B_{21}y. \end{aligned} \tag{8}$$

This is a differential equation for y and an algebraic relation for z, which can be evaluated once the differential part has been solved. Naturally, initial conditions are only allowed for y. So (7) is supplemented by

$$y(0)=y^0. \tag{9}$$

In view of (8) it is natural to define asymptotic stability in such a way that only y is concerned. A simplified version of a definition in [2, p. 78] is the following: Equation (7) is called *contractive* if there is a $c>0$ and a symmetric positively definite matrix S such that

$$(S\bar{y})^Ty\leq -c|y|^2 \tag{10}$$

for all $y,\bar{y}$ with $\bar{y}=(B_{11}-B_{12}B_{22}^{-1}B_{21})y$. If there is no algebraic part in (7), the well-known notion of contractivity for explicit systems is restated (cf. [5, p. 191]). For contractive dae's we obtain the exponential decay of solutions: There exists a $\beta>0$ such that

$$(Sy(t))^Ty(t)\leq e^{-\beta(t-t_0)}(Sy(t_0))^Ty(t_0), t\geq t_0.$$

The second equation of (8) provides a similar estimate for z. With the notion of contractivity at hand it is now straightforward to introduce a generalization of the B-stability. The essential result has been given above.

Let us now consider the index 2 case. In order to avoid technical expense we consider the special case of index 2 Hessenberg systems, which we obtain by setting $B_{22}(t)\equiv 0$ in (7). The general case is treated in [6]. Assume in the following $B_{21}(t)B_{12}(t)$ to be nonsingular for all $t\geq 0$. Define

$$H(t)=B_{12}(t)(B_{21}(t)B_{12}(t))^{-1}B_{21}(t). \tag{11}$$

It is easy to see that $H(t)$ is a projection. Multiplying the second row of (7) by $B_{12}(B_{21}B_{12})^{-1}$ one obtains $Hy=0$ (Note $B_{22}=0$!). Multiplication of the first row by B_{21} yields $z=(B_{21}B_{12})^{-1}B_{21}(y'-B_{11}y)$. Finally, multiplication by $I-H$ leads to $(I-H)y'=(I-H)B_{11}y$. Therefore, (7) is equivalent to

$$\begin{aligned} [(I-H)y]' &= [(I-H)B_{11}-H'](I-H)y\\ Hy &= 0\\ z &= (B_{21}B_{12})^{-1}B_{21}([(I-H)y]'+(Hy)'-B_{11}y). \end{aligned} \tag{12}$$

Now the solution of (7) consists of three parts: $(I-H)y$, Hy, and z. While $(I-H)y$ is given by a differential equation, the others are given by algebraic relations. Note the differentiation on the right-hand side of (12) for determining z. Analogously to the index 1 case, notions of asymptotic stability should rely on $(I-H)y$ only and neither on z nor y as a whole. A detailed elaboration can be found in [6].

5. Discretization

The k-step BDF method applied to (1) reads

$$F(\frac{1}{h}\sum_{j=0}^{k}\alpha_j x_{l-j}, x_l, t_l) = 0, l \geq k. \tag{13}$$

At each step, (13) provides an approximation x_l of the exact solution value $x(t_l)$, $t_l = t_0 + lh$. Define $B_{11,l} = B_{11}(t_l)$ etc. Suppose now $B_{22} = 0$ and $B_{21}B_{12}$ to be nonsingular, i.e. (7) is an index 2 Hessenberg system. Then (13) applied to (7) yields

$$\begin{array}{rcl} \frac{1}{h}\sum_{j=0}^{k}\alpha_j y_{l-j} & = & B_{11,l}y_l + B_{12,l}z_l \\ 0 & = & B_{21,l}y_l. \end{array} \tag{14}$$

The latter row yields $H_l y_l = 0$ immediately. Using

$$(I - H_l)\sum_{j=0}^{k}\alpha_j y_{l-j} = \sum_{j=0}^{k}\alpha_j (I - H_{l-j})y_{l-j} + \sum_{j=0}^{k}\alpha_j (H_{l-j} - H_l)y_{l-j}$$

one has the following equivalent of (14)

$$\begin{array}{rcl} \frac{1}{h}\sum_{j=0}^{k}\alpha_j (I - H_{l-j})y_{l-j} & = & \frac{1}{h}\sum_{j=0}^{k}\alpha_j (H_l - H_{l-j})y_{l-j} + (I - H_l)B_{11,l}y_l \\ H_l y_l & = & 0 \\ z_l & = & (B_{21,l}B_{12,l})^{-1}\left(\frac{1}{h}\sum_{j=0}^{k}\alpha_j y_{l-j} - B_{11,l}x_l\right). \end{array} \tag{15}$$

A comparison of (12) and (15) shows that the BDF discretization and splitting commute if and only if H is constant. If this is true, the BDF methods preserve their asymptotic stability properties. Note that the same is true for implicit Runge-Kutta methods and their projected counterparts.

In our numerical example (6) it holds that

$$H(t) = \begin{pmatrix} 1 - \eta t & 1 \\ \eta t(1 - \eta t) & \eta t \end{pmatrix}.$$

This matrix is constant if $\eta = 0$. In this case (6) has constant coefficients. If the subspaces characterized by H change sufficiently fast, the asymptotic stability of BDF and Runge-Kutta methods may get lost.

As a conclusion the authors would like to mention that the observed effects are far from being understood completely. Even the question of a well-motivated test equation is open. What does, e.g., stiffness mean in the present context? A first idea was recently developed for index 2 Hessenberg systems [9]. Moreover, the discussion concerning linear equations should be considered as a prerequisite for discussing nonlinear dae's – even if they are autonomous.

6. References

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