Defect-based a-posteriori error estimation for differential-algebraic equations

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We show how the QDeC estimator, an efficient and asymptotically correct a-posteriori error estimator for collocation solutions to ODE systems, can be extended to differential-algebraic equations of index 1.

1 Problem setting

We consider linear systems of DAEs of index 1,

$$A(t)(D(t)x(t))' + B(t)x(t) = g(t), \quad t \in [a,b], \tag{1}$$

with appropriately smooth data $A(t) \in \mathbf{R}^{m\times n},\ B(t) \in \mathbf{R}^{m\times m}$ and constant $D(t) = D \in \mathbf{R}^{n\times m}$. For the purpose of this analysis, we assume that (1) is well-posed as an initial value problem, with smooth solution $x^*(t)$. We assume

$$m > n, \quad \text{and} \quad \ker A(t) = \{0\}, \quad \operatorname{im} D = \mathbf{R}^n, \quad t \in [a,b]. \tag{2}$$

Conditions (2) imply that $(AD)(t) \in \mathbf{R}^{m\times m}$ is singular, with rank $(AD)(t) \equiv n.$

The requirement that $D(t)$ be constant is not a real restriction, as any such system with varying $D(t)$ can be rewritten by introducing a new variable $u(t) = D(t)x(t)$, resulting in a larger system of the type (1) for $\hat{x}(t) := (x(t), u(t))^T$ with a constant matrix $\hat{D}(t) \equiv \hat{D}$, see [4].

We consider collocation solutions $p(t)$ for (1), defined by

$$A(t_{ij})(Dp)'(t_{ij}) + B(t_{ij})p(t_{ij}) = g(t_{ij}), \tag{3}$$

where $p(t)$ is represented by a polynomial $p_i(t)$ of degree $\le s$ on each subinterval $[\tau_i, \tau_{i+1}]$, and

$$p_{i-1}(\tau_i) = p_i(\tau_i), \quad \tau_0 = a,\ h_i := \tau_{i+1} - \tau_i > 0,\ \tau_N = b, \quad t_{ij} := \tau_i + c_j h_i, 0 < c_1 < \ldots c_j < \ldots < c_s = 1, \tag{4}$$

for $i = 0 \ldots N-1,\ j = 1 \ldots s$. Note, in particular, that $c_s = 1$ is essential for our analysis. We also assume that s is even, which will be necessary to guarantee the asymptotic correctness of our error estimator to be defined in Section 2. We also denote $h := \max_{i=0\ldots N-1} h_i$.

2 Defect-based error estimation

In the context of regular and singular ODEs, a method for computing an a-posteriori estimate ϵ of the global error $e := p - x^*$ was proposed in [2] and implemented in [1]. This method is based on the defect correction principle [6, 7]. In particular, for a special realization of the defect, an efficient, asymptotically correct error estimator, the *QDeC estimator*, was designed and analyzed in [2, 3] for collocation solutions on arbitrary grids. These ideas are now extended to the DAE context, which turns out not to be straightforward because of the coupling between differential and algebraic components.

A naive application of the procedure proposed in [6] would be based on the pointwise defect

$$d(t) := A(t)(Dp)'(t) + B(t)p(t) - g(t), \quad t \in [a,b], \tag{5}$$

of the approximate solution $p(t)$. However, as pointed out in [2] in the ODE context, the resulting method for error estimation does not lead to successful results. For collocation this is obvious: Since, by definition of the collocation solution, the defect $d(t_{ij})$ vanishes at each point $t_{ij}, i = 0 \ldots N-1,\ j = 1 \ldots s$, the right hand side of the backward Euler scheme (7) used to compute the error estimate $\epsilon_{ij}, i = 0 \ldots N-1, j = 1 \ldots s$, would always be zero, and consequently $\epsilon_{ij} \equiv 0$.

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Table 1 Error of collocation, error of error estimate, empirical orders for both solution components, at $t = 1$

N	e_1	ord $_{e_1}$	$\epsilon_1 - e_1$	ord $_{\epsilon_1 - e_1}$	e_2	ord $_{e_2}$	$\epsilon_2 - e_2$	ord $_{\epsilon_2 - e_2}$
4	−2.466 e−06	3.8	8.513 e−08	4.6	2.906 e−05	3.8	−7.927 e−07	4.6
8	−1.634 e−07	3.9	2.989 e−09	4.8	1.522 e−06	3.9	−2.783 e−08	4.8
16	−1.051 e−08	4.0	9.886 e−11	4.9	1.074 e−08	4.0	1.074 e−10	5.1
32	−6.664 e−10	4.0	3.180 e−12	5.0	6.734 e−10	4.0	3.311 e−12	5.0

In our QDeC method, a *modified defect* is used instead which is essentially an approximate integral mean of $d(t)$ between each pair of successive collocation points,

$$\bar{d}_{ij} := \sum_{k=0}^{s} \alpha_{jk}\, d(t_{ik}) = \frac{1}{h_{ij}} \int_{t_{i,j-1}}^{t_{ij}} d(t)dt + \mathcal{O}(h^{s+1}), \quad h_{ij} := t_{ij} - t_{i,j-1}, \tag{6}$$

for $i = 0 \ldots N-1,\ j = 1 \ldots s$, where the α_{jk} are appropriate quadrature coefficients.

In the linear case considered here, our error estimate $\epsilon_{ij} \approx e(t_{ij})$ is defined as the solution of the Euler-type difference scheme

$$A(t_{ij})\, \frac{D\epsilon_{ij} - D\epsilon_{i,j-1}}{h_{ij}} + B(t_{ij})\epsilon_{ij} = \bar{d}_{ij}, \tag{7}$$

with the inhomogeneous term given by (6) and with homogeneous initial conditions.

3 Analysis of asymptotic correctness

We have been able to show that the idea of weighting the defect according to (6), which is motivated by the integration inherent in the [numerical] solution of an ODE, does not compromise the quality of the global error estimate for the algebraic components.

Theorem 3.1 *While the global error of the collocation method* (3) *is of order h^s, i.e.*

$$e(t) = p(t) - x^*(t) = \mathcal{O}(h^s), \tag{8}$$

the QDeC estimate ϵ_{ij} of the global error (8) *defined via the modified defect* (6) *and the auxiliary scheme* (7) *is asymptotically correct, i.e.*

$$\epsilon_{ij} - e(t_{ij}) = \mathcal{O}(h^{s+1}). \tag{9}$$

Proof. Our analysis is based on decoupling the index 1 problem (1) into an associated *inherent ODE* and a system of purely algebraic equations according to the ideas from [5]. For the discrete systems (3) and (7) a similar decoupling argument is used. For details of the proof we refer to [4]. □

4 Numerical example

We consider the initial value problem

$$\begin{pmatrix} e^t \\ e^t \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \end{pmatrix} x'(t) + \begin{pmatrix} e^t(1+\cos^2 t) & \cos^2 t \\ e^t(-1+\cos^2 t) & -\cos^2 t \end{pmatrix} x(t) = \begin{pmatrix} \sin^2 t(1-\cos t) - \sin t \\ \sin^2 t(-1-\cos t) - \sin t \end{pmatrix}, \tag{10}$$

on $[a, b] = [0, 1]$ with initial condition $x(0) = (1, -1)^T$. We use a realization of our method in MATLAB, based on collocation at equidistant nodes with $s = 4$, on $N = 2, 4, 8, 16, 32$ subintervals of length $1/N$. In Table 1 the asymptotical order $\epsilon - e = \mathcal{O}(h^{s+1})$ is clearly visible.

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