Quadrature-defect-based a-posteriori error estimates for differential-algebraic equations

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DAE with properly stated leading term

Problem class

Consider a DAE with properly stated leading term (according to Balla, März 2002) of tractability index 1

$$\mathbf{A}(t)(\mathbf{D}(t)\mathbf{x}(t))' + \mathbf{B}(t)\mathbf{x}(t) \;=\; \mathbf{g}(t), t \in [0,1],$$

posed as IVP, where

$\mathbf{A}(t) \in \mathbb{R}^{m\times n}$, $\mathbf{D}(t) \in \mathbb{R}^{n\times m}$, $\mathbf{B}(t) \in \mathbb{R}^{m\times m}$, $n \leq m$,
$\mathbf{x}(t)$, $\mathbf{g}(t) \;\in\; \mathbb{R}^m$
$\ker \mathbf{A}(t) = \{0\}$, $\operatorname{im} \mathbf{D}(t) = \mathbb{R}^n$, all functions sufficiently smooth.

DAE with properly stated leading term

Extended system

Assumption $D(t) \equiv \mathrm{const}$ is not restrictive, because

- such a system can be rewritten as

$$\begin{aligned} \mathbf{A}(t)\mathbf{u}'(t) + \mathbf{B}(t)\mathbf{x}(t) &= \mathbf{g}(t) \\ \mathbf{u}(t) - \mathbf{D}(t)\mathbf{x}(t) &= 0 \end{aligned}$$

- or

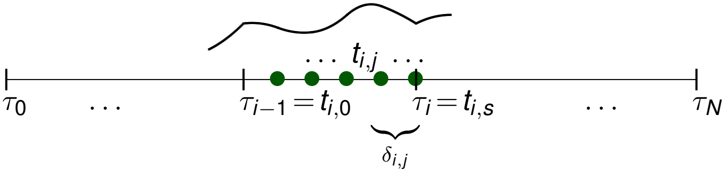
$$\underbrace{\begin{pmatrix} \mathbf{A}(t) \\ 0 \end{pmatrix}}_{A(t)} \left[\underbrace{\begin{pmatrix} 0 & I \end{pmatrix}}_{D} \underbrace{\begin{pmatrix} \mathbf{x}(t) \\ \mathbf{u}(t) \end{pmatrix}}_{x(t)} \right]' + \underbrace{\begin{pmatrix} \mathbf{B}(t) & 0 \\ \mathbf{D}(t) & -I \end{pmatrix}}_{B(t)} \underbrace{\begin{pmatrix} \mathbf{x}(t) \\ \mathbf{u}(t) \end{pmatrix}}_{x(t)} = \underbrace{\begin{pmatrix} \mathbf{g}(t) \\ 0 \end{pmatrix}}_{g(t)}$$

Method class
Collocation

We consider collocation methods for the numerical solution of such DAEs, i. e.

$$\hat{F}(x) := A(t_{i,j})(Dx(t_{i,j}))' + B(t_{i,j})x(t_{i,j}) - g(t_{i,j}),$$
$$i = 1, \ldots, N, \quad j = 1, \ldots, s$$

for continuous piecewise polynomial functions x of degree $\leq s$, s even.



Abstract setting (nonlinear)

Original problem, working scheme, auxiliary scheme

Consider

- $F^*(x) = 0$ ... original problem, solution x^*
- $\hat{F}(x) = 0$ ... working scheme, solution $\hat{x}$
- $F^{\rm def}(x)$ ... defect-defining operator, typically restriction of F^* to discrete grid; this operator is not inverted numerically
- $\tilde{F}(x) = 0$ ... auxiliary scheme, solution $\tilde{x}$
  $\tilde{F}$ is assumed to be 'cheap to solve', plays auxiliary role in error estimation

  ($F^* \approx F^{\rm def} \approx \hat{F} \approx \tilde{F}$)
- $\hat{x}$ is computed by solving $\hat{F}(x) = 0$

  ... wish to estimate the (global) error $\hat{e} := \hat{x} - x^*$

Defect-based a-posteriori error estimation

DeC approach: Estimate global error using auxiliary scheme

Basic idea due to Zadunaisky 1976, Stetter 1978:

To estimate $\hat{e} = \hat{x} - x^*$, proceed as follows

- Compute defect (residual) $\hat{d} := F^{\mathrm{def}}(\hat{x})$
- Solve $\tilde{F}(x) = 0 \longrightarrow \tilde{x}$
- Solve $\tilde{F}(x) = \hat{d} \longrightarrow \tilde{x}^{\mathrm{def}}$
- Estimate $\hat{e}$:

$$\hat{e} = \hat{x} - x^* \approx F^{*\,-1}\underbrace{F^{\mathrm{def}}(\hat{x})}_{=\,\hat{d}} - F^{*\,-1}\underbrace{F^{\mathrm{def}}(x^*)}_{\approx\,0}$$

$$\approx \tilde{F}^{-1}(\hat{d}) - \tilde{F}^{-1}(0) = \tilde{x}^{\mathrm{def}} - \tilde{x}$$

- I.e.: error estimate $\hat{\epsilon} := \tilde{x}^{\mathrm{def}} - \tilde{x} \approx \hat{x} - x^* =$ error

Auxiliary scheme and pointwise defect

$\tilde{F}$ = backward Euler-like

$\tilde{F}(x) = 0$ ... low order discretization scheme

In particular: Consider backward Euler-like scheme over collocation nodes,

$$A(t_{i,j})\frac{D\tilde{x}_{i,j} - D\tilde{x}_{i,j-1}}{\delta_{i,j}} + B(t_{i,j})\tilde{x}_{i,j} - g(t_{i,j}) \;=\; 0,$$
$$i = 1,\dots,N,\; j = 1,\dots,s$$

$$A(t_{i,j})\frac{D\tilde{x}^{\mathrm{def}}{}_{i,j} - D\tilde{x}^{\mathrm{def}}{}_{i,j-1}}{\delta_{i,j}} + B(t_{i,j})\tilde{x}^{\mathrm{def}}_{i,j} - g(t_{i,j}) \;=\; \hat{d}_{i,j}$$
$$i = 1,\dots,N,\; j = 1,\dots,s$$

Defect-based a-posteriori error estimation

Choice of F^{def}

Choice of F^{def}

- Define point-wise defect

$$\hat{d}^{\circ}(t) := A(t)D\hat{x}'(t) + B(t)\hat{x}(t) - g(t)$$

$\hat{d}^{\circ}_{i,j} = 0$ at all points evaluated in $\tilde{F}(\hat{d}^{\circ}) \Rightarrow$ estimate would always be zero.

- Use modified defect or quadrature defect, therefore QDeC (Auzinger, Koch, Weinmüller 2002 in ODE context)

$$F^{\mathrm{def}}(\hat{x})(t_{i,j}) := \hat{d}_{i,j} := \sum_{k=0}^{s} \alpha_{jk}\hat{d}^{\circ}(t_{i,k}) = \frac{1}{\delta_{i,j}}\int_{t_{i,j-1}}^{t_{i,j}} \hat{d}^{\circ}(t)dt + \mathcal{O}(h^{s+1})$$

In this sum $\alpha_{j,0}\hat{d}^{\circ}(t_{i,0})$ is only non-zero term!

Defect-based a-posteriori error estimation
Main result

Main result

$$\hat{e} = \hat{x} - x^* = \mathcal{O}(h^s)$$

$\hat{\epsilon} = \tilde{x}^{\mathrm{def}} - \tilde{x}$ is an asymptotically correct estimate for the error $\hat{e} = \hat{x} - x^*$, i. e.

$$\hat{\epsilon} - \hat{e} = \mathcal{O}(h^{s+1}).$$

Numerical example
Problem

- Initial value problem

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

  on $[0,1]$ with initial condition $x(0) = (1,-1)^T$.

- We use collocation at equidistant points with $s = 4$ on $N = 2,4,8,16,32$ intervals.
  Asymptotical order $\hat{\epsilon} - \hat{e} = \mathcal{O}(h^{s+1})$ is clearly visible.

Numerical example

Results tabular, component 1

- First component, at $t = 1$:

N	$\hat{e}$	$\mathrm{ord}_{\hat{e}}$	$\hat{\epsilon} - \hat{e}$	$\mathrm{ord}_{\hat{\epsilon}-\hat{e}}$
4	-2.466e−06	3.8	8.513e−08	4.6
8	-1.634e−07	3.9	2.989e−09	4.8
16	-1.051e−08	4.0	9.886e−11	4.9
32	-6.664e−10	4.0	3.180e−12	5.0

- First component, maximum absolute values over all collocation points $\in [0, 1]$:

N	$\hat{e}$	$\mathrm{ord}_{\hat{e}}$	$\hat{\epsilon} - \hat{e}$	$\mathrm{ord}_{\hat{\epsilon}-\hat{e}}$
4	2.732e−06	4.0	1.272e−07	5.3
8	1.711e−07	4.0	3.578e−09	5.2
16	1.074e−08	4.0	1.074e−10	5.1
32	6.734e−10	4.0	3.311e−12	5.0

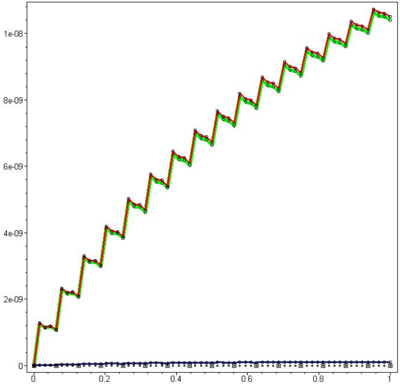
Numerical example

Results tabular, component 2

- Second component, at $t = 1$:

N	$\hat{e}$	$\mathrm{ord}_{\hat{e}}$	$\hat{\epsilon} - \hat{e}$	$\mathrm{ord}_{\hat{\epsilon}-\hat{e}}$
4	2.906e−05	3.8	-7.927e−07	4.6
8	1.522e−06	3.9	-2.783e−08	4.8
16	9.788e−08	4.0	-9.206e−10	4.9
32	6.205e−09	4.0	-2.961e−12	5.0

Numerical example
Results graphical



error $|\hat{e}_1(t)| = |\hat{x}_1(t) - x^*{}_1(t)|$

error estimate $|\hat{\epsilon}_1(t)|$

deviation of error estimate $|\hat{\epsilon}_1(t) - \hat{e}_1(t)|$

Other examples

Other numerical experiments indicate that

- singularities of the first kind do not compromise asymptotical correctness (theoretically established in the ODE case)
- with use of interior collocation points asymptotical correctness is lost, but estimate still gives reasonable approximation of error (preliminary)

Decoupling of Index 1 DAEs
Definition of matrices

Index 1 DAEs with constant $\operatorname{im} D(t)$ can be decoupled into a pure ODE (inherent ODE) and a purely algebraic equation:

- Let Q be a linear projector of $\mathbb{R}^n$ onto $\ker D$,
- D^- a generalized reflexive inverse of D such that

$$D^- D = I - Q, \quad DD^- = I, \quad DD^- D = D, \quad D^- DD^- = D^-$$

- $G(t) = A(t)D + B(t)Q, \quad (\exists G^{-1} \Leftrightarrow \mathit{index} = 1)$
- $N(t) = G(t)^{-1} B(t) D^-$.

Decoupling of Index 1 DAEs
Inherent ODE

- Premultiplying our system with $DG(t)^{-1}$ and $QG(t)^{-1}$, respectively, we obtain

$$\begin{aligned} Dx^{*\prime}(t)) + DN(t)(Dx^*(t)) - DG(t)^{-1}g(t) &= 0, \\ Qx^*(t) + QN(t)(Dx^*(t)) - QG(t)^{-1}g(t) &= 0, \end{aligned}$$

  i. e. the inherent ODE for $Dx(t)$ and an algebraic equation expressing $Qx(t)$ in terms of $Dx(t)$, with

-

$$x^*(t) = (I - Q)x^*(t) + Qx^*(t) = D^- Dx^*(t) + Qx^*(t).$$

Decoupling of Index 1 DAEs

Decoupled collocation and error

- Collocation equations decouple in exactly the same way:

$$\begin{aligned} D\hat{x}'(t_{i,j})) + DN(t_{i,j})\, D\hat{x}(t_{i,j}) - DG(t_{i,j})^{-1} g(t_{i,j}) &= 0, \\ Q\hat{x}(t_{i,j}) + QN(t_{i,j})\, D\hat{x}(t_{i,j}) - QG(t_{i,j})^{-1} g(t_{i,j}) &= 0, \end{aligned}$$

$$i = 1, \ldots, N, \quad j = 1, \ldots, s$$

- Theory of collocation for ODEs and polynomial interpolation argument:
  $D\hat{e}(t),\ D\hat{e}'(t), Q\hat{e}(t), \hat{e}(t) = \mathcal{O}(h^s)$,
- and $\hat{d}^\circ(t_{i,j}) = \mathcal{O}(h^s) \;\Rightarrow\; \hat{d}(t_{i,j}) = \mathcal{O}(h^s)$.

Analysis of deviation

Decoupling of defect definition

- Pointwise defect

$$DG(t)^{-1}\hat{d}^{\circ}(t) = D\hat{x}'(t) + DN(t)D\hat{x}(t) - DG(t)^{-1}g(t) = DG(t)^{-1}F^{*}(\hat{x})$$
$$QG(t)^{-1}\hat{d}^{\circ}(t) = Q\hat{x}(t) + QN(t)D\hat{x}(t) - QG(t)^{-1}g(t) = QG(t)^{-1}F^{*}(\hat{x})$$

Note that $QG(t)^{-1}\hat{d}^{\circ}(t_{i,j}) = 0\,\forall\, i = 1, \ldots, N,\ j = 0, \ldots, s$ owing to collocation conditions and the continuity conditions $\hat{x}(t_{i,0}) = \hat{x}(t_{i-1,s})$.

Analysis of deviation
Differential component

Combining the above equations we obtain for $r := \hat{\epsilon} - \hat{e}$:

$$\frac{Dr_{i,j} - Dr_{i,j-1}}{\delta_{i,j}} = -DN(t_{i,j})Dr_{i,j}$$

$$\underbrace{-DN(t_{i,j})D\hat{e}(t_{i,j}) + \sum_{k=0}^{s} \alpha_{jk} DN(t_{i,k})D\hat{e}(t_{i,k})}_{\leq C\delta_{i,j}(\|D\hat{e}\|+\|D\hat{e}'\|)=\mathcal{O}(h^{s+1})} + \mathcal{O}(h^{s+1})$$

$$+ \sum_{k=0}^{s} \alpha_{jk} \underbrace{\left(DG(t_{i,j})^{-1} - DG(t_{i,k})^{-1}\right)}_{\mathcal{O}(h)} \underbrace{\hat{d}^{\circ}(t_{i,k})}_{\mathcal{O}(h^s)}$$

The claimed order $Dr = \mathcal{O}(h^{s+1})$ now follows from the stability of the backward Euler scheme.

Analysis of deviation
Algebraic component

For the algebraic component we have

$$
\begin{aligned}
Qr_{i,j} &= -QN(t_{i,j})Dr_{i,j} + QG(t_{i,j})^{-1}\hat{d}_{i,j} \\
&= -QN(t_{i,j})Dr_{i,j} + \sum_{k=0}^{s} \alpha_{jk} \underbrace{\left(QG(t_{i,j})^{-1} - QG(t_{i,k})^{-1}\right)}_{\mathcal{O}(h)} \underbrace{\hat{d}^{\circ}(t_{i,k})}_{\mathcal{O}(h^s)} + \\
&\qquad + \sum_{k=0}^{s} \alpha_{jk} \underbrace{QG(t_{i,k})^{-1}\hat{d}^{\circ}(t_{i,k})}_{=0}
\end{aligned}
$$

$QG(t_{i,j})^{-1}\hat{d}^{\circ}(t_{i,j}) = 0 \,\forall\, i = 1, \ldots, N,\ j = 0, \ldots, s$ owing to the collocation and continuity conditions $\hat{x}(t_{i,0}) = \hat{x}(t_{i-1,s})$.

Conclusions and ongoing research

Conclusions

Conclusion

- Defect correction provides a basis for inexpensive and reliable error estimate for DAEs
- Interplay between working schemes and defect evaluation is essential
- In some particular cases asymptotic correctness established
- In other cases numerical evidence suggests asymptotic correctness or acceptable approximation

Conclusions and ongoing research

Open questions

Ongoing research

- Index 2 or higher index problems
- Essential singularities (theory for collocation not yet available)
- Realization in a nonlinear setting, combination with Newton method
- etc.

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