Defect-based a-posteriori error estimation for implicit ODEs and DAEs

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Outline

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   - Defect definition
   - Modification: Integral means of defect
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   - Collocation and QDeC/BEUL or mixed estimate
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Abstract setting (nonlinear)

Original problem, working scheme, auxiliary scheme

Consider

- $F^*(u) = 0$ ... original problem, solution u^*
- $\hat{F}(u) = 0$ ... working scheme, solution $\hat{u}$
- $\tilde{F}(u) = 0$ ... auxiliary scheme, solution $\tilde{u}$

Note: $F^* \approx \hat{F} \approx \tilde{F}$

- De facto we are in discrete setting, i.e., $F^*(u) = 0$ is a very accurate (possibly very expensive) discretization of a continous problem which we wish do not wish to solve
- $\hat{u}$ is computed by solving $\hat{F}(u) = 0$

  ... wish to estimate the (global) error $\hat{e} := \hat{u} - u^*$
- $\tilde{F}$ is assumed to be 'cheaply to solve', plays auxiliary role in error estimation

Defect-based a-posteriori error estimation

DeC approach: Estimate global error using auxiliary scheme

Basic idea due to Zadunaisky, Stetter:

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

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

$$\hat{e} = \hat{u} - u^* = F^{*-1} \underbrace{F^*(\hat{u})}_{= \hat{d}} - F^{*-1} \underbrace{F^*(u^*)}_{= 0}$$

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

- I.e.: error estimate $\hat{\epsilon} := \tilde{u}_{def} - \tilde{u} \approx \hat{u} - u^*$ = error
- Linear case: Simply compute $\hat{\epsilon} := \tilde{F}^{-1}\hat{d}$

Collocation for explicit ODE system

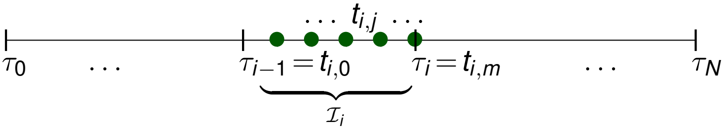
$\hat{F}$ = collocation method

- $\hat{F}(u) = 0$ ... high order discretization for explicit ODE system $y'(t) = f(t, y(t))$ (IVP od BVP)

  In particular: Consider piecewise polynomial collocation

  $$\hat{u} = (\ldots, \hat{u}(t_{i,j}), \ldots), \quad \text{where} \quad \hat{u}'(t_{i,j}) = f(t_{i,j}, \hat{u}(t_{i,j})) \quad \forall\, i, j$$

- [Non]equidistant mesh $\{\tau_0, \ldots, \tau_N\}$, collocation intervals $\mathcal{I}_i := [\tau_{i-1}, \tau_i]$
- Collocation (degree m) at nodes • $t_{i,j} \in \mathcal{I}_i,\ j = 1 \ldots m$



- Coll. nodes • may be nonequidistant; $h_{i,j} := t_{i,j} - t_{i,j-1}$

Auxiliary scheme and pointwise defect

$\tilde{F}$ = BEUL (backward Euler); use pointwise defect $\hat{d}$ of $\hat{u}$

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

  In particular: Consider BEUL over collocation nodes,

$$\frac{\tilde{u}_{i,j} - \tilde{u}_{i,j-1}}{h_{i,j}} = f(t_{i,j}, \tilde{u}_{i,j}) \quad \forall\, i,j$$

- F^* is 'implicitly' defined by specifying the defect $\hat{d}$:
  - Compute pointwise (differential) defect of $\hat{u}$ w.r.t. ODE at all grid points $t_{i,j}$

$$\hat{d}_{i,j} := \hat{u}'(t_{i,j}) - f(t_{i,j}, \hat{u}(t_{i,j})) \quad \longrightarrow \quad \hat{d} = (\ldots, \hat{d}_{i,j}, \ldots)$$

  - ... i.e.: $F^* \sim$ collocation scheme of higher order $m+1$

- Auxiliary step: Solve BEUL scheme, with additional inhomogeneity defined by defect $\hat{d}$

Use of pointwise defect makes non sense

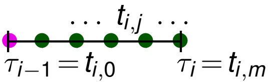
$\hat{d}$ vanishes at collocation nodes

- But: This makes no sense, because BEUL evaluates $\hat{d}$ at collocation nodes, i.e. at the zeros of $\hat{d}(t)$:

  By definition of $\hat{u}$,

  $\hat{d}_{i,j} = 0$ at collocation nodes • $\Longrightarrow$ error estimate $\equiv 0$

- However, $\hat{d}(t) \not\equiv 0$; in particular, $\hat{d}_{i,0} \neq 0$ at left endpoint $\tau_{i-1} = t_{i,0}$ • of $\mathcal{I}_i$:



- $\Longrightarrow$ We have to use defect information in another way

- Note: Use of forward Euler or box scheme instead of BEUL does not help us.

Defect-defining scheme F^* is not appropriate

Heuristic argument

- Collocation error satisfies $\hat{e}(t) := (\hat{u} - u^*)(t)$ satisfies

$$\hat{e} = \mathcal{O}(h^m), \quad \hat{e}' = \mathcal{O}(h^m), \quad \hat{e}'' = \mathcal{O}(h^{m-1}),$$

- Note:
  - F^* corresponds to collocation scheme (of higher order), involves a term with 1st derivative (like in ODE)
  - $\tilde{F}$ = difference scheme (BEUL or any one-step scheme), involves 1st difference quotient
  - $\Longrightarrow$ $\tilde{F} - F^*$ depends on second derivative $\hat{e}''$ of error function $\hat{e}(t)$
  - $\hat{e}''$ is of reduced order $\mathcal{O}(h^{m-1})$
  - $\Longrightarrow$ $\tilde{F} - F^*$ is not small enough asymptotically

How to make the estimate work: QDeC approach

Use local integral means of $\hat{d}(t)$

- The consequence: modify defect, i.e.
- Modify F^* in such a way that $\tilde{F} - F^*$ sufficiently 'similar'
- I.e.: Replace pointwise (differential) defect values $\hat{d}_{i,j} = \hat{u}'(t_{i,j}) - f(t_{i,j}, \hat{u}(t_{i,j}))$ by local integral means
$$\hat{\bar{d}}_{i,j} := \fint_{t_{i,j-1}}^{t_{i,j}} \hat{d}(t)\,dt = \frac{\hat{u}_{i,j} - \hat{u}_{i,j-1}}{h_{i,j}} - \fint_{t_{i,j-1}}^{t_{i,j}} f(t, \hat{u}(t))\,dt$$
- In practice: Use appropriate quadrature formula for $\fint$ – coefficients related to Runge-Kutta formalism
- ... corresponds to a re-formulation of F^* as a difference scheme involving a 1st difference just like in $\tilde{F}$
- $\Longrightarrow$ $\tilde{F} - F^*$ is merely a weighted sum of f - values
- Proof of asymptotic correctness: O.K.:
Error of estimate: $\hat{\epsilon} - \hat{e} = \mathcal{O}(h^{m+1})$ $\surd$

Linear implicit system with varying mass matrix

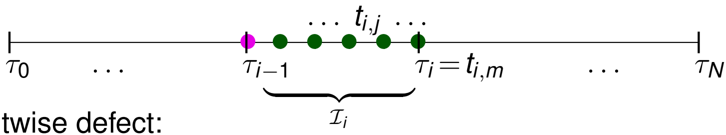
Generalization of the above procedure

- Consider linear case:

$$\boldsymbol{A}(\boldsymbol{t})\, y'(t) + B(t)\, y(t) \;=\; g(t)$$

- Collocation:

$$\boldsymbol{A}(\boldsymbol{t_{i,j}})\, \hat{u}'(t_{i,j}) + B(t_{i,j})\, \hat{u}(t_{i,j}) \;=\; g(t_{i,j}) \quad \text{at} \quad t_{i,j} \; \bullet$$



- Pointwise defect:

$$\hat{d}(t) \;:=\; \boldsymbol{A}(\boldsymbol{t})\, \hat{u}'(t) - B(t)\, \hat{u}(t) - g(t) \;\neq\; 0 \quad \text{at} \quad t = \tau_{i-1} = t_{i,0} \; \bullet$$

- Integrated defect:

$$\hat{\hat{d}}_{i,j} \;:=\; \int_{t_{i,j-1}}^{t_{i,j}} \hat{d}(t)\, dt$$

Integrated defect and auxiliary scheme

Attention: $A = A(t)$

- Note:

$$\begin{aligned}\hat{\hat{d}}_{i,j} &= \int_{t_{i,j-1}}^{t_{i,j}} \hat{d}(t)\,dt = \int_{t_{i,j-1}}^{t_{i,j}} A(t)\,\hat{u}'(t)\,dt + \ldots \\ &= \int_{t_{i,j-1}}^{t_{i,j}} (\,(A\,\hat{u}')(t) - A'(t)\,\hat{u}(t)\,)\,dt + \ldots \\ &= \frac{(A\,\hat{u})(t_{i,j}) - (A\,\hat{u})(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \int_{t_{i,j-1}}^{t_{i,j}} A'(t)\,\hat{u}(t)\,dt + \ldots\end{aligned}$$

- ¿ What auxiliary scheme is appropriate ?

  Analysis shows: Any stable, consistent one-step scheme is O.K., e.g. BEUL: Error estimate $\hat{\epsilon} \approx \hat{e}$ computed from

$$A_{i,j}\,\frac{\hat{\epsilon}_{i,j} - \hat{\epsilon}_{i,j-1}}{h_{i,j}} + B_{i,j}\,\hat{\epsilon}_{i,j} = \hat{\hat{d}}_{i,j}$$

  is asymptotically correct $\surd$

Collocation for DAEs

Use stiffly stable collocation scheme

- Now consider DAE case ($A(t)$ singular) :
  Use of right end node $\tau_i = t_{i,m}$ for collocation means: the scheme is stiffly stable – usually the most beneficial choice in the DAE case
- Analysis of QDeC estimate cited above:
  No explicit assumption about rank of $A(t)$, but we need
  $$\hat{e}(t) = \mathcal{O}(h^m), \quad \hat{e}'(t) = \mathcal{O}(h^m)$$
- Numerical tests in Maple 10 –
  programming is simple: collocation equations are set up symbolically, system to be solved is extracted using `coeff`
- Note: Here, defect is integrated exactly (effect of quadrature is masked, but will also have to be considered)

A simple numerical example

Index 1 DAE with constant coefficients

- Initial value problem

$$\begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix} u'(t) + \begin{pmatrix} 1 & 2 \\ 2 & 3 \end{pmatrix} u(t) = \begin{pmatrix} \sin(10\,t) \\ \cos(t) \end{pmatrix},$$

  with consistent initial condition

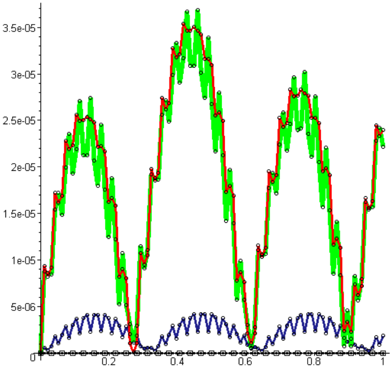
- Equidistant collocation ($m=3$) + QDeC/BEUL estimate; results displayed for $\|\cdot\|_2$ at $t=1$:

N	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
4	1.364e−02		7.750e−03	
8	1.570e−03	3.1	5.966e−05	7.0
16	1.927e−04	3.0	2.224e−06	1.4
32	2.399e−05	3.0	1.944e−07	3.5

Index 1 DAE with constant coefficients

2-norm of error and QDeC/BEUL estimate

$m = 3, \quad N = 32$



error $\|\hat{e}(t)\|_2 = \|\hat{u}(t) - u^*(t)\|_2$

error estimate $\|\hat{\epsilon}(t)\|_2$

error of error estimate $\|\hat{\epsilon}(t) - \hat{e}(t)\|_2$

Index 1 DAEs with constant coefficients

Stiffly stable scheme exact in algebraic component

- Note: For stiffly stable collocation, algebraic equation is exactly reproduced at collocation nodes
- $\Longrightarrow$ Integration of defect (essential for differential component !) is not really reasonable for algebraic component

  Asymptotic order is O.K (interpolation error), but overall reduced accuracy is to be expected
- $\Longrightarrow$ Use mixed strategy, with pointwise defect (= 0 at collocation nodes) in algebraic component
- We see: Heuristic idea behind DeC estimator is simple – but precise definition of the defect is essential, also depends on the auxiliary scheme used
- More general DAEs: discussed below

Index 1 DAE with constant coefficients

Results for mixed DeC/BEUL estimate

- Example from above ($m = 3$)
- Mixed DeC/BEUL estimate: Error estimate is more precise, asymptotic order

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

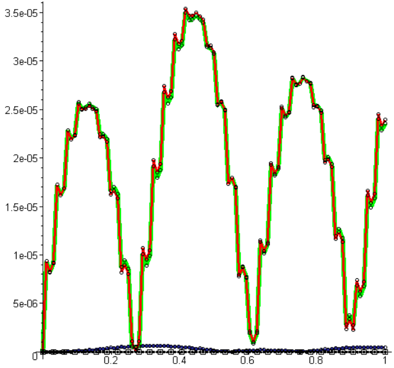
is clearly visible:

N	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
4	1.364e−02		2.105e−03	
8	1.570e−03	3.1	1.176e−04	4.2
16	1.927e−04	3.0	7.214e−06	4.0
32	2.399e−05	3.0	4.504e−07	4.0

Index 1 DAE with constant coefficients

2-norm of error and mixed DeC/BEUL estimate

$m = 3, \quad N = 32$



error $\|\hat{e}(t)\|_2 = \|\hat{u}(t) - u^*(t)\|_2$

error estimate $\|\hat{\epsilon}(t)\|_2$

error of error estimate $\|\hat{\epsilon}(t) - \hat{e}(t)\|_2$

Index 1 DAEs with variable coefficients

Properly stated formulation

- Consider variable coefficient Index 1 case

$$A(t)\,u'(t) + B(t)\,u(t) \;=\; g(t)$$

- ¿ 'Index = 1 for variable coefficients ? ' –
  … Most natural definition due to R. März et.al.:
  'Properly stated form' with 'tractability index' $\boldsymbol{i}_t = 1$:
- Assume that $A(t)$ can be written as

$A(t) = E(t)\,D(t)$, where $E(t) \in \mathbb{R}^{n\times s}$, $D(t) \in \mathbb{R}^{s\times n}$ in C^1,

with

$$\ker E(t) \oplus \operatorname{im} D(t) \;=\; \mathbb{R}^s\,,$$

and such that $\exists$ C^1 projector $R(t)$ with

$$\ker R(t) \;=\; \ker E(t), \qquad \operatorname{im} R(t) \;=\; \operatorname{im} D(t).$$

Properly stated formulation, $\boldsymbol{i}_t = 1$

Use stiffly stable scheme

- DAE has tractability index $\boldsymbol{i}_t = 1$ if (essentially; omit some technical details) it can be decoupled into the equivalent form

$$E(t)\,(Rv)'(t) + B(t)\,u(t) \;=\; g(t),$$
$$D(t)\,u(t) \;=\; v(t),$$

  with an inherent ODE and a purely algebraic equation.
- Important: Application of stiffly stable scheme is equivalent to direct application to ($U = (u, v)$)

$$\begin{pmatrix} 0 & E(t) \\ 0 & 0 \end{pmatrix} U'(t) + \begin{pmatrix} B(t) & 0 \\ D(t) & -I \end{pmatrix} U(t) \;=\; \begin{pmatrix} g(t) \\ 0 \end{pmatrix}.$$

- Convergence theory: $\surd$ with stage order in general. (Here: We do not discuss possible superconvergence effects.)

Properly stated formulation, $\boldsymbol{i_t = 1}$

Stiffly stable scheme and QDeC/BEUL or mixed estimator

Numerical evidence is the same as for constant coefficients:

- QDeC/BEUL estimate is asymptotically correct,

$$\hat{\epsilon} - \hat{e} = \mathcal{O}(h^{m+1}) \quad \surd$$

- Stiffly stable collocation scheme does not propagate any error in the algebraic component, i.e.

$$D(t_{i,j})\,\hat{u}_{i,j} \equiv \hat{v}_{i,j}$$

  $\Longrightarrow$ it makes sense to use the mixed estimate, with zero defect in the algebraic component: Again, asymptotic order is the same, accuracy of estimator is slightly better

- Analysis (including nonlinear problems) will be based on a combination of our argument for the implicit case and the convergence theory for stiffly stable collocation schemes by Higueras / März.

Index 2 case:

Preliminary analysis: Consider simple model

- Simplest index 2 DAE: Solution obtained by differentiation of a given data function $g(t)$, or slighly more general:

$$A\,u'(t) + B\,u(t) = \begin{pmatrix} f(t) \\ g(t) \end{pmatrix},$$

with

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

- Stiffly stable collocation yields stage order $\mathcal{O}(h^m)$, but
- QDeC/BEUL or mixed estimate is not asymptotically correct for $m > 1$
- However: For $m = 1$ we obtain

$$\hat{\epsilon} - \hat{e} = \mathcal{O}(h^2) = \mathcal{O}(h^{m+1}) \quad \checkmark$$

Index 2 case: Model problem analysis

QDeC/BEUL or mixed estimate asymptotically correct for $m = 1$

- Explanation: Consider special case $f(t) = 0$ and mixed estimator
- Algebraic equation $u_2(t) = g(t)$ is exactly reproduced by collocation: $\hat{u}_2(t_{i,j}) = g(t_{i,j})$, pointwise defect $= 0$

  ... equivalent to piecewise linear interpolation, with

  $$(\hat{u}_2 - g)(t) = \mathcal{O}(h^2), \quad (\hat{u}_2' - g')(t) = \mathcal{O}(h)$$

- (Integrated) Qdefect in first component reads

$$\begin{aligned} (\hat{\bar{d}}_1)_{i,j} &= \int_{t_{i,j-1}}^{t_{i,j}} (\hat{u}_2'(t) - \hat{u}_1(t))\, dt \\ &= \frac{g_{i,j} - g_{i,j-1}}{h_{i,j}} - \int_{t_{i,j-1}}^{t_{i,j}} \hat{u}_1(t)\, dt \end{aligned}$$

$\longrightarrow$

Index 2 case: Model problem investigation

Mixed estimate asymptotically correct for $m = 1$

- $\longrightarrow$ Mixed estimator, first component of BEUL scheme:

$$\frac{(\hat{\epsilon}_2)_{i,j} - (\hat{\epsilon}_2)_{i,j-1}}{h_{i,j}} - (\hat{\epsilon}_1)_{i,j} = \frac{g_{i,j+1} - g_{i,j}}{h_{i,j}} - \int_{t_{i,j-1}}^{t_{i,j}} \hat{u}_1(t)\,dt$$

with $(\hat{\epsilon}_2)_{i,j} \equiv 0 \; (\equiv (\hat{e}_2)_{i,j}) \implies$ error estimate $\hat{\epsilon}$ satisfies

$$(\hat{\epsilon}_1)_{i,j} = \int_{t_{i,j-1}}^{t_{i,j}} (\hat{u}_1(t) - g'(t))\,dt$$

- Compared with error $\hat{e} = \hat{u} - u^*$ to be estimated,

$$(\hat{e}_1)_{i,j} = (\hat{u}_1)_{i,j} - (u_1^*)_{i,j} = (\hat{u}_1)(t_{i,j}) - g'(t_{i,j}),$$

we conclude

$$\hat{\epsilon}_1 - \hat{e}_1 = \mathcal{O}(h^2) \quad \surd \qquad \text{because} \quad \hat{u}_1 - g' = \mathcal{O}(h)\,.$$

□

Index 2 case: Numerical evidence and outlook

QDeC/BEUL estimate O.K. for $m = 1$; ¿ $m > 1$?

- Numerical evidence shows:
  - Again, mixed estimate performs slightly better than pure QDeC estimate; asymptotic order is the same
  - Behavior observed for model problem carries over to more general (variable coefficient) examples
- Case $m > 1$: Possible remedy: Choose

  $$\tilde{F} = \hat{F},$$

  i.e. the estimator is computed from a second application of the underlying collocation scheme, with defect added (currently being tested).
- More experiments and analysis are under preparation.

*** Many thanks for your attention! ***