Accurate and efficient a-posteriori error estimation for implicit and singular boundary value problems

Defect correction techniques

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Outline

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 $\hat{\varepsilon} := \tilde{u}_{def} - \tilde{u} \approx \hat{u} - u^*$ = error
- Can also proceed using local error estimates (similar procedure)

Collocation for boundary value problems

$\hat{F}$ = collocation method

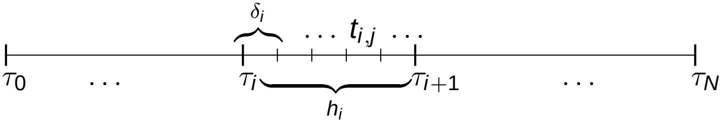
- $\hat{F}(u) = 0$ ... high order discretization scheme of boundary value problem (BVP) for nonlinear ODE $y'(t) = f(t, y(t))$
  In particular: Consider piecewise polynomial collocation

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

- Nonequidistant mesh, collocation at interior nodes of

  $$\Delta := \{t_{i,j} = \tau_i + j\delta_i,\ i = 0, \ldots, N-1,\ j = 0, \ldots, m+1\},$$

  with 'outer' and 'inner' stepsizes h_i and $\delta_i = \frac{h_i}{m+1}$



- Collocation degree m ;
  nodes may also be nonequidistant

Collocation for boundary value problems

$\tilde{F}$ = box scheme; defect via higher order interpolation of $\hat{u}$

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

  In particular: Consider box scheme w.r.t. collocation grid,

$$\frac{\tilde{u}_{i,j} - \tilde{u}_{i,j-1}}{\delta_i} = \frac{1}{2}\big(f(t_{i,j-1}, \tilde{u}_{i,j-1}) + f(t_{i,j}, \tilde{u}_{i,j})\big) \quad \forall\, i, j$$

- F^* is 'implicitly' defined by specifying the defect $\hat{d}$:
  - Interpolate $\hat{u}$ by piecewise polynomial $\hat{v}(t)$ of higher degree $m+1$
  - Compute pointwise (differential) defect w.r.t. given ODE,

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

  - ... i.e.: $F^* \sim$ collocation scheme of higher order
- Auxiliary step: Solve box scheme, with additional inhomogeneity defined by defect $\hat{d}$

Collocation for boundary value problems

Straightforward idea does not work. ¿What has gone wrong?

- We know a-priori: $\hat{e} = O(h^m)$ $\quad$ (h ... maximal stepsize)
- Implementation of error estimate described above yields $\hat{\varepsilon} = O(h^m)$, but
$$\hat{\varepsilon} - \hat{e} \neq O(h^k) \quad \text{with } k > m,$$
i.e., error estimate is not asymptotically correct
- What has gone wrong? $\longrightarrow$ Note:
  - F^* corresponds to collocation scheme, involves a term with 1st derivative (like in ODE)
  - $\tilde{F}$ is difference scheme, involves 1st difference quotient
  - $\Longrightarrow$ $\tilde{F} - F^*$ depends on second derivative of error function $\hat{e}(t) = (\hat{u} - u^*)(t)$
  - $(\hat{u} - u^*)''$ is of reduced order $O(h^{m-1})$
  - $\Longrightarrow$ $\tilde{F} - F^*$ is not 'small enough' asymptotically

Collocation for boundary value problems

How to make the estimate work: QDeC approach

- The consequence: modify defect, i.e.
- Modify F^* in such a way that $\tilde{F} - F^*$ sufficiently similar
- $\longrightarrow$ Replace pointwise (differential) defect values $\hat{d}_{i,j} = \hat{v}'(t_{i,j}) - f(t_{i,j}, \hat{v}(t_{i,j}))$ by their local integral means

$$\hat{D}_{i,j} := \fint_{t_{i,j-1}}^{t_{i,j}} \hat{d}(t)\,dt = \frac{\hat{v}_{i,j} - \hat{v}_{i,j-1}}{\delta_i} - \fint_{t_{i,j-1}}^{t_{i,j}} f(t, \hat{v}(t))\,dt$$

- In practice: Use sufficiently accurate quadrature formulas; coefficients related to Runge-Kutta formalism
- This 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 only a weighted sum of f - values
- Proof of asymptotic correctness: O.K.

Collocation for boundary value problems

Numerical example: QDeC estimator asymptotically correct

- Example: Boundary value problem on $[0,1]$

$$u'(t) = \begin{pmatrix} 0 & 1 \\ 4 & 0 \end{pmatrix} u(t) - 3 \begin{pmatrix} 0 \\ \exp(t) \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} u(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} u(1) = \begin{pmatrix} 1 \\ e \end{pmatrix}$$

- Collocation ($m = 4$) + QDeC error estimate :

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/4	1.740e−06		6.574e−08	
1/8	1.064e−07	4.0	1.916e−09	5.1
1/16	6.617e−09	4.0	5.803e−11	5.1
1/32	4.130e−10	4.0	1.750e−12	5.0

Singular ODEs

Performance of QDeC estimate in singular case

- Singular ODEs :

$$u'(t) = t^{-\alpha} A(t)u(t) + f(t, u(t))$$

- Collocation / QDeC estimate successfully applicable to BVPs with singularity of the first kind ($\alpha = 1$)

  $\longrightarrow$ Proof: O.K.

- Essential singularities ($\alpha > 1$) :
  - O.K., but less accurate due to reduced smoothness of collocation error
  - Alternative: Mesh halving – slightly more robust but significantly more expensive

Singular ODEs

Numerical example: QDeC estimator in presence of essential singularity

- Example: Essential singularity ($\alpha = 3$), terminal value problem on $[0,1]$

$$u'(t) = t^{-3}u(t) + (1 - t^{-3})e^t, \quad u(1) = e$$

- Collocation ($m = 4$) + QDeC error estimate:

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{coll}}$	$\mathrm{err}_{\mathrm{est}}$	$\mathrm{ord}_{\mathrm{est}}$
1/16	1.106e−10		2.814e−11	
1/32	6.796e−12	4.0	1.203e−12	4.4
1/64	4.208e−13	4.0	4.266e−14	4.6
1/128	2.953e−14	3.8	1.442e−14	4.8

Implicit problems

Under consideration: Implicit ODEs (linear, nonlinear, DAEs, ...)

- $\hat{F}$ = collocation for implicit ODE systems,
  e.g. linearly implicit with mass matrix $M(t)$,
  $$M(t_{i,j})u'(t_{i,j}) = f(t_{i,j}, u(t_{i,j}))$$
- $\tilde{F}$ = box scheme:
  $$M(t_{i,j-\frac{1}{2}})\,\frac{\tilde{u}_{i,j} - \tilde{u}_{i,j-1}}{\delta_i} = \tfrac{1}{2}\big(f(t_{i,j-1}, \tilde{u}_{i,j-1}) + f(t_{i,j}, \tilde{u}_{i,j})\big)$$
- Let $\hat{v}$ ... higher order interpolant of $\hat{u}$; pointwise defect
  $$\hat{d}_{i,j} = M(t_{i,j})\hat{v}'(t_{i,j}) - f(t_{i,j}, \hat{v}(t_{i,j}))$$
- ... equivalent to explicit case if $M(t)$ regular
- Interesting case: $M(t)$ has reduced rank $\longrightarrow$
  Question: How to modify defect and/or auxiliary scheme to ensure asymptotic correctness of error estimate

Implicit problems

Differential-algebraic systems

- Consider

$$A(Du)'(t) = f(t,u(t)), \quad A,D \ \ldots \text{ full rank}$$

(A, D rectangular in general)

- … with $v := D\,u$ this is equivalent to implicit ODE system with singular mass matrix:

$$\begin{pmatrix} 0 & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} u'(t) \\ v'(t) \end{pmatrix} = \begin{pmatrix} D\,u(t) - v(t) \\ f(t,u(t)) \end{pmatrix}$$

- … Collocation: O.K. e.g. with Radau IIa nodes $\rightarrow \hat{u}, \hat{v}, \hat{d}$
- Error estimator:
  - Use auxiliary scheme $\tilde{F}$ = backward Euler on fine grid
  - Use local quadrature means of defect $\hat{d}$
    (defect in algebraic component remains zero)
  - For varying A, further modification may be necessary

Collocation for boundary value problems

Numerical example: DAE, Radau IIa

- Example: Boundary value problem on $[0, 1]$

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} (u_1'(t) - u_2'(t)) = \begin{pmatrix} 1-t^2 & 0 \\ 0 & -t^2 \end{pmatrix} u(t) + \begin{pmatrix} g(t) \\ g(t) \end{pmatrix},$$

$$(g(t) = \sinh t + t^2(t^2-1)\cosh t),$$

$$u_1(0) = 0, \quad u_1(1) - u_2(1) = \cosh 1$$

- Radau IIa collocation ($m = 2$):

h	$\mathrm{err}_{\mathrm{coll}}$	$\mathrm{ord}_{\mathrm{est}}$
1/10	3.538e−06	
1/20	4.465e−07	3.0
1/40	5.605e−08	3.0
1/80	7.019e−09	3.0

- Error estimator not yet implemented . . .

Choice of auxiliary scheme and of defect

Defect needs to be defined carefully

- Appropriate choice of auxiliary scheme and defect is problem-dependent
- Interpolation (as basis for defect definition) should be of local type (efficiency!)
- Approximation of derivatives should be similar for auxiliary scheme $\tilde{F}$ and defect-defining scheme F^*
- Must be applicable to non-uniform meshes $\longrightarrow$ Adaptive mesh selection aiming at equidistribution of global error
- For PDEs, a number of error estimation principle exists (e.g. residual-based, smoothing)
  - Finite volume schemes, Finite element methods
  - *DeC involves some additional effort –
  - expect gain concerning reliability, robustness

Conclusion, acknowledgments

NSDE group at Vienna University of Technology

- NSDE research group: MATLAB code `sbvp`,
  especially designed for singular BVPs,
  collocation + adaptive mesh based on QDeC estimate
- See
  - `www.math.tuwien.ac.at/nsde/`
  - `www.mathworks.com/matlabcentral/fileexchange/`
    (download)
- People:
  - Ernst Karner
  - Othmar Koch
  - Dirk Praetorius
  - Ewa Weinmüller
  - ...