On the stability and error structure of BDF schemes applied to sectorial problems

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W. Auzinger F. Kramer

w.auzinger@tuwien.ac.at Felix.Kramer@gmx.at

Institute for Analysis and Scientific Computing

Vienna University of Technology

Introduction

We consider k-step BDF schemes applied to evolution equations

$$y(t) = Ay(t) + f(t), \qquad y(t_0) = y_0,$$

where A is maximal sectorial in Hilbert space $\mathcal{H}$;
$h > 0$; $t_\nu = \nu h$. We discuss:

(I) Explicit stability bounds

(II) Asymptotic error expansion for BDF 2, for smooth $y(t)$ (generalization to $k > 2$ will be 'merely technical')

Essentially, (I) provides quantitative versions of known, qualitative bounds, based on estimates for the separation of characteristic roots. (II) is an extension of prior work on one-step schemes, e.g. backward Euler.

Characteristic polynomials and discrete resolvent

Let ρ and σ be the characteristic polynomials of a k-step BDF scheme,

$$\rho(\zeta) = \sum_{j=1}^{k} \frac{1}{j}\, \zeta^{k-j} (\zeta - 1)^j, \quad \sigma(\zeta) = \zeta^k$$

For scalar $A = \lambda$, $\mu := h\lambda$, let

$$p(\zeta) = p(\zeta; \mu) := \rho(\zeta) - \mu\, \sigma(\zeta),$$

$$r(\zeta) = r(\zeta; \mu) := p^{-1}(\zeta)$$

$r(\zeta)$ is called the discrete resolvent of the scheme, providing a representation of the discrete solution.

Location of characteristic roots (i)

Proposition 1 [3]: For $k = 2 \ldots 5$ and arbitrary μ in the stability region of the k-step BDF scheme, any root of $p(\zeta) = p(\zeta;\mu)$ which is contained in the annulus

$$\mathcal{A}_k := \{ \zeta \in \mathbb{C} : \; a_k < |\zeta| \leq 1 \}$$

is simple and solitary within $\mathcal{A}_k$, i.e., $\mathcal{A}_k$ contains no other root.

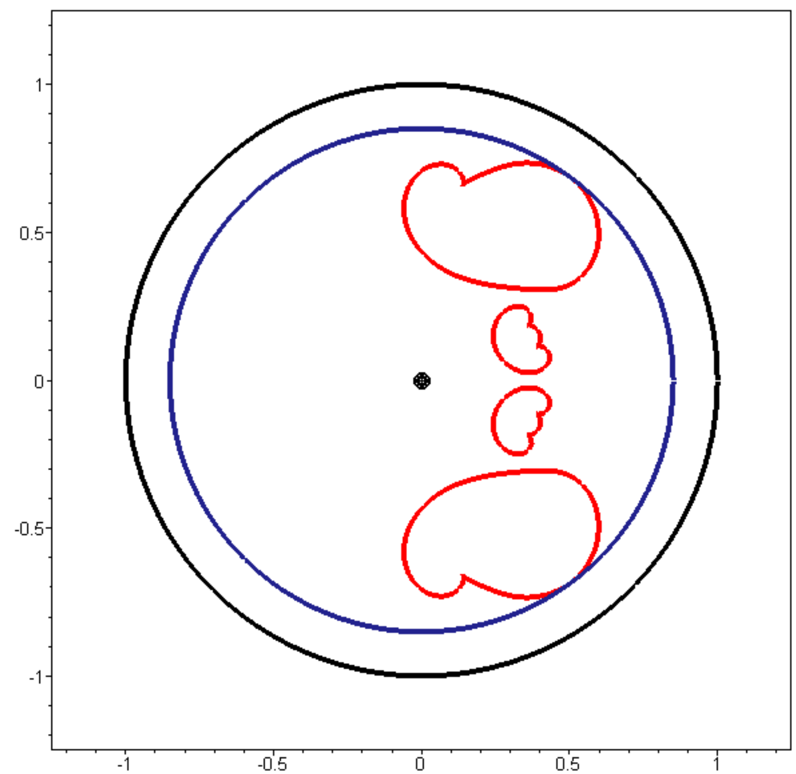
Here, $a_k = \dfrac{1}{|1-\omega_k|}, \; \omega_k = e^{2\pi i/k}$.

k	a_k	
2	$\frac{1}{2}$	$=$ 0.5
3	$\frac{1}{\sqrt{3}}$	$\approx$ 0.5774
4	$\frac{1}{\sqrt{2}}$	$\approx$ 0.7071
5	$\frac{\sqrt{5+\sqrt{5}}}{\sqrt{10}}$	$\approx$ 0.8507

Location of characteristic roots (ii)

Remark: Due to stiff stability, all roots tend to zero for $\mu \to \infty$; Proposition 1 refers to moderate-sized values of $\mu = h\lambda$. It enables quantitative stability estimates, uniform w.r.t. μ in the stability region, see [3].

- $k = 5$:



Problem class

We assume A to be densely defined and θ-sectorial, i.e.

$$\langle Au, u\rangle \in \mathcal{T}_\theta, \qquad \mathcal{T}_\theta := \{z \in \mathbb{C} : \ |\text{arg}(-z)| \le \theta\}$$

equivalent to the resolvent inequality

$$\|(zI - hA)^{-1}\| \le \frac{1}{\text{dist}(z, \mathcal{T}_\theta)}, \quad \forall z \in \mathbb{C} \setminus \mathcal{T}_\theta.$$

- Characteristic polynomial and discrete resolvent (with hA taking the role of μ):

$$\begin{aligned} P(\zeta) &= \rho(\zeta)I - \sigma(\zeta)hA, \\ R(\zeta) &= P^{-1}(\zeta) = \sum_{\nu=k}^{\infty} \zeta^{-\nu} R_\nu(hA) \end{aligned}$$

Discrete variation of constants

For sector $\mathcal{T}_\theta \subset$ stability region, the coefficients R_ν admit the Cauchy representation

$$R_\nu = \frac{1}{2\pi i} \oint_\Gamma \zeta^{\nu-1} R(\zeta) d\zeta, \quad \Gamma \text{ outside unit circle.}$$

$\Rightarrow$ BDF solution $\eta_\nu,\ \nu \geq k$, with initial values $\eta_0, \ldots, \eta_{k-1}$:

$$\eta_\nu = -\sum_{j=k}^{\min\{2k-1,\nu\}} R_{\nu+k-j}(hA) \Big(\sum_{\ell=0}^{2k-1-j} \alpha_\ell\, \eta_{j-k+\ell} \Big) + h \sum_{j=k}^{\nu} R_{\nu+k-j}(hA) f_j$$

The $R_\nu = R_\nu(hA)$ satisfy the homogeneous difference equation, with $R_0 = \alpha_0^{-1} I$ and $R_1 = \ldots = R_{k-1} = 0$.

A quantitative discrete resolvent estimate

Let $2 \le k \le 5$, A θ-sectorial with $\theta \le \alpha =$ stability angle; $\alpha_k =$ coefficients of $\rho(\zeta)$; $a_k =$ inner radii of $\mathcal{A}_k$

Proposition 2 [1] :

$$\|R(\zeta)\| \le \frac{b_k}{|\zeta|^{k-1}(|\zeta|-1)} \;\; \forall\, |\zeta| > 1, \qquad b_k = \frac{1}{\alpha_k (1-a_k)^{k-1}}\,.$$

Proof: Extended, quantitative version of the estimate given in [7], based on information about the separation of characteristic roots (Proposition 1). □

Proposition 3 [1] : Let $n := \text{dim}(\mathcal{H})$.

$$\|R_\nu(hA)\| \le e\, b_k \min\{\nu, kn\} \quad \forall\, \nu \ge k.$$

Proof: As in [7], estimating the Cauchy integrals for R_ν. □

Remarks

- Proposition 3 enables stability estimates via discrete variation of constants.
- For another scaling of the discrete resolvent,

$$\hat{R}(\zeta) := (a_k I - hA) R(\zeta),$$

analogous estimates can be derived (and will be used).

- Related work has been done in [5], where *discrete damping properties* are studied for the error of BDF applied to $y' = Ay$. Independently of the smoothness of $y(t)$, there is an order reduction at the first grid points which is damped out algebraically with increasing ν.
- Damping properties of the discrete resolvent are also essential in the following.

The BDF 2 method (A-stable, G-stable)

- For $k=2$, the uniform bounds

$$\|R_\nu(hA)\| \le \tfrac{3}{2}\,, \quad \|\hat{R}_\nu(hA)\| \le \tfrac{9}{4}\,,$$

can easily be concluded from G-stability.

- Precise estimates for the characteristic roots $\zeta_{1,2}(\mu)$:

Lemma 1 [1]: For all $\mu \in \mathbb{C}^-$,

$$|\zeta_{1,2}(\mu)| = \left|\frac{1}{2 \mp \sqrt{1+2\mu}}\right| \le \frac{1}{\sqrt{1-2\,\mathrm{Re}\,\mu}} =: \delta(\mu)\,.$$

For $\mu \in \mathcal{T}_\theta$ with $\mathrm{Re}\,\mu \ge -\frac{1}{4}$,

$$|\zeta_1(\mu)| \le e^{\tau\,\mathrm{Re}\,\mu}, \quad \tau = 2\ln(\tfrac{3}{2}) \approx 0.81,$$

and ζ_2 is uniformly strictly smaller than ζ_1 (depending on θ).

‘Scalar damping’ for BDF 2

Lemma 1 implies quantitative damping estimates for the scalar discrete resolvent (proof via Cauchy representation):

Lemma 2 [1]: For $\mu \in \mathcal{T}_\theta$ with $\mathrm{Re}\,\mu \geq -\frac{1}{4}$,

$$|r_\nu(\mu)| \leq C(\theta) e^{\tau(\nu-2)\mathrm{Re}\,\mu}, \quad \nu \geq 2,$$

with $\tau \approx 0.81$ as above.

For $\mathrm{Re}\,\mu \leq -\frac{1}{4}$,

$$|r_\nu(\mu)| \leq \frac{e^2}{3 - 2\,\mathrm{Re}\,\mu}\,\nu\,\delta(\mu)^\nu, \quad \nu \geq 2,$$

with $\delta(\mu) < 1$ as above, $\delta(\mu) \to 0$ for $\mu \to \infty$.

Asymptotic error expansion for BDF 2

Problem is assumed to be sectorial and non-degenerate (strongly elliptic), with bounded inverse A^{-1}. Assume smooth solution $y(t)$; but inhomogeneity f need not be bounded. We only require $A^{-1}f$ to be bounded.

- Ansatz

$$\eta_\nu - y(t_\nu) = h^2 e_2(t_\nu) + h^3 e_3(t_\nu) + \varepsilon_\nu$$

together with local error expansion yields

$$e_2' = Ae_2 + \tfrac{1}{3}\, y''', \quad e_3' = Ae_3 - \tfrac{1}{4}\, y^{IV},$$

and

$$\tfrac{1}{2}\,\varepsilon_{\nu-2} - 2\,\varepsilon_{\nu-1} + (\tfrac{3}{2}I - hA)\varepsilon_\nu = h\, i_\nu,$$

where i_ν is a collection of formally $\mathcal{O}(h^4)$ Taylor remainders depending on derivatives of y, e_2 and e_3.

The principal error functions $e_2(t)$ and $e_3(t)$

- With $e_2(0) = e_3(0) = 0$ we obtain bounded solutions $e_2(t)$, $e_3(t)$, but

$$
\begin{aligned}
e_2'''(0) &= y^V(0) - \tfrac{2}{3}\, f^{IV}(0) - \tfrac{1}{3}\, A f'''(0), \\
e_3''(0) &= -\tfrac{1}{2}\, y^V(0) + \tfrac{1}{4}\, f^{IV}(0),
\end{aligned}
$$

are not bounded and influence the inhomogeneity i_ν in the difference equation for the remainder ε_ν.

- Thus, ε_ν is only 'formally $\mathcal{O}(h^4)$' – it remains to be estimated. The following results are similar as in [2] for the backward Euler scheme, with a considerably higher technical effort. (For the special case of selfadjoint A, the analysis is similar but reduces to spectral estimates.)

Estimation of the remainder ε_ν (i)

- Smooth and bounded contributions from e_2 and e_3 (via i_ν) can be estimated by conventional stability argument, using bounds for $R_\nu(hA)$ and $\hat{R}_\nu(hA)$

- 'Critical terms' in ε_ν result from unbounded terms $\hat{e}_2'''(0)$, $\hat{e}_3''(0)$ in $e_2'''(0)$, $e_3''(0)$. They can be represented as

$$\begin{aligned}\hat{\varepsilon}_{\nu,2} &= h^4\,\Omega_\nu \hat{I}_2\,\hat{e}_2'''(0),\\ \hat{\varepsilon}_{\nu,3} &= h^4\,\Omega_\nu \hat{I}_3\,\hat{e}_3''(0),\end{aligned}$$

where

$$\begin{aligned}\hat{I}_2 &= -(hA)^{-3}(\tfrac{1}{2}\,I - 2\,e^{hA} + (\tfrac{3}{2}I - hA)e^{2hA}),\\ \hat{I}_3 &= -hA\,\hat{I}_2\,,\end{aligned}$$

and Ω_ν satisfies

$$\tfrac{1}{2}\,\Omega_{\nu-2} - 2\,\Omega_{\nu-1} + (\tfrac{3}{2}I - hA)\Omega_\nu = e^{t_{\nu-2}A}.$$

Estimation of the remainder ε_ν (ii)

- The critical terms can be rewritten as ([1])

$$\begin{aligned} \hat{\varepsilon}_{\nu,2} &= h^4 (hA)^{-3} (\tilde{E}_\nu - e^{t_\nu A}) \hat{e}_2'''(0), \\ \hat{\varepsilon}_{\nu,3} &= -h^5 (hA)^{-3} (\tilde{E}_\nu - e^{t_\nu A}) A \, \hat{e}_3''(0), \end{aligned}$$

where $\tilde{E}_\nu$ is the BDF approximation to the operator exponential, i.e.

$$\tfrac{1}{2} \tilde{E}_{\nu-2} - 2 \tilde{E}_{\nu-1} + (\tfrac{3}{2} I - hA) \tilde{E}_\nu = 0, \quad \nu \geq 2,$$

with $\tilde{E}_0 = I$, $\tilde{E}_1 = e^{hA}$.

This representation follows from the difference equation for Ω_ν together with the fact that $\hat{I}_2$ and $\hat{I}_3$ are essentially local truncation errors w.r.t. e^{tA}.

Estimation of the remainder ε_ν (iii)

- Due to the occurrence of A and A^2 in $\hat{e}_2'''(0)$ and $\hat{e}_3''(0)$, a simple stability estimate is too weak. We now combine techniques from [2] and [5].

- Sharp estimation of

$$(\tilde{E}_\nu - e^{t_\nu A}) \cdot A^p$$

is accomplished by

– Considering the scalar problem ($hA \sim \mu \in \mathcal{T}_\theta$), and making use of the distribution of characteristic roots and/or damping properties of the scalar discrete resolvent (see above),

– and applying a spectral argument (A selfadjoint) or a Cauchy estimate near the boundary of $\mathcal{T}_\theta$, using the resolvent inequality characterizing sectorial A.

Main result

Proposition 4 [2] :
For $\eta_0 = y(0)$ and exact or sufficiently accurate initial value $\eta_1 \approx y(h)$, the global error of BDF 2 satisfies

$$\eta_\nu - y(t_\nu) = h^2 e_2(t_\nu) + h^3 e_3(t_\nu) + \varepsilon_\nu,$$

with smooth functions $e_2(t)$, $e_3(t)$ independent of h, and

$$\varepsilon_\nu = \hat{\varepsilon}_\nu + \mathcal{O}(h^4) = \mathcal{O}(h^3),$$

where the $\mathcal{O}(h^4)$ - term depends on certain derivatives of $y(t)$, and

$$\|\hat{\varepsilon}_\nu\| \leq \Big(C_0 + \frac{C_1}{t_\nu}\Big) h^4,$$

with an order reduction $\mathcal{O}(h^4) \to \mathcal{O}(h^3)$ at the first grid points which is damped out algebraically with increasing ν.

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