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

Time Integration of Evolution Equations
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We consider $k$-step BDF schemes applied to evolution equations

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

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 $\rho$ and $\sigma$ 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.
Proposition 1 [3]: For \( k = 2 \ldots 5 \) and arbitrary \( \mu \) 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, \( a_k = \frac{1}{|1 - \omega_k|} \), \( \omega_k = e^{2\pi i/k} \).

<table>
<thead>
<tr>
<th>( k )</th>
<th>( a_k )</th>
</tr>
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<tbody>
<tr>
<td>2</td>
<td>( \frac{1}{2} )  = 0.5</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{1}{\sqrt{3}} )  \approx 0.5774</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{1}{\sqrt{2}} )  \approx 0.7071</td>
</tr>
<tr>
<td>5</td>
<td>( \frac{\sqrt{5+\sqrt{5}}}{\sqrt{10}} ) \approx 0.8507</td>
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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. $\mu$ in the stability region, see [3].

$\bullet \ k = 5:$

![Diagram of characteristic roots](image-url)
Problem class

We assume $A$ to be densely defined and $\theta$-sectorial, i.e.

$$\langle Au, u \rangle \in \mathcal{T}_\theta,$$

$$\mathcal{T}_\theta := \{ z \in \mathbb{C} : |\arg(-z)| \leq \theta \}$$

equivalent to the resolvent inequality

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

- Characteristic polynomial and discrete resolvent (with $hA$ taking the role of $\mu$):

$$P(\zeta) = \rho(\zeta)I - \sigma(\zeta)hA,$$

$$R(\zeta) = P^{-1}(\zeta) = \sum_{\nu=k}^{\infty} \zeta^{-\nu} R_\nu(hA)$$
Discrete variation of constants

For sector $\mathcal{S}_\theta \subset$ stability region, the coefficients $R_\nu$ 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 $\eta_0, \ldots, \eta_{k-1}$:

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

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

Proposition 2 [1]:

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

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 $n := \dim(\mathcal{H})$.

$$\| R_\nu(hA) \| \leq e b_k \min\{\nu, k n\} \quad \forall \nu \geq k.$$ 

Proof: As in [7], estimating the Cauchy integrals for $R_\nu$. □
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 \( \nu \).
- 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

\[
\| R_\nu(hA) \| \leq \frac{3}{2}, \quad \| \hat{R}_\nu(hA) \| \leq \frac{9}{4},
\]

can easily be concluded from G-stability.

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

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

\[
|\zeta_{1,2}(\mu)| = \left| \frac{1}{2 \mp \sqrt{1 + 2\mu}} \right| \leq \frac{1}{\sqrt{1 - 2\Re \mu}} =: \delta(\mu).
\]

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

\[
|\zeta_1(\mu)| \leq e^{\tau \Re \mu}, \quad \tau = 2 \ln\left(\frac{3}{2}\right) \approx 0.81,
\]

and $\zeta_2$ is uniformly strictly smaller than $\zeta_1$ (depending on $\theta$).
‘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 \( \Re \mu \geq -\frac{1}{4} \),

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

with \( \tau \approx 0.81 \) as above.

For \( \Re \mu \leq -\frac{1}{4} \),

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

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
  \[ e_2' = A e_2 + \frac{1}{3} y''' , \quad e_3' = A e_3 - \frac{1}{4} y^{IV} , \]

  and
  \[
  \frac{1}{2} \varepsilon_{\nu - 2} - 2 \varepsilon_{\nu - 1} + \left( \frac{3}{2} I - h A \right) \varepsilon_{\nu} = h i_{\nu},
  \]

  where $i_{\nu}$ is a collection of formally $O(h^4)$ 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

$$
e'''_2(0) = y^V(0) - \frac{2}{3} f^{IV}(0) - \frac{1}{3} A f'''(0),$$
$$e''_3(0) = -\frac{1}{2} y^V(0) + \frac{1}{4} f^{IV}(0),$$

are not bounded and influence the inhomogeneity $i_\nu$ in the difference equation for the remainder $\varepsilon_\nu$.

- Thus, $\varepsilon_\nu$ is only ‘formally $O(h^4)$’ – 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 $\varepsilon_\nu$ (i)

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

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

$$
\hat{\varepsilon}_{\nu,2} = h^4 \Omega_\nu \hat{I}_2 \hat{e}_2'''(0),
$$

$$
\hat{\varepsilon}_{\nu,3} = h^4 \Omega_\nu \hat{I}_3 \hat{e}_3''(0),
$$

where

$$
\hat{I}_2 = -(hA)^{-3} \left( \frac{1}{2} I - 2 e^{hA} + \left( \frac{3}{2} I - hA \right) e^{2hA} \right),
$$

$$
\hat{I}_3 = -hA \hat{I}_2,
$$

and $\Omega_\nu$ satisfies

$$
\frac{1}{2} \Omega_{\nu-2} - 2 \Omega_{\nu-1} + \left( \frac{3}{2} I - hA \right) \Omega_\nu = e^{t_\nu - 2A}.
$$
Estimation of the remainder $\varepsilon_\nu$ (ii)

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

$$
\hat{\varepsilon}_{\nu,2} = h^4 (hA)^{-3} (\tilde{E}_\nu - e^{t\nu A}) \hat{e}_2'''(0), \\
\hat{\varepsilon}_{\nu,3} = -h^5 (hA)^{-3} (\tilde{E}_\nu - e^{t\nu A}) A \hat{e}_3''(0),
$$

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

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

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

This representation follows from the difference equation for $\Omega_\nu$ 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 $\varepsilon_{\nu}$ (iii)

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

- Sharp estimation of

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

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

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

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

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

with an order reduction $O(h^4) \rightarrow O(h^3)$ at the first grid points which is damped out algebraically with increasing $\nu$. 
References


