Backward difference formula: The energy technique for subdiffusion equation

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Abstract Based on the equivalence of A-stability and G-stability, the energy technique of the six-step BDF method for the heat equation has been discussed in [Akrivis, Chen, Yu, Zhou, Math. Comp., Revised]. Unfortunately, this theory is hard to extend the time-fractional PDEs. In this work, we consider three types of subdiffusion models, namely single-term, multi-term and distributed order fractional diffusion equations. We present a novel and concise stability analysis of time stepping schemes generated by $k$-step backward difference formula (BDF$k$), for approximately solving the subdiffusion equation. The analysis mainly relies on the energy technique by applying Grenander-Szegő theorem. This kind of argument has been widely used to confirm the stability of various A-stable schemes (e.g., $k = 1, 2$). However, it is not an easy task for the higher-order BDF methods, due to the loss the A-stability. The core object of this paper is to fill in this gap.

Keywords Subdiffusion equation · backward difference formula · stability analysis · energy technique

This work was supported by NSFC 11601206 and Hong Kong RGC grant (No. 25300818).

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1 Introduction

Let $T > 0, \rho \in H$, and consider the single-term subdiffusion, for which the governing equation is given by \[ \frac{\partial^{\alpha,\sigma} u(t)}{\partial t} + A u(t) = 0, \quad 0 < t < T, \] \[ u(0) = \rho, \] (1.1)

where $\sigma > 0, A$ is a positive definite, selfadjoint, linear operator on a Hilbert space $(H, \langle \cdot, \cdot \rangle)$ with domain $D(A)$ dense in $H$. Let $\| \cdot \|$ denote the norm on $H$ induced by the inner product $(\cdot, \cdot)$, and introduce on $V, V := D(A^{1/2})$, the norm $\| \cdot \|$ by $\| v \| := |A^{1/2}v|$. We identify $H$ with its dual, and denote by $V'$ the dual of $V$, and by $\| \cdot \|$, the dual norm on $V', \| v \|_* = |A^{-1/2}v|$. We shall use the notation $(\cdot, \cdot)$ also for the antiduality pairing between $V$ and $V'$. Here $\frac{\partial^{\alpha,\sigma}}{\partial t}$, with $\alpha \in (0, 1)$, denotes the fractional substantial derivative in time variable \[ \frac{\partial^{\alpha,\sigma} u(t)}{\partial t} = \frac{1}{\Gamma(1-\alpha)} \left[ \frac{\partial}{\partial t} + \sigma \right] \int_0^t (t-s)^{-\alpha} e^{-\sigma(t-s)} u(s) ds. \] (1.2)

In addition, under the initial condition $u(0) = \rho$, the fractional substantial derivative $\frac{\partial^{\alpha,\sigma}}{\partial t} (u(t) - e^{-\sigma t} \rho)$ in the model (1.1) is identical with the usual Caputo fractional substantial derivative. The time-fractional diffusion model (1.1) could be derived by using the continuous time random walk, describing anomalous diffusion process [23]. They have recently attracted a lot of attention in physics and chemistry (diffusion in different media, reactions, mixing in hydrodynamic flows), biology (from the motion of animals to that of subcellular structures in the crowded environment inside cells), and many other disciplines [23, 32].

Our purpose in this paper is to discuss the stability for the more general initial boundary value problem

\[ \begin{cases} P(\partial_t) (u(t) - e^{-\sigma t} \rho) + A u(t) = 0, & 0 < t < T, \\ u(0) = \rho, \end{cases} \] (1.3)

where $P(\partial_t) u$ denotes a fractional substantial differential operator of the form

\[ P(\partial_t) u(t) = \int_0^1 \frac{\partial^{\alpha,\sigma} u(t)}{\partial \alpha} d\nu(\alpha), \] (1.4)

with $\nu(\alpha)$ a positive measure on $[0, 1]$. We remark that it is reduced to fractional order differential operators if $\alpha = 0$ in (1.1). These more general models, including in addition to the single-term model (1.1), multi-term and distributed order models are reviewed briefly. In the multi-term model,

\[ P(\partial_t) u(t) = \sum_{i=1}^m b_i \frac{\partial^{\alpha_i,\sigma}}{\partial t} u(t), \]

where the constants $b_i$ are positive and $0 < \alpha_0 < \ldots < \alpha_i < 1$. It becomes the single-term subdiffusion model (1.1) when $m = 1$. In the distributed order model,

\[ P(\partial_t) u(t) = \int_0^1 \frac{\partial^{\alpha,\sigma} u(t)}{\partial \alpha} d\mu(\alpha), \]
where $\mu (\alpha )$ is a nonnegative weight function. Formally, the multi-term subdiffusion model can be seen as the distributed order subdiffusion model associated with the weight function $\mu (\alpha ) = \sum_{i=1}^{m} b_i \delta (\alpha - \alpha_i)$, where $\delta$ is the Dirac-delta function.

Stability of the A-stable one- and/or two-step BDF methods can be easily proved by the energy method. The powerful Nevanlinna–Odeh multiplier technique [31] extends the applicability of the energy method to the non A-stable three-, four- and five-step BDF methods. Using results from Dahlquist’s G-stability theory [14], Liu constructs the new telescope formulas for the BDFk ($k = 3, 4, 5$) schemes of parabolic equations [26], but it fails to BDF6. According to G-stability theory and Nevanlinna-Odeh multipliers [31], Lubich et al. analyze the BDF methods up to order five for parabolic equations [27]. Based on the cerebrated equivalence of A-stability and G-stability [17], Akrivis et al. construct new multipliers and analyze the BDF method for parabolic equations [1]. Recently, the energy technique for the six-step BDF method is first established for the heat equations [2], which also shows that no Nevanlinna-Odeh multiplier exists.

However, as the mentioned above, the G-stability theory [26] or the equivalence of A-stability and G-stability [2] are not easy to extend to subdiffusion equation. Using fractional backward difference formula, error analysis of up to sixth order temporal accuracy for fractional ordinary differential equation has been discussed [10] with the starting quadrature weights schemes. A few years later, based on operational calculus with sectorial operator, nonsmooth data error estimates for fractional evolution equations have been studied in [13] and extended to [20] including fractional substantial PDEs [35] to restore up to six-order. Under the time regularity assumption, high order finite difference method (BDF2) for the anomalous diffusion equation has been studied in [25] by analyzing the properties of the coefficients. Using Grenander-Szegö theorem, stability and convergence for time-fractional subdiffusion equation have been provided in [15] and also developed in [12] for BDF2. To the best of our knowledge, we are unaware of any other published works on stability analysis of BDF$k$ ($k \geq 3$) schemes for subdiffusion equation by the energy technique. This gap in the research literature is the motivation for our work. In this paper, we introduce multipliers satisfying the positivity property (P) and the A-stability property (A) for the BDF$k$ ($k \geq 3$) method and establish a novel stability analysis for time-fractional subdiffusion equation by the energy technique.

An outline of the paper is as follows. In Section 2, we recall the BDF$k$ (corrected) schemes for the model (1.1) and introduce multipliers. In Section 3, we provide some relevant lemmas and prove the positivity property (P) and the A-stability property (A) for the BDF$k$ ($k \geq 3$) method that are needed for the subsequent stability analysis. In Section 4, we use the multipliers in combination with the Grenander–Szegö theorem to establish stability for the BDF$k$ corrected scheme by the energy technique.

2 Multipliers and up to six-step BDF method

Let $N \in \mathbb{N}$, $\tau := T/N$ be the time step, and $t_n := n\tau, n = 0, \ldots , N$, be a uniform partition of the interval $[0, T]$. The fractional substantial derivative $\partial_t^{\alpha,\alpha} \varphi(t_n)$ can be
approximated by [10]
\[
\partial_\tau^\alpha \phi^n := \frac{1}{\tau^\alpha} \sum_{j=0}^n g_j \phi^{n-j} \tag{2.1}
\]
with \(\phi^n = \varphi(t_n)\), where the coefficients \(\{g_j\}_{j=0}^n\) are determined by the \((k\text{-step})\) BDF method generating power series \(g(\zeta)\),
\[
g(\zeta) = \left( \sum_{j=1}^k \frac{1}{j!} (1 - e^{-\sigma_\tau \zeta})^j \right)^\alpha = \sum_{j=0}^\infty g_j \zeta^j, \quad g_j = e^{-\sigma_\tau \tau} l_j^k, \tag{2.2}
\]
It should be noted that there are several ways to compute the coefficients \(l_j^k\). For example, it can be calculated efficiently by the fast Fourier transform or recursion in [32, Chapter 7]; or direct calculation in [8, 9]. Here we introduce the simple and efficient formulas to compute \(l_j^k\) with linearly computational count, see Appendix.

We recursively define a sequence of approximations \(u^n\) to the nodal values \(u(t_n)\) by the \(k\text{-step}\) BDF method. Correspondingly, the BDF\(k\) scheme for solving (1.3) seeks approximations \(u^n, n = 1, \ldots, N\) to the analytic solution \(u(t_n)\) by [10]

**BDF\(k\) scheme**
\[
P(\partial_\tau) (u^n - e^{-\sigma_\tau \tau} \rho) + A u^n = 0, \quad u^0 = \rho.
\]
The low regularity of the solution of (1.1) implies the above standard BDF\(k\) scheme only yields a first-order accuracy [34, 36]. To restore the \(k\text{-th}\) order accuracy for BDF\(k\), the BDF\(k\) scheme has been corrected at the starting \(k - 1\) steps by [35]

**BDF\(k\) corrected scheme**
\[
P(\partial_\tau) (u^n - e^{-\sigma_\tau \tau} \rho) + A u^n = -e^{-\sigma_\tau \tau} \omega_n^{(k)} A \rho, \quad 1 \leq n \leq k - 1,
\]
\[
P(\partial_\tau) (u^n - e^{-\sigma_\tau \tau} \rho) + A u^n = 0, \quad k \leq n \leq N, \tag{2.3}
\]
where the coefficients \(\omega_n^{(k)}\) are given in Table 2.1. Taking \(w^n := u^n - e^{-\sigma_\tau \tau} \rho\) with \(w^0 = 0\), we can rewrite (2.3) as
\[
P(\partial_\tau) w^n + A w^n = -e^{-\sigma_\tau \tau} \left( 1 + \omega_n^{(k)} \right) A \rho, \quad 1 \leq n \leq k - 1,
\]
\[
P(\partial_\tau) w^n + A w^n = -e^{-\sigma_\tau \tau} A \rho, \quad k \leq n \leq N. \tag{2.4}
\]

### 2.1 Multipliers for BDF methods

From the A-stable definition [17, 31], we introduce the following definition.

**Definition 2.1 (A-stability)** Let \(g(\zeta)\) be the generating power series of the \(k\text{-step}\) BDF method defined in (2.2). Let \(\mu(\zeta) = 1 - \mu_1 e^{-\sigma_\tau \zeta} - \cdots - \mu_k (e^{-\sigma_\tau \zeta})^k\) be a polynomial, with real coefficients and roots outside the unit disk. In addition, the generating power series \(g\) and polynomials \(\mu\) have no common divisor. Then, we call the \(k\text{-step}\) scheme described by the pair \((g, \mu)\) is A-stable if
\[
\Re \left( \frac{g(\zeta)}{\mu(\zeta)} \right) > 0 \quad \text{for} \ |\zeta| < 1. \tag{A}
\]
Table 2.1 The coefficients $a_n^{(k)}$.

| BDFk | $a_1^{(k)}$ | $a_2^{(k)}$ | $a_3^{(k)}$ | $a_4^{(k)}$ | $a_5^{(k)}$ |
|------|-------------|-------------|-------------|-------------|-------------|
| $k = 2$ | $\frac{1}{2}$ | 0 | 0 | 0 | 0 |
| $k = 3$ | $\frac{1}{12}$ | $-\frac{5}{12}$ | 0 | 0 | 0 |
| $k = 4$ | $\frac{1}{24}$ | $-\frac{7}{24}$ | $\frac{3}{8}$ | 0 | 0 |
| $k = 5$ | $\frac{1181}{720}$ | $-\frac{127}{80}$ | $\frac{341}{240}$ | $-\frac{251}{720}$ | 0 |
| $k = 6$ | $\frac{2837}{1440}$ | $-\frac{2543}{720}$ | $\frac{17}{10}$ | $-\frac{1201}{720}$ | 0 |

Now, $g(\zeta)/\mu(\zeta)$ is holomorphic inside the unit disk in the complex plane, and

$$\lim_{|\zeta| \to 0} \frac{g(\zeta)}{\mu(\zeta)} = g_0 > 0.$$ 

Therefore, using the maximum principle for harmonic functions, the A-stability property (A) is equivalent to

$$\text{Re} \frac{g(\zeta)}{\mu(\zeta)} \geq 0 \quad \forall \zeta \in \mathcal{H},$$

with $\mathcal{H}$ the unit circle in the complex plane, $\mathcal{H} := \{ \zeta \in \mathbb{C} : |\zeta| = 1 \}$.

**Definition 2.2 (Multipliers)** Let $g(\zeta)$ be the generating power series of the $k$-step BDF method defined in (2.2). Consider a $k$-tuple $(\mu_1, \ldots, \mu_k)$ of real numbers such that with the given $g(\zeta)$ and $\mu(\zeta) := 1 - \mu_1 e^{-\sigma \tau \zeta} - \cdots - \mu_k (e^{-\sigma \tau \zeta})^k$, and the pair $(g, \mu)$ satisfies the A-stability condition (A), and, in addition, the generating power series $g$ and polynomials $\mu$ have no common divisor. Then, we call $(\mu_1, \ldots, \mu_k)$ simply multiplier if it satisfies the positivity property

$$1 - \mu_1 e^{-\sigma \tau \cos x} - \cdots - \mu_k (e^{-\sigma \tau \cos x})^k > 0 \quad \forall x \in \mathbb{R}.$$  

(P)

In this paper, the simply multiplier $(\mu_1, \ldots, \mu_k)$ for the $k$-step BDF method list in the following, see Table 2.2.

Table 2.2 Multipliers for the up to six-step BDF method.

| BDFk | $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_4$ | $\mu_5$ | $\mu_6$ |
|------|---------|---------|---------|---------|---------|---------|
| $k = 3$ | $\frac{1}{3}$ | 0 | 0 | 0 | 0 | 0 |
| $k = 4$ | $\frac{1}{4}$ | 0 | 0 | 0 | 0 | 0 |
| $k = 5$ | 1 | $-\frac{1}{3}$ | 0 | 0 | 0 | 0 |
| $k = 6$ | $\frac{43}{30}$ | $-\frac{2}{3}$ | $\frac{1}{5}$ | 0 | 0 | 0 |
Remark 2.1 From [17,31], we know that the A-stability is equivalent to G-stability for parabolic equation. However, this equivalence property is still an open question for subdiffusion equation and awaits further investigation.

For simplicity, we denote by \( \langle \cdot, \cdot \rangle \) the inner product on \( V, \langle w, v \rangle := (A^{1/2}w, A^{1/2}v) \).

To prove stability of the method by the energy technique, we test \( (2.4) \) by \( v^\sigma = w^\sigma - \mu_1 e^{-\sigma \tau} w^{\sigma-1} - \cdots - \mu_k e^{-\sigma k \tau} w^{\sigma-k} \) and obtain

\[
(P \left( \partial_\tau \right) w^\sigma, v^\sigma) + \langle w^\sigma, v^\sigma \rangle = -e^{-\sigma \tau} \left( 1 + \frac{\mu_1 (k)}{2} \right) \langle \rho, v^\sigma \rangle. \tag{2.5}
\]

For the first term on the left hand side of \( (2.5) \), from \( (1.4) \), we have

\[
(P \left( \partial_\tau \right) w^\sigma, v^\sigma) = \int_0^1 \partial_{\alpha}^\sigma \partial_{\tau}^\alpha w^\sigma d\nu (\alpha), v^\sigma = \int_0^1 \left( \partial_{\alpha}^\sigma \partial_{\tau}^\alpha w^\sigma, v^\sigma \right) d\nu (\alpha)
\]

\[
= \frac{1}{\tau^2} \int_0^1 \left( \sum_{j=0}^n g_j^k w^{\sigma-j}, v^\sigma \right) d\nu (\alpha). \tag{2.6}
\]

We consider the integrand of \( (2.6) \) for our subsequent discussion.

Case 1: \( k = 3,4 \). Taking \( v^\sigma = w^\sigma - \mu_1 e^{-\sigma \tau} w^{\sigma-1} \) with \( \mu_1 = 1/2 \), we have

\[
\begin{align*}
\sum_{j=0}^n g_j^k w^{\sigma-j} &= g^k_0 (w^\sigma - \mu_1 e^{-\sigma \tau} w^{\sigma-1}) + \left( g^k_1 + \frac{1}{2} e^{-\sigma \tau} g^k_0 \right) (w^{\sigma-1} - \mu_1 e^{-\sigma \tau} w^{\sigma-2}) + \cdots \\
&\quad \quad + \left( g^k_{n-1} + \frac{1}{2} e^{-\sigma \tau} g^k_{n-2} + \frac{3}{2} e^{-2\sigma \tau} g^k_{n-3} + \cdots + \frac{n}{2^{n-1}} e^{-(n-1)\sigma \tau} g^k_0 \right) \\
&\quad \quad \quad \times (w^1 - \mu_1 e^{-\sigma \tau} w^0) \\
&= \sum_{j=0}^n g_j^k w^{\sigma-j}
\end{align*}
\]

with

\[
q_j^k = \sum_{m=0}^j \frac{1}{2^m} e^{-\sigma m \tau} g^k_{j-m}. \tag{2.7}
\]

Case 2: \( k = 5 \). Taking \( v^\sigma = w^\sigma - \mu_1 e^{-\sigma \tau} w^{\sigma-1} - \mu_2 e^{-2\sigma \tau} w^{\sigma-2} \) with \( \mu_1 = 1, \mu_2 = -1/4 \), it yields

\[
\begin{align*}
\sum_{j=0}^n g_j^k w^{\sigma-j} &= g^k_0 (w^\sigma - \mu_1 e^{-\sigma \tau} w^{\sigma-1} - \mu_2 e^{-2\sigma \tau} w^{\sigma-2}) + \left( g^k_1 + e^{-\sigma \tau} g^k_0 \right) \\
&\quad \quad \quad \quad \quad \times (w^{\sigma-1} - \mu_1 e^{-\sigma \tau} w^{\sigma-2} - \mu_2 e^{-2\sigma \tau} w^{\sigma-3}) + \cdots \\
&\quad \quad \quad \quad \quad + \left( g^k_{n-1} + e^{-\sigma \tau} g^k_{n-2} + \frac{3}{2} e^{-2\sigma \tau} g^k_{n-3} + \cdots + \frac{n}{2^{n-1}} e^{-(n-1)\sigma \tau} g^k_0 \right) \\
&\quad \quad \quad \quad \quad \times (w^1 - \mu_1 e^{-\sigma \tau} w^0 - \mu_2 e^{-2\sigma \tau} w^1) \\
&= \sum_{j=0}^n g_j^k w^{\sigma-j}
\end{align*}
\]
with the starting values \( w^{-1} = 0 \) \(^{[29]} \) and

\[
q_j^k = \sum_{m=0}^j \frac{m+1}{2^m} e^{-\sigma m \tau} g_{j-m}^k.
\]  

(2.8)

Case 3: \( k = 6 \). Taking \( \nu^2 = w^\mu - \mu_1 e^{-\sigma \tau w^{\mu-1}} - \mu_2 e^{-2\sigma \tau w^{\mu-2}} - \mu_3 e^{-3\sigma \tau w^{\mu-3}} \) with \( \mu_1 = 43/30, \mu_2 = -2/3, \mu_3 = 1/10 \), there exists

\[
\begin{align*}
\sum_{j=0}^n g_j^k w^{n-j} \\
= g_0^k (w^n - \mu_1 e^{-\sigma \tau w^{\mu-1}} - \mu_2 e^{-2\sigma \tau w^{\mu-2}} - \mu_3 e^{-3\sigma \tau w^{\mu-3}}) \\
+ \left( g_1^k + \frac{43}{30} e^{-\sigma \tau} g_0^k \right) (w^{n-1} - \mu_1 e^{-\sigma \tau w^{\mu-2}} - \mu_2 e^{-2\sigma \tau w^{\mu-3}} - \mu_3 e^{-3\sigma \tau w^{\mu-4}}) + \cdots \\
+ \left( g_{n-1}^k + \frac{43}{30} e^{-\sigma \tau} g_{n-2}^k + \cdots + \frac{243 \times 18^m - 15^m + 25 \times 10^{m-2}}{30^m} e^{-(n-1)\sigma \tau} g_0^k \right) \\
\times (w^1 - \mu_1 e^{-\sigma \tau w^0} - \mu_2 e^{-2\sigma \tau w^1} - \mu_3 e^{-3\sigma \tau w^2}) = \sum_{j=0}^{n-1} q_j^k \nu^{n-j}
\end{align*}
\]

with the starting values \( w^{-1} = w^{-2} = 0 \) and

\[
q_j^k = \sum_{m=0}^j \frac{243 \times 18^m - 15^m + 25 \times 10^{m-2}}{30^m} e^{-\sigma m \tau} g_{j-m}^k.
\]  

(2.9)

Therefore, E.q. (2.6) can be written in the following equivalent form

\[
(P (\partial_{\alpha}) w, \nu) = \frac{1}{\tau^\alpha} \int_0^1 \left( \sum_{j=0}^{n-1} q_j^k \nu^{n-j}, \nu \right) d\nu (\alpha).
\]  

(2.10)

To prove stability of the method by the energy technique for (2.5). First, we sum over \( n \) and subsequently estimate the sum of each terms. The integrand of the first term on the left-hand side can be estimated from below using Lemmas \(3.5-3.8\); this is the motivation for the requirement \([A]\). In view of the Grenander–Szegö theorem, the condition \([P]\) ensures that symmetric band Toeplitz matrices, with generating function the positive trigonometric polynomial \( 1 - \mu_1 e^{-\sigma \tau \cos \alpha} - \cdots - \mu_4 e^{-\sigma k \tau \cos(k \alpha)}, \) are positive definite; see Lemma \(3.3\).

### 3 Positivity property (P) and A-stability property (A)

Before we proceed, for the reader’s convenience, we recall the notion of the generating function of an \( n \times n \) Toeplitz matrix \( T_\nu \) as well as an auxiliary result, the Grenander–Szegö theorem.

**Definition 3.1** \([33\text{ p. 27}]\) A matrix \( A \in \mathbb{R}^{n \times n} \) is said to be positive definite in \( \mathbb{R}^n \) if \( (Ax, x) > 0, \forall x \in \mathbb{R}^n, x \neq 0. \)
Lemma 3.1 [33, p. 28] A real matrix $A$ of order $n$ is positive definite if and only if its symmetric part $H = \frac{A + A^T}{2}$ is positive definite. Let $H \in \mathbb{R}^{n \times n}$ be symmetric. Then $H$ is positive definite if and only if the eigenvalues of $H$ are positive.

Definition 3.2 [7, p. 13] (the generating function of a Toeplitz matrix) Consider the $n \times n$ Toeplitz matrix $T_n = (t_{ij}) \in \mathbb{R}^{n \times n}$ with diagonal entries $t_0$, subdiagonal entries $t_1$, superdiagonal entries $t_{-1}$, and so on, and $(n, 1)$ and $(1, n)$ entries $t_{n-1}$ and $t_{1-n}$, respectively, i.e., the entries $t_{ij} = t_{i-j}$, $i = 1, \ldots, n$, are constant along the diagonals of $T_n$. Let $t_{n+1}, \ldots, t_{n-1}$ be the Fourier coefficients of the trigonometric polynomial $f(x)$, i.e.,

$$t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)e^{-ikx} \, dx, \quad k = 1, \ldots, n-1.$$ 

Then, $f(x) = \sum_{k=1-n}^{n-1} t_k e^{ikx}$, is called generating function of $T_n$.

Lemma 3.2 [7, p. 13–15] (the Grenander–Szegő theorem) Let $T_n$ be given in Definition 3.2 with a generating function $f(x)$. Then, the smallest and largest eigenvalues $\lambda_{\min}(T_n)$ and $\lambda_{\max}(T_n)$, respectively, of $T_n$ are bounded as follows

$$f_{\min} \leq \lambda_{\min}(T_n) \leq \lambda_{\max}(T_n) \leq f_{\max},$$

with $f_{\min}$ and $f_{\max}$ the minimum and maximum of $f(x)$, respectively. In particular, if $f_{\min}$ is positive, then $T_n$ is positive definite.

3.1 Checking the positivity property (P) in space direction

In this subsection, we prove the positivity property (P) in space direction.

Lemma 3.3 For any positive integer $N$, it holds that

$$\sum_{n=1}^{N} \left\langle w^n, w^n - \sum_{j=1}^{k} \mu_j e^{-\sigma j^2} w^{n-j} \right\rangle \geq c_k \sum_{n=1}^{N} \|w^n\|^2, \quad k = 3, 4, 5, 6,$$

where $(c_3, c_4, c_5, c_6) = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$.

Proof We prove the desired results by the following three cases.

Case 1: Let $k = 3, 4$. With this notation $\mu_0 := -1/2, \mu_1 := 1/2, \mu_2 = \mu_3 = \mu_4 = 0$, we have

$$\sum_{n=1}^{N} \left\langle w^n, w^n - \mu_1 e^{-\sigma j^2} w^{n-1} \right\rangle = \frac{1}{2} \sum_{n=1}^{N} \|w^n\|^2 + \sum_{i,j=1}^{N} \ell_{i,j} \left\langle w^i, w^j \right\rangle.$$

Here the lower triangular Toeplitz matrix $L = (\ell_{ij}) \in \mathbb{R}^{N \times N}$ with entries

$$\ell_{i,j} = -\mu_1 e^{-\sigma j^2}, \quad j = 0, 1, \quad i = j + 1, \ldots, N,$$

and all other entries equal zero. From Definition 3.2 we know that the generating function of $(L + L^T)/2$ is

$$f(x) = \frac{1}{2} \left( 1 - e^{-\sigma \cos x} \right) \quad \forall x \in \mathbb{R}.$$
Using Lemma 3.1 and 3.2 it implies that \( L \) is semipositive definite. Then we have
\[
\sum_{n=1}^{N} \langle w^n, w^n - \mu_1 e^{-\sigma \tau} w^{n-1} \rangle \geq \frac{1}{2} \sum_{n=1}^{N} \| w^n \|^2.
\]

Case 2: Let \( k = 5 \). With this notation \( \mu_0 := -3/4, \mu_1 := 1, \mu_2 := -1/4, \mu_3 = \mu_4 = \mu_5 = 0 \), we obtain
\[
\sum_{n=1}^{N} \langle w^n, w^n - \mu_1 e^{-\sigma \tau} w^{n-1} - \mu_2 e^{-2\sigma \tau} w^{n-2} \rangle = \frac{1}{4} \sum_{n=1}^{N} \| w^n \|^2 + \sum_{i,j=1}^{N} \ell_{i,j} \langle w^i, w^j \rangle.
\]

Here, we introduce the lower triangular Toeplitz matrix \( L_1 = (\ell_{ij}) \in \mathbb{R}^{N \times N} \) with entries
\[
\ell_{i,i-j} = -\mu_j e^{-\sigma \tau}, \quad j = 0, 1, 2, \quad i = j + 1, \ldots, N,
\]
and all other entries equal zero. From Definition 3.2 we know that the generating function of \((L_1 + L_1^T)/2\) is
\[
f(x) = \frac{3}{4} - e^{-\sigma \tau} \cos x + \frac{1}{4} e^{-2\sigma \tau} \cos(2x) \geq \frac{1}{2} \left( 1 - e^{-\sigma \tau} \cos x \right)^2 \quad \forall x \in \mathbb{R}.
\]

Using Lemma 3.1 and 3.2 it implies that \( L_1 \) is semipositive definite. Then we have
\[
\sum_{n=1}^{N} \langle w^n, w^n - \mu_1 e^{-\sigma \tau} w^{n-1} - \mu_2 e^{-2\sigma \tau} w^{n-2} \rangle \geq \frac{1}{4} \sum_{n=1}^{N} \| w^n \|^2.
\]

Case 3: Let \( k = 6 \). With this notation \( \mu_0 := -23/24, \mu_1 := 43/30, \mu_2 := -2/3, \mu_3 = 1/10, \mu_4 = \mu_5 = \mu_6 = 0 \), it yields
\[
\sum_{n=1}^{N} \langle w^n, w^n - \mu_1 e^{-\sigma \tau} w^{n-1} - \mu_2 e^{-2\sigma \tau} w^{n-2} - \mu_3 e^{-3\sigma \tau} w^{n-3} \rangle = \frac{1}{24} \sum_{n=1}^{N} \| w^n \|^2 + \sum_{i,j=1}^{N} \ell_{i,j} \langle w^i, w^j \rangle.
\]

To this end, we introduce the lower triangular Toeplitz matrix \( L_2 = (\ell_{ij}) \in \mathbb{R}^{N \times N} \) with entries
\[
\ell_{i,i-j} = -\mu_j e^{-\sigma \tau}, \quad j = 0, 1, 2, 3, \quad i = j + 1, \ldots, N,
\]
and all other entries equal zero. According to Definition 3.2 the generating function of \((L_2 + L_2^T)/2\) is
\[
f(x) = \frac{23}{24} - \frac{43}{30} e^{-\sigma \tau} \cos x + \frac{2}{3} e^{-2\sigma \tau} \cos(2x) - \frac{1}{10} e^{-3\sigma \tau} \cos(3x)
\]
\[
= -\frac{2}{5} (e^{-\sigma \tau} \cos x)^3 + \frac{4}{5} (e^{-\sigma \tau} \cos x)^2 - \frac{43}{30} e^{-\sigma \tau} \cos x + \frac{3}{10} e^{-3\sigma \tau} \cos x
\]
\[
- \frac{2}{3} e^{-2\sigma \tau} + \frac{23}{24} \quad \forall x \in \mathbb{R}.
\]
Let $\xi = e^{-\sigma \tau} \cos x$, $\lambda = e^{-2\sigma \tau}$, it leads to
\[
f(x) = -\frac{2}{5} \xi^3 + \frac{4}{3} \xi^2 - \frac{43}{30} \lambda \xi - \frac{2}{3} \lambda + \frac{23}{24}, \quad \xi \in [-1, 1], \quad \lambda \in (0, 1].
\]
Clearly, $f(x)$ is decreasing with respect to $\lambda$, it yields
\[
f(x) \geq -\frac{2}{5} \xi^3 + \frac{4}{3} \xi^2 - \frac{17}{15} \xi + \frac{7}{24}, \quad \xi \in [-1, 1].
\]
Hence, we consider the polynomial $p$,
\[
p(\xi) := -\frac{2}{5} \xi^3 + \frac{4}{3} \xi^2 - \frac{17}{15} \xi + \frac{7}{24}, \quad \xi \in [-1, 1].
\]
It is easily seen that $p$ attains its minimum at $\xi^* = (20 - \sqrt{94})/18$ and
\[p(\xi^*) > 0.004785 > 0.\]
Using Lemma 3.1 and 3.2, it implies that $L_2$ is positive definite. Then we obtain
\[
\sum_{n=1}^{N} \langle v_n^p, w_n^p - \mu_1 e^{-\sigma \tau} w_n^{p-1} - \mu_2 e^{-2\sigma \tau} w_n^{p-2} - \mu_3 e^{-3\sigma \tau} w_n^{p-3} \rangle \geq \frac{1}{24} \sum_{n=1}^{N} \| w_n^p \|^2.
\]
The proof is completed.

### 3.2 Checking the A-stability property (A) in time direction

The G-stability theory or the equivalence of A-stability and G-stability are used to analyze the stability of BDF methods for parabolic equation. However, it is not easy to extend to subdiffusion equation. In this subsection, we prove the A-stability property $\mathbf{A}$ in time direction for subdiffusion equation. It is well-known that BDF $k$ $(k \geq 3)$ is not A-stable [17, p.251], which underlies the main technical difficulty in carrying out a rigorous stability analysis by the energy technique. Based on the generating power series $g(\xi)$ in (2.2), we construct a novel generating power series
\[
q(\xi) = g(\xi) / \mu(\xi) = \sum_{j=0}^{\infty} q_j^k \xi^j,
\]
where $q_j^k$ is given in (2.7)-(2.9). According to [12, 19, 37] and Definition 2.1, we have the following results.

**Lemma 3.4** *Let* $\{q_j^k\}_{j=0}^{\infty}$ *be a sequence of real numbers such that* $q(\xi) = \sum_{j=0}^{\infty} q_j^k \xi^j$ *is analytic in the unit disk* $S = \{\xi \in \mathbb{C} : |\xi| \leq 1\}$. *Then for any positive integer* $N$ *and for any* $(v^1, \ldots, v^N)$
\[
\sum_{n=1}^{N} \left( \sum_{j=0}^{n-1} q_j^k v^{n-j}, v^n \right) \geq 0,
\]
*if and only if* $\text{Re} q(\xi) \geq 0$, *if and only if* $\text{arg} (q(\xi)) \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.  


Correspondingly, the \( k \)-step schemes described by the pair \((g, \mu)\) are all \(A\)-stable, see the following Lemmas 3.5-3.8.

**Lemma 3.5 (BDF3)** Let \( q_k^j \) be defined by (2.7). Then for any positive integer \( N \), it holds that
\[
\sum_{n=1}^N \left( \sum_{j=0}^{n-1} q_k^j v^{n-j}, v^n \right) \geq 0.
\]

**Proof** From (2.7) and (3.1), we can check that
\[
q(\zeta) = \left( \frac{11}{6} - 3e^{-\sigma \tau \zeta} + \frac{2}{3}(e^{-\sigma \tau \zeta})^2 - \frac{1}{3}(e^{-\sigma \tau \zeta})^3 \right)_{\alpha}.
\]
Taking \( z = e^{-\sigma \tau \zeta} \), it leads to
\[
\left( \frac{11}{6} - 7z + \frac{2}{3}z^2 \right)_{\alpha} = \left( 1 - z \right)_{\alpha} \left( \frac{11}{6} - 7z + \frac{2}{3}z^2 \right)_{\alpha}.
\]

Next we apply the Grenander-Szegö theorem to obtain the desired result. Let \( z = e^{ix} \). Here we just need to consider its principal value on \( x \in [0, \pi] \), since \( x \in [\pi, 2\pi] \) can be similarly discussed. Then
\[
(1 - z)_{\alpha} = \left( 2 \sin \frac{x}{2} \right)_{\alpha} e^{i\theta_1}
\]
with \( \theta_1 = \arctan -\frac{\sin x}{1 - \cos x} = \frac{\pi - x}{2} \leq 0 \).
\[
\left( \frac{11}{6} - 7z + \frac{2}{3}z^2 \right)_{\alpha} = (a_3 - ib_3)_{\alpha} = (a_3^2 + b_3^2)^{\frac{\alpha}{2}} e^{i\alpha \theta_2},
\]
where
\[
a_3 = \frac{1}{6} (11 - 7 \cos x + 2 \cos(2x)) > 0, \quad b_3 = \frac{1}{6} (7 \sin x - 2 \sin(2x)) \geq 0,
\]
\[
\theta_2 = \arctan -\frac{7 \sin x - 2 \sin(2x)}{11 - 7 \cos x + 2 \cos(2x)} \leq 0.
\]
Moreover, we get
\[
\frac{1}{1 - \frac{1}{2} \zeta} = \frac{1}{\sqrt{\frac{1}{2} \cos x}} e^{i\theta_3}, \quad \theta_3 = \arctan \frac{\frac{1}{2} \sin x}{1 - \frac{1}{2} \cos x} \leq \arctan 1 = \frac{\pi}{4}.
\]
From Lemma 3.3 we need to prove
\[
\text{Re} \left\{ \left( \frac{11}{6} - 3z + \frac{2}{3}z^2 - \frac{1}{3}z^3 \right)_{\alpha} \right\} \geq 0,
\]
which is equal to prove
\[
\arg\left\{ \frac{\left( \frac{11}{3} \frac{7}{5} \frac{1}{2} \frac{3}{4} \right)}{1 - \frac{z}{2}} \right\} \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right].
\]

According to the above equations, we have
\[
\arg\left\{ \frac{\left( \frac{11}{3} \frac{7}{5} \frac{1}{2} \frac{3}{4} \right)}{1 - \frac{z}{2}} \right\} = \arg\left\{ \left( 1 - \frac{z}{2} \right) \alpha \right\} + \arg\left\{ \left( \frac{11}{6} \frac{7}{6} \right) \alpha \right\} + \arg\left\{ \frac{1}{1 - \frac{z}{2}} \right\}
\]
\[
= \alpha \theta_1 + \alpha \theta_2 + \theta_3.
\]

Since \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 \leq \theta_2 < \theta_3 \leq \frac{\pi}{4} \) and \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 \geq \theta_1 + \theta_2 + \theta_3 \). Next we just need to prove
\[
g(x) = (\theta_1 + \theta_2 + \theta_3)(x) \geq -\frac{\pi}{4}.
\]
With \( y = \cos x \), it yields
\[
g'(x) = 4 \left( \frac{88y^2 - 182y + 130}{5 - 4y} \right) h(y)
\]
with \( h(y) = -88y^3 + 262y^2 - 230y + 65, y \in [-1,1] \). It is easily seen that \( h \) attains its minimum at \( y^* = \frac{131 - \sqrt{1981}}{132} \) and
\[
h(y^*) > 2.02 > 0.
\]
Moreover, combining with \( (88y^2 - 182y + 130)(5 - 4y) > 0 \), it implies that \( g'(x) \) is positive, \( g(x) \geq g(0) = -\frac{\pi}{4} \). The proof is completed.

**Lemma 3.6** (BDF4) Let \( q_j^k \) be defined by (2.7). Then for any positive integer \( N \), it holds that
\[
\sum_{n=1}^{N} \left( \sum_{j=0}^{n-1} q_j^k \right)^n \geq 0.
\]

**Proof** From (2.7) and (3.1), there exists
\[
g(\zeta) = \left( \frac{25}{12} - 4e^{-\sigma \tau \zeta} + 3(e^{-\sigma \tau \zeta})^2 - \frac{3}{4} (e^{-\sigma \tau \zeta})^3 \right)^{\alpha} \.
\]
Taking \( z = e^{-\sigma \tau \zeta} \), it leads to
\[
\left( \frac{25}{12} - 4z + 3z^2 - \frac{3}{4} z^3 \right)^{\alpha} = \left( 1 - \frac{z}{2} \right)^{\alpha} \left( \frac{25}{12} - \frac{21}{12} z + \frac{13}{12} z^2 - \frac{z}{4} z^3 \right)^{\alpha}.
\]

Next we apply the Grenander-Szegö theorem to obtain the desired result. Let \( z = e^{i\alpha} \). Here we just need to consider its principal value on \( x \in [0,\pi] \). It is easy to compute that
\[
(1 - z)^{\alpha} = \left( 2 \sin \frac{x}{2} \right)^{\alpha} e^{i\alpha \theta_1}.
\]
with \( \theta_1 = \arctan \frac{\sin(x)}{1 - \cos x} = \frac{\pi - x}{4} \leq 0 \); and
\[
\left( \frac{25}{12} \frac{23}{12} z^3 + \frac{13}{12} z^2 - \frac{1}{4} z^3 \right)^\alpha = (a_4 - ib_4)^\alpha = (a_4^2 + b_4^2)^\frac{\alpha}{2} e^{i\alpha \theta_2}
\]
with
\[
a_4 = \frac{1}{12} (25 - 23 \cos x + 13 \cos(2x) - 3 \cos(3x)) > 0,
b_4 = \frac{1}{12} (23 \sin x - 13 \sin(2x) + 3 \sin(3x)) \geq 0, 
\theta_2 = \arctan \frac{-(23 \sin x - 13 \sin(2x) + 3 \sin(3x))}{25 - 23 \cos x + 13 \cos(2x) - 3 \cos(3x)} \leq 0.
\]
Moreover, we get
\[
\frac{1}{1 - \frac{1}{4} z} = \frac{1}{\sqrt{\frac{5}{4} - \cos x}} e^{i\theta_1}, \quad \theta_3 = \arctan \frac{1}{4} \sin(x) \frac{1}{1 - \frac{1}{2} \cos x} \leq \arctan 1 = \frac{\pi}{4}.
\]
From Lemma 3.3 we need to prove
\[
\text{Re} \left\{ \left( \frac{25}{12} \frac{23}{12} z^3 + \frac{13}{12} z^2 - \frac{1}{4} z^3 \right)^\alpha \right\} \geq 0,
\]
which is equal to prove
\[
\arg \left\{ \left( \frac{25}{12} \frac{23}{12} z^3 + \frac{13}{12} z^2 - \frac{1}{4} z^3 \right)^\alpha \right\} \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right] .
\]
According to the above equations, we get
\[
\arg \left\{ \left( \frac{25}{12} \frac{23}{12} z^3 + \frac{13}{12} z^2 - \frac{1}{4} z^3 \right)^\alpha \right\} 
= \arg \left\{ (1 - z)^\alpha \right\} + \arg \left\{ \left( \frac{25}{12} \frac{23}{12} z^3 + \frac{13}{12} z^2 - \frac{1}{4} z^3 \right)^\alpha \right\} + \arg \left\{ \frac{1}{1 - \frac{1}{4} z} \right\}
= \alpha \theta_1 + \alpha \theta_2 + \theta_3 .
\]
Since \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 \leq \theta_3 \leq \frac{\pi}{4} \) and \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 \geq \theta_1 + \theta_2 + \theta_3 \). Next we only need to prove \( g(x) = (\theta_1 + \theta_2 + \theta_3) > \frac{\pi}{2} \). With \( y := \cos x \), we have
\[
g'(x) = \frac{8}{(-600y^4 + 1576y^2 - 1376y + 544)(5 - 4y)} h(y) .
\]
Here \( h(y) = 450y^4 - 1601y^3 + 1949y^2 - 862y + 82 \), \( y \in (-1, 1) \) has the roots \( y_1 \approx 0.1288 \) with \( y_1 \approx 1.4416 \), \( y_2 \approx 0.7664 \). In further, we have \( h(y) > 0 \) if \( y \in (-1, y_1) \) and \( h(y) < 0 \) if \( y \in (y_1, y_2) \) and \( h(y) > 0 \) if \( y \in (y_2, 1) \). Moreover, combining with \( (-600y^4 + 1576y^2 - 1376y + 544)(5 - 4y) > 0 \), it implies that \( g'(x) > 0 \)
Moreover, we get

\[ g(x^*) > -1.37 > -\frac{\pi}{2}. \]

On the other hand, it can be easily checked that \( g(0) = -\frac{\pi}{2} \) and \( g(\pi) = 0 \). Hence, we have \( g(x) \geq -\frac{\pi}{2} \). The proof is completed.

**Lemma 3.7 (BDF5)** Let \( q^j \) be defined by (2.8). Then for any positive integer \( N \), it holds that

\[
\sum_{n=1}^{N} \left( \sum_{j=0}^{n-1} q^j \right)^2 \geq 0.
\]

**Proof** From (2.8) and (3.1), it yields

\[ q(\xi) = \frac{137}{60} - 5e^{-\pi \xi} + 5(e^{-\pi \xi})^2 - 10(e^{-\pi \xi})^3 + \frac{5}{3}(e^{-\pi \xi})^4 - \frac{1}{3}(e^{-\pi \xi})^5. \]

Taking \( z = e^{-\pi \xi} \), it leads to

\[ \frac{(137/60 - 5z + 5z^2 - 10z^3 + 5z^4 - 1/3z^5)}{(1 - 1/3z)^2} = \frac{(1 - z)^\alpha (137/60 - 163/60z + 5z^2 - 63z^3 + 4z^4)}{(1 - 1/3z)^2}. \]

We next apply the Grenander-Szegö theorem to prove the desired result. Let \( z = e^{i\theta} \) with \( x \in [0, \pi] \), it yields

\[ (1 - z)^\alpha = \left( 2 \sin \frac{x}{2} \right)^\alpha e^{i\alpha \theta_1} \]

with \( \theta_1 = \arctan \frac{-\sin(x)}{1 - \cos(x)} = \frac{-\pi}{2} \leq 0 \); and

\[ \left( \frac{137}{60} - \frac{163}{60}z^2 + \frac{5}{3}z^3 + z^4 \right)^\alpha = (a_5 + ib_5)^\alpha = (a_5 + b_5)^\frac{\alpha}{2} e^{i\alpha \theta_2} \]

with

\[ a_5 = \frac{1}{60} \left( 137 - 163 \cos x + 137 \cos(2x) - 63 \cos(3x) + 12 \cos(4x) \right) > 0, \]

\[ b_5 = \frac{1}{60} \left( 163 \sin x - 137 \sin(2x) + 63 \sin(3x) - 12 \sin(4x) \right) \geq 0, \]

\[ \theta_2 = \arctan \frac{(163 \sin x - 137 \sin(2x) + 63 \sin(3x) - 12 \sin(4x))}{137 - 163 \cos x + 137 \cos(2x) - 63 \cos(3x) + 12 \cos(4x)} \leq 0. \]

Moreover, we get

\[ \frac{1}{(1 - 1/3z)^2} = \frac{1}{\frac{x}{2} - \cos x} e^{i\theta_3}, \quad \theta_3 = 2 \arctan \frac{\frac{x}{2} - \cos x}{1 - \frac{x}{2} \cos x} \leq 2 \arctan 1 = \frac{\pi}{2}. \]
From Lemma 3.8 we need to prove

$$\text{Re} \left\{ \frac{\left( \frac{137}{60} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{4}z^4 - \frac{1}{5}z^5 \right)^{\alpha}}{(1 - \frac{1}{2}z)^2} \right\} \geq 0,$$

which is equal to prove

$$\arg \left\{ \frac{\left( \frac{137}{60} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{4}z^4 - \frac{1}{5}z^5 \right)^{\alpha}}{(1 - \frac{1}{2}z)^2} \right\} \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right].$$

According to the above equations, we have

$$\arg \left\{ \frac{\left( \frac{137}{60} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{4}z^4 - \frac{1}{5}z^5 \right)^{\alpha}}{(1 - \frac{1}{2}z)^2} \right\} = \alpha \theta_1 + \alpha \theta_2 + \theta_3.$$

Since $\alpha \theta_1 + \alpha \theta_2 + \theta_3 \leq \theta_3 \leq \frac{\pi}{2}$ and $\alpha \theta_1 + \alpha \theta_2 + \theta_3 \geq \theta_1 + \theta_2 + \theta_3$. Next we need to prove $g(x) = (\theta_1 + \theta_2 + \theta_3)(x) \geq -\frac{\pi}{2}$. With $y := \cos x$, we have

$$g'(x) = \frac{4}{(6576y^4 - 21174y^3 + 24106y^2 - 11144y + 2536)(5 - 4y)}h(y).$$

Here $h(y) = -9864y^5 + 42348y^6 - 66272y^7 + 43985y^8 - 8407y - 1343$, $y \in (-1, 1)$ and the roots are $y_1 \approx -0.0996$ with $x_1 \approx 1.6705$, $y_2 \approx 0.6531$ with $x_2 \approx 0.8591$, respectively. In further, we have $h(y) > 0$ if $y \in (-1, y_1)$ and $h(y) < 0$ if $y \in (y_1, y_2)$ and $h(y) > 0$ if $y \in (y_2, 1)$. Moreover, combining with

$$(6576y^4 - 21174y^3 + 24106y^2 - 11144y + 2536)(5 - 4y) > 0,$$

it implies that $g'(x) > 0$ if $x \in (x_1, \pi)$ and $g'(x) < 0$ if $x \in (x_2, x_1)$ and $g'(x) > 0$ if $x \in (0, x_2)$. Therefore, the function $g$ attains its minimum at $x^* = x_1$ and

$$g(x^*) > -1.33 > -\frac{\pi}{2}.$$

On the other hand, it can be easily checked that $g(0) = -\frac{\pi}{2}$ and $g(\pi) = 0$. Hence, we have $g(x) \geq -\frac{\pi}{2}$. The proof is completed.

**Lemma 3.8 (BDF6)** Let $q^j_i$ be defined by 2.9. Then for any positive integer $N$, it holds that

$$\sum_{n=1}^{N} \left( \sum_{j=0}^{n-1} q^j_i \alpha_{n-j}, \alpha^n \right) \geq 0.$$
Proof From (2.9) and (3.1), we get \( q(\zeta) = \frac{\sigma(\zeta)}{\mu(\zeta)} \) with
\[
g_6(\zeta) = \left( \frac{147}{60} - 6e^{-\sigma \zeta} + \frac{15}{2} (e^{-\sigma \zeta})^2 - \frac{20}{3} (e^{-\sigma \zeta})^3 + \frac{15}{4} (e^{-\sigma \zeta})^4 \right)
- \frac{6}{5} (e^{-\sigma \zeta})^5 + \frac{1}{6} (e^{-\sigma \zeta})^6
\]
and \( \mu_6(\zeta) = (1 - \frac{2}{3} e^{-\sigma \zeta})(1 - \frac{1}{2} e^{-\sigma \zeta})(1 - \frac{1}{4} e^{-\sigma \zeta})(1 - \frac{1}{6} e^{-\sigma \zeta}) \).

Taking \( z = e^{-\sigma \zeta} \), it leads to
\[
(1 - \frac{4}{3} z)^\alpha = \left( \frac{147}{60} - 6z + \frac{15}{2} z^2 - \frac{20}{3} z^3 + \frac{15}{4} z^4 - \frac{6}{5} z^5 + \frac{1}{6} z^6 \right)^\alpha
\]
\[
\left(1 - \frac{3}{2} z\right)^\alpha(1 - \frac{5}{2} z)(1 - \frac{5}{2} z)^\alpha
\]
\[
\left(1 - \frac{5}{2} z\right)^\alpha(1 - \frac{7}{2} z)(1 - \frac{7}{2} z)^\alpha.
\]

Next we apply the Grenander-Szegö theorem to obtain the desired result. Let \( z = e^{ix} \) with \( x \in [0, \pi] \), we have
\[
(1 - z)^\alpha = \left( 2 \sin \frac{x}{2} \right)^\alpha e^{i\alpha \theta_1}
\]
with \( \theta_1 = \arctan \left( \frac{-\sin(x)}{1 - \cos x} \right) = \frac{-\pi}{2} \leq 0 \); and
\[
\left( \frac{147}{60} - \frac{213}{60} z + \frac{237}{60} z^2 - \frac{163}{60} z^3 + \frac{62}{60} z^4 - \frac{10}{60} z^5 \right)^\alpha
= (a_6 - ib_6)^\alpha = (a_6 + b_6)^\alpha = e^{i\alpha \theta_2}
\]
with
\[
a_6(x) = \frac{1}{60} \left( 147 - 213 \cos x + 237 \cos(2x) - 163 \cos(3x) + 62 \cos(4x) - 10 \cos(5x) \right),
\]
\[
b_6(x) = \frac{1}{60} \left( 213 \sin x - 237 \sin(2x) + 163 \sin(3x) - 62 \sin(4x) + 10 \sin(5x) \right) \geq 0,
\]
and \( \theta_2 = \arctan \left( \frac{b_6(x)}{a_6(x)} \right) \leq 0, \ a_6(x) \geq 0, \) or \( \theta_2 = \arctan \left( \frac{b_6(x)}{a_6(x)} - \pi \right) \leq 0, \ a_6(x) \leq 0. \)
Furthermore, there exists
\[
\frac{1}{1 - \frac{3}{5} z} = \frac{1}{\sqrt{\frac{14}{25} - \frac{6}{5} \cos x}} e^{i\theta_1}, \ \theta_1 = \arctan \left( \frac{1}{3} \sin x \right) \frac{1}{1 - \frac{3}{5} \cos x} > 0,
\]
\[
\frac{1}{1 - \frac{4}{5} z} = \frac{1}{\sqrt{\frac{5}{9} - \frac{2}{3} \cos x}} e^{i\theta_2}, \ \theta_2 = \arctan \left( \frac{1}{4} \sin x \right) \frac{1}{1 - \frac{4}{5} \cos x} > 0,
\]
\[
\frac{1}{1 - \frac{5}{6} z} = \frac{1}{\sqrt{\frac{10}{9} - \frac{2}{5} \cos x}} e^{i\theta_3}, \ \theta_3 = \arctan \left( \frac{1}{5} \sin x \right) \frac{1}{1 - \frac{5}{6} \cos x} > 0.
\]
From Lemma [3.4] we need to prove
\[
\text{Re} \left\{ \left( \frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{7}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6 \right) \alpha \right\} \geq 0,
\]
which is equal to prove
\[
\arg \left\{ \left( \frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{7}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6 \right) \alpha \right\} \in \left[ -\frac{\pi}{2}, \frac{\pi}{2} \right].
\]
According to the above equations, we have
\[
\begin{align*}
\arg \left\{ \left( \frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{7}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6 \right) \alpha \right\} &= \arg \left\{ \left( \frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{7}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6 \right) \right\} \\
&= \arg \left\{ \frac{1}{1 - \frac{3}{5}z} \right\} + \arg \left\{ \frac{1}{1 - \frac{1}{2}z} \right\} + \arg \left\{ \frac{1}{1 - \frac{1}{2}z} \right\} \\
&= \alpha \theta_1 + \alpha \theta_2 + \theta_3 + \theta_4 + \theta_5.
\end{align*}
\]
Since \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 + \theta_4 + \theta_5 \geq \theta_1 + \theta_2 + \theta_3 + \theta_4 + \theta_5 \) and \( \alpha \theta_1 + \alpha \theta_2 + \theta_3 + \theta_4 + \theta_5 \leq \theta_3 + \theta_4 + \theta_5 < \frac{\pi}{2} \). In fact, \( \delta(x) = \theta_3 + \theta_4 + \theta_5 < \frac{\pi}{2} \) follows by taking \( \cos x = y \), we have
\[
\delta'(x) = \frac{2}{(17 - 15y)(5 - 4y)(5 - 3y)}p(y).
\]
Here \( p(y) = 135y^3 - 429y^2 + 420y - 120, y (-1, 1) \) has the root \( y_1 \approx 0.5041 \) with \( x_1 \approx 1.0425 \). In further, we obtain \( p(y) < 0 \) if \( y \in (-1, y_1) \) and \( p(y) > 0 \) if \( y \in (y_1, 1) \). Moreover, combining with \( (17 - 15y)(5 - 4y)(5 - 3y) > 0 \), it implies that \( \delta'(x) < 0 \) if \( x \in (x_1, \pi) \) and \( \delta'(x) > 0 \) if \( x \in (0, x_1) \). Therefore, the function \( \delta \) attains its maximum at \( x^* = x_1 \) and
\[
\delta(x^*) < 1.5 < \frac{\pi}{2}.
\]
Next we just need to prove \( g(x) = \theta_1 + \theta_2 + \theta_3 + \theta_4 + \theta_5 \geq -\frac{\pi}{2} \). With \( y := \cos x \), we obtain \( g'(x) = 4b(y)/C_y \). Here
\[
C_y = \begin{vmatrix}
-11760y^5 + 44976y^4 - 64374y^3 + 40906y^2 - 9944y + 1096 \\
\times (5 - 4y)(5 - 3y)(17 - 15y) > 0, \forall y \in [-1, 1]; \\
\end{vmatrix}
\]
and
\[
h(y) = 793800y^8 - 6314580y^7 + 20885463y^6 - 37146627y^5 + 38067828y^4 \\
- 21920022y^3 + 5908998y^2 - 72525y - 199635, y \in [-1, 1],
\]
which has the roots \( y_1 \approx -0.1391 \) with \( x_1 \approx 1.7103, y_2 \approx 0.5015 \) with \( x_2 \approx 1.0455 \). In further, we have \( h(y) > 0 \) if \( y \in (-1, y_1) \) and \( h(y) < 0 \) if \( y \in (y_1, y_2) \) and \( h(y) > 0 \).
Fig. 3.1 Argument of generating power series \( q(\zeta) \) with \( \sigma = 0 \) in (3.1).

if \( y \in (y_2, 1) \). It implies that \( g'(x) > 0 \) if \( x \in (x_1, \pi) \) and \( g'(x) < 0 \) if \( x \in (x_2, x_1) \) and \( g'(x) > 0 \) if \( x \in (0, x_2) \). Therefore, the function \( g \) attains its minimum at \( x^* = x_1 \) with \( a_6(x_1) < 0 \) and

\[
g(x^*) > -1.566 > -\frac{\pi}{2}.
\]

On the other hand, it can be easily checked that \( g(0) = -\frac{\pi}{2} \) and \( g(\pi) = 0 \). Hence, we have \( g(x) \geq -\frac{\pi}{2} \). The proof is completed.

Remark 3.1 From (3.1) and Lemmas 3.5-3.8, it yields

\[
\max \arg (q(\zeta)) \leq \frac{\pi}{2}, \quad \alpha \in [0, 1], \quad k = 3, 4, 5, 6.
\]

Figure 3.1 also shows that the argument of \( q(\zeta) \) are less than or equal to \( \frac{\pi}{2} \).

4 Stability analysis

In this section we prove stability of the up to six-step BDF method (2.3) by the energy technique for subdiffusion equation. The novelty is the simplicity of the proof, the main advantage of the energy technique. The result is well known if \( \alpha = 1 \). Proofs by other stability techniques are significantly more involved. For example, by a spectral
Let $\tilde{u}^n$ be the approximate solution of $u^n$, which is the exact solution of BDF$k$ corrected scheme (2.3) with $\varepsilon^n = \tilde{u}^n - u^n$. Then the BDF$k$ corrected scheme (2.3) with $k = 3, 4, 5, 6$ is stable in the sense that

$$\tau \sum_{n=1}^{N} \|\varepsilon^n\|^2 \leq C \tau \sum_{n=1}^{N} \|\varepsilon^0\|^2$$

and

$$\tau \sum_{n=1}^{N} \|\eta^n\| \leq C \tau \sum_{n=1}^{N} \|\varepsilon^0\|.$$

Proof

Let $\tilde{u}^n$ be the approximate solution of $u^n$, which is the exact solution of BDF$k$ corrected scheme (2.3) with $k = 3, 4, 5, 6$. Putting $\varepsilon^n = \tilde{u}^n - u^n$, we have

$$P(\partial_\tau) (\varepsilon^n - e^{-\sigma \tau} \varepsilon^0) + A \varepsilon^n = -e^{-\sigma \tau} (\alpha_n^{(k)}) A \varepsilon^0.$$

Let $\eta^n = \varepsilon^n - e^{-\sigma \tau} \varepsilon^0$ with $\eta^0 = 0$, it yields

$$P(\partial_\tau) \eta^n + A \eta^n = -e^{-\sigma \tau} (1 + (\alpha_n^{(k)}) A \varepsilon^0.$$

(4.1)

Taking in (4.1) the inner product with $\nu^n = \eta^n - \mu_1 e^{-\sigma \tau} \eta^{n-1} - \ldots - \mu_k e^{-\sigma \varepsilon \tau} \eta^{n-k}$, we have

$$\langle P(\partial_\tau) \eta^n, \nu^n \rangle + \langle \eta^n, \nu^n \rangle = -e^{-\sigma \tau} (1 + (\alpha_n^{(k)}) \langle \varepsilon^0, \nu^n \rangle \leq 1 + (\alpha_n^{(k)}) \|\varepsilon^0\| \cdot \|\nu^n\|.$$

Multiplying the above inequality by $\tau$ and summing up for $n$ from 1 to $N$, we get

$$\tau \sum_{n=1}^{N} \langle P(\partial_\tau) \eta^n, \nu^n \rangle + \tau \sum_{n=1}^{N} \langle \eta^n, \nu^n \rangle \leq C \tau \sum_{n=1}^{N} \|\varepsilon^0\| \cdot \|\nu^n\|.$$

According to (2.10), Lemmas 3.5, 3.8, and the above inequality, it implies that

$$\tau \sum_{n=1}^{N} \langle \eta^n, \nu^n \rangle \leq C \tau \sum_{n=1}^{N} \left( \frac{\|\varepsilon^0\|^2}{4\varepsilon} + \varepsilon \|\nu^n\|^2 \right) \forall \varepsilon > 0.$$

(4.2)

Next we prove the following inequality (4.3) for three cases: $k = 3, 4; k = 5; \text{and } k = 6$.

$$\tau \sum_{n=1}^{N} \|\eta^n\|^2 \leq C \tau \sum_{n=1}^{N} \|\varepsilon^0\|^2.$$

(4.3)

Case 1: Let $k = 3, 4$ with $\nu^n = \eta^n - \frac{1}{2} e^{-\sigma \tau} \eta^{n-1}$. Using (4.2), Lemma 3.3, we have

$$\frac{1}{2} \tau \sum_{n=1}^{N} \|\eta^n\|^2 \leq C \tau \sum_{n=1}^{N} \left( \frac{\|\varepsilon^0\|^2}{4\varepsilon} + \varepsilon_1 \|\nu^n\|^2 \right) \leq C \tau \sum_{n=1}^{N} \|\varepsilon^0\|^2 + \frac{5}{2} \varepsilon_1 \tau \sum_{n=1}^{N} \|\eta^n\|^2.$$


By choosing a sufficiently small $\varepsilon_1$, the desired result (4.3) is obtained.

Case 2: Let $k = 5$ with $\eta^n = \eta^{n-1} + \frac{1}{4}e^{-2\sigma \varepsilon \eta^{n-2}}$. According to (4.2), Lemma 3.3, we obtain

$$1 - \frac{N}{4} \sum_{n=1}^{N} \| \eta^n \|^2 \leq C \tau \sum_{n=1}^{N} \left( \frac{\| e^0 \|^2}{4 \varepsilon_2} + \| \varepsilon^n \|^2 \right) \leq C \tau \sum_{n=1}^{N} \frac{\| e^0 \|^2}{4 \varepsilon_2} + \frac{25}{4} C \varepsilon_2 \tau \sum_{n=1}^{N} \| \eta^n \|^2.$$

By choosing sufficiently small $\varepsilon_2$, the desired result (4.3) is obtained.

Case 3: Let $k = 6$ with $\eta^n = \eta^{n-1} + \frac{1}{16}e^{-3\sigma \varepsilon \eta^{n-2}} - \frac{1}{16}e^{-2\sigma \varepsilon \eta^{n-1}} + \frac{1}{4}e^{-\sigma \varepsilon \eta^n}$. From (4.2), Lemma 3.3, it yields

$$\frac{1}{24} \sum_{n=1}^{N} \| \eta^n \|^2 \leq C \tau \sum_{n=1}^{N} \left( \frac{\| e^0 \|^2}{4 \varepsilon_3} + \| \varepsilon^n \|^2 \right) \leq C \tau \sum_{n=1}^{N} \frac{\| e^0 \|^2}{4 \varepsilon_3} + \frac{44}{3} C \varepsilon_3 \tau \sum_{n=1}^{N} \| \eta^n \|^2.$$

By choosing a sufficiently small $\varepsilon_3$, the desired result (4.3) is obtained.

On the one hand, there exists

$$\| e^n \|^2 = \| e^{-\sigma n \varepsilon} e^0 + e^n - e^{-\sigma n \varepsilon} e^0 \|^2 \leq 2 \left( \| e^0 \|^2 + \| e^n \|^2 \right).$$

From (4.3) and the above inequality, we get

$$\tau \sum_{n=1}^{N} \| e^n \|^2 \leq 2 (C + 1) \tau \sum_{n=1}^{N} \| e^0 \|^2.$$

On the other hand, using Cauchy-Schwarz inequality and (4.3), it yields

$$\left( \tau \sum_{n=1}^{N} \| e^n \|^2 \right)^2 \leq \left( \tau \sum_{n=1}^{N} 1 \right) \left( \tau \sum_{n=1}^{N} \| \eta^n \|^2 \right) \leq C \tau^2 \| e^0 \|^2,$$

which leads to

$$\tau \sum_{n=1}^{N} \| e^n \| - \tau \sum_{n=1}^{N} \| e^{-\sigma n \varepsilon} e^0 \| \leq \tau \sum_{n=1}^{N} \| e^n - e^{-\sigma n \varepsilon} e^0 \| = \tau \sum_{n=1}^{N} \| e^n \| \leq C \tau \| e^0 \|,$$

i.e.,

$$\tau \sum_{n=1}^{N} \| e^n \| \leq (C + 1) T \| e^0 \|.$$

The proof is completed.

Appendix

Let

$$g(\zeta) = \left( \sum_{j=1}^{\infty} \frac{1}{(1 - e^{-\sigma \varepsilon})^j} \right) = \sum_{j=0}^{\infty} g_j \zeta^j, \quad g_j = e^{-\sigma j \varepsilon}.$$
- **BDF1**

\[ t_j^0 = 1, \ t_j^k = \left( 1 - \frac{\alpha + 1}{j} \right) t_j^{k-1}, \ j \geq 1. \]

- **BDF2**

\[ t_0^k = \left( \frac{3}{2} \right)^{\frac{\alpha}{2}}, \ t_1^k = -\left( \frac{3}{2} \right)^{\frac{\alpha}{2}} 4^{\frac{3}{2}} \alpha, \]

\[ t_j^k = \frac{4}{3} \left( 1 - \frac{\alpha + 1}{j} \right) t_j^{k-1} + \frac{1}{3} \left( 2\left( \frac{\alpha + 1}{j} \right) - 1 \right) t_j^{k-2}, \ j \geq 2. \]

- **BDF3**

\[ t_0^k = \left( \frac{11}{6} \right)^{\alpha}, \ t_1^k = -\left( \frac{11}{6} \right)^{\alpha} \frac{18}{11} \alpha, \ t_2^k = \left( \frac{11}{6} \right)^{\alpha} \left( \frac{162}{121} \alpha^2 - \frac{63}{121} \alpha \right), \]

\[ t_j^k = \frac{18}{11} \left( 1 - \frac{\alpha + 1}{j} \right) t_j^{k-1} + \frac{18}{22} \left( \frac{2\left( \alpha + 1 \right)}{j} - 1 \right) t_j^{k-2} + \frac{2}{11} \left( 1 - \frac{3\left( \alpha + 1 \right)}{j} \right) t_j^{k-3}, \ j \geq 3. \]

- **BDF4**

\[ t_0^k = \left( \frac{25}{12} \right)^{\alpha}, \ t_1^k = -\left( \frac{25}{12} \right)^{\alpha} \frac{48}{25} \alpha, \ t_2^k = \left( \frac{25}{12} \right)^{\alpha} \left( \frac{1152}{625} \alpha^2 - \frac{252}{625} \alpha \right), \]

\[ t_j^k = \frac{48}{25} \left( 1 - \frac{\alpha + 1}{j} \right) t_j^{k-1} + \frac{36}{25} \left( \frac{2\left( \alpha + 1 \right)}{j} - 1 \right) t_j^{k-2} + \frac{16}{25} \left( 1 - \frac{3\left( \alpha + 1 \right)}{j} \right) t_j^{k-3} + \frac{3}{25} \left( \frac{4\left( \alpha + 1 \right)}{j} - 1 \right) t_j^{k-4}, \ j \geq 4. \]

- **BDF5**

\[ t_0^k = \left( \frac{137}{60} \right)^{\alpha}, \ t_1^k = -\left( \frac{137}{60} \right)^{\alpha} \frac{300}{137} \alpha, \ t_2^k = \left( \frac{137}{60} \right)^{\alpha} \left( \frac{450000}{18769} \alpha^2 - \frac{3900}{18769} \alpha \right), \]

\[ t_j^k = \frac{137}{60} \left( 1 - \frac{\alpha + 1}{j} \right) t_j^{k-1} + \frac{300}{137} \left( \frac{2\left( \alpha + 1 \right)}{j} - 1 \right) t_j^{k-2} + \frac{200}{137} \left( 1 - \frac{3\left( \alpha + 1 \right)}{j} \right) t_j^{k-3} + \frac{75}{137} \left( \frac{4\left( \alpha + 1 \right)}{j} - 1 \right) t_j^{k-4} + \frac{12}{137} \left( 1 - \frac{5\left( \alpha + 1 \right)}{j} \right) t_j^{k-5}, \ j \geq 5. \]
\begin{align*}
l_k^0 &= \left(\frac{147}{60}\right)^\alpha, \quad l_k^1 = -\left(\frac{147}{60}\right)^\alpha \frac{360}{147} \alpha, \\
l_k^2 &= \left(\frac{147}{60}\right)^\alpha \left(-\frac{288000}{117649} \alpha^3 - \frac{18000}{117649} \alpha^2 + \frac{42400}{117649} \alpha\right), \\
l_k^3 &= \left(\frac{147}{60}\right)^\alpha \left(\frac{8640000}{5764801} \alpha^4 + \frac{1080000}{5764801} \alpha^3 + \frac{1707250}{5764801} \alpha^2 - \frac{2603575}{5764801} \alpha\right), \\
l_k^4 &= \left(\frac{147}{60}\right)^\alpha \left(-\frac{20736000}{282475249} \alpha^5 - \frac{43200000}{282475249} \alpha^4 - \frac{14730000}{40353607} \alpha^3 + \frac{310309000}{282475249} \alpha^2 - \frac{94994224}{282475249} \alpha\right), \\
l_k^5 &= \left(\frac{147}{60}\right)^\alpha \left(\frac{360}{147} \left(1 - \frac{\alpha + 1}{j}\right) l_{j-1}^5 + \frac{450}{147} \left(\frac{2(\alpha + 1)}{j} - 1\right) l_{j-2}^5 + \frac{400}{147} \left(1 - \frac{3(\alpha + 1)}{j}\right) l_{j-3}^5\right) \\
&\quad + \frac{225}{147} \left(\frac{4(\alpha + 1)}{j} - 1\right) l_{j-4}^5 + \frac{72}{147} \left(1 - \frac{5(\alpha + 1)}{j}\right) l_{j-5}^5 \\
&\quad + \frac{10}{147} \left(\frac{6(\alpha + 1)}{j} - 1\right) l_{j-6}^5, \quad j \geq 6.
\end{align*}

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