Convergence and stability of boundary value methods for ordinary differential equations

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Abstract

A usual way to approximate the solution of initial value problems for ordinary differential equations is the use of a linear multistep formula. If the formula has k steps, k values are needed to obtain the discrete solution. The continuous problem provides only the initial value. It is customary to impose the additional k - 1 conditions at the successive k - 1 initial points. However, the class of methods obtained in this way suffers from heavy limitations summarized by the two Dahlquist barriers. It is also possible to impose the additional conditions at different grid-points. For example, some conditions can be imposed at the initial points and the remaining ones at the final points. The obtained methods, called boundary value methods (BVMs), do not have barriers whatsoever. In this paper the question of convergence of BVMs is discussed, along with the linear stability theory. Some numerical examples on stiff test problems are also presented.

Keywords: Boundary value methods; Linear multistep formulae; Stability

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1. Introduction

A common way to approximate the solution of the problem

\[ y' = f(t, y), \quad t \in [t_0, T], \quad y(t_0) = y_0, \]  

is the use of a k-step linear multistep formula:

\[ \sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \]  

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over the partition
\[ t_i = t_0 + ih, \quad i = 0, \ldots, N + k_2 - 1, \quad h = (T - t_0)/(N + k_2 - 1). \]

Here \( y_n \) is the discrete approximation to \( y(t_n) \) and \( f_n = f(t_n, y_n) \). The \( k \) conditions required by scheme (2) are usually obtained by fixing the values \( y_0, \ldots, y_{k-1} \) of the discrete solution. Since only \( y_0 \) is provided by the continuous problem, the remaining values \( y_1, \ldots, y_{k-1} \) need to be found. We shall refer to the class of such methods as Initial Value Methods (IVMs). This approach is very straightforward, although it suffers from heavy theoretical limitations, summarized by the two well-known Dahlquist barriers.

A less-known approach is to fix the values
\[ y_0, \ldots, y_{k_1-1}, \quad y_N, \ldots, y_{N+k_2-1}, \quad k_1 + k_2 = k, \]
of the discrete solution. The continuous initial value problem (1) is then approximated by means of a discrete boundary value problem. We call the methods obtained in this way Boundary Value Methods (BVMs) with \((k_1, k_2)\)-boundary conditions. We observe that for \( k_1 = k \) and \( k_2 = 0 \) one obtains the IVMs, which may be regarded as particular BVMs. For earlier references on this approach see, for example [4, 6].

2. Discrete boundary value problems

In order to discuss the behavior of the solutions given by BVMs, we need to analyze in more detail the solution of a linear discrete boundary value problem. For simplicity, we shall analyse the case of a homogeneous equation [3, 5, 10], although the results can be generalized to non-homogeneous equations [8]. Then, let
\[ \sum_{i=0}^{k} p_i y_{n+i} = 0, \quad n = 0, \ldots, N - k_1 - 1, \]
\[ y_0, \ldots, y_{k_1-1}, \quad y_N, \ldots, y_{N+k_2-1} \text{ fixed,} \tag{3} \]
be a given discrete boundary value problem. Moreover, let \( p(z) = \sum_{i=0}^{k} p_i z^i \) be the characteristic polynomial associated with the difference equation, whose zeros are
\[ |z_1| \leq \cdots \leq |z_k|. \]
The following result holds true.

**Theorem 1.** Suppose that \(|z_{k_1-1}| < |z_{k_1}| < |z_{k_1+1}|, |z_{k_1+1}| > 1\). Then, the solution of problem (3) is given by
\[ y_n = z_1^n (\gamma + O(|z_{k_1-1}/z_{k_1}|n)) + O(|z_{k_1}/z_{k_1+1}|^{N-n}) + O(|z_{k_1+1}|^{-N}) + O(|z_{k_1+1}|^{-(N-n)}), \]
where \( \gamma \) depends only on \( y_0, \ldots, y_{k_1-1} \).
Proof. We shall prove the results in the simpler case where $p(z)$ has only simple zeros. The general solution of the difference equation (3) is given by

$$y_n = e_i^T D_i^n c_i + c_k, z_k^n + e_f^T D_f^n c_f,$$

where

$$D_i = \text{diag}(z_1, \ldots, z_{k_1-1}), \quad D_f = \text{diag}(z_{k_1}, \ldots, z_k),$$

$$e_i = (1, \ldots, 1)^T \in \mathbb{R}^{k_1-1}, \quad e_f = (1, \ldots, 1)^T \in \mathbb{R}^{k_2}.$$

The entries of the two vectors $c_i$ and $c_f$ and the scalar $c_k$ must be determined in order to satisfy the boundary conditions. In matrix form they are:

$$
\begin{pmatrix}
1 & e_i^T & e_f^T \\
 w_{k_1-1} z_k, & U_{k_1-1} D_i & V_{k_1-1} D_f \\
 w_k z_k & U_k D_i^N & V_k D_f^N
\end{pmatrix}
\begin{pmatrix}
c_k \\
c_i \\
c_f
\end{pmatrix}
= 
\begin{pmatrix}
y_0 \\
y_i \\
y_f
\end{pmatrix},
$$

where

$$U_j = \begin{pmatrix} 1 & \ldots & 1 \\ z_1 & \ldots & z_{k_1-1} \\ \vdots & \ddots & \vdots \\ z_{j-1} & \ldots & z_{k_1-1} \end{pmatrix}, \quad V_j = \begin{pmatrix} 1 & \ldots & 1 \\ z_{k_1+1} & \ldots & z_k \\ \vdots & \ddots & \vdots \\ z_{j-1} & \ldots & z_{k_1+1} \end{pmatrix},$$

$$w_f = (1, z_{k_1}, \ldots, z_{k_1}^j)^T, \quad y_i = (y_1, \ldots, y_{k_1-1})^T, \quad y_f = (y_N, \ldots, y_{N+k_2-1})^T. \quad \text{The coefficient matrix } G \text{ can be factored as follows:}$$

$$G = \begin{pmatrix}
1 & e_i^T & e_f^T \\
 w_{k_1-1} z_k, & U_{k_1-1} D_i & V_{k_1-1} D_f \\
 w_k z_k^N & U_k D_i^N & V_k D_f^N
\end{pmatrix}
= \begin{pmatrix}
1 & e_i^T & e_f^T \\
 w_{k_1-1} z_k, & I_i & B_1 \\
 w_k z_k^N & H & I_f
\end{pmatrix},$$

where $I_i$ and $I_f$ are the identity matrices of size $k_1 - 1$ and $k_2$, respectively, and

$$B_1 = U_{k_1-1} D_i - z_k, w_{k_1-1} e_i^T, \quad B_2 = V_{k_1-1} D_f - z_k, w_{k_1-1} e_f^T,$$

$$H = (U_k z_k D_f - z_k, w_k e_i^T) B_1^{-1}$$

$$= -z_k^N (w_k e_i^T + O((z_{k_1-1}/z_k)^{N})) B_1^{-1} = O(|z_k|^N),$$

$$C = V_k D_f^N - z_k^N w_k e_f^T - H B_2 = (V_k + O((z_k/z_{k_1+1})^N)) D_f^N.$$
From the above relations, it follows that

\[
G^{-1} = \begin{pmatrix}
1 + z_k e_i^T B_1^{-1} w_{k-1} + w^T C^{-1} \nu & w^T C^{-1} H - e_i^T B_1^{-1} & -w^T C^{-1} \\
B_1^{-1} (B_2 C^{-1} \nu - z_k w_{k-1}) & B_1^{-1} (I_1 + B_2 C^{-1} H) & -B_1^{-1} B_2 C^{-1} \\
-C^{-1} \nu & -C^{-1} H & C^{-1}
\end{pmatrix},
\]

where \( w^T = e_i^T - e_i^T B_1^{-1} B_2 \) and \( v = z_k^N w_k - z_k H w_{k-1} = O(|z_k|^N) \). Then, one verifies that

\[
c_k = (1 + z_k e_i^T B_1^{-1} w_{k-1} + O(|z_k/z_{k+1}|^N)) y_0
\]

\[
- (e_i^T B_1^{-1} + O(|z_k/z_{k+1}|^N)) y_i + O(|z_k+1|^{-N})
\]

\[
= \gamma + O(|z_k/z_{k+1}|^N) + O(|z_k+1|^{-N}),
\]

\[
c_i = -B_1^{-1} ((z_k w_{k-1} + O(|z_k/z_{k+1}|^N)) y_0 - (I_i + O(|z_k/z_{k+1}|^N)) y_i + O(|z_k+1|^{-N})
\]

\[
= \delta + O(|z_k/z_{k+1}|^N) + O(|z_k+1|^{-N}),
\]

\[
c_f = D_f^{-N} (V_{k-1}^{-1} + O(|z_k/z_{k+1}|^N)) (y_f + O(|z_k|^N))
\]

\[
= D_f^{-N} (\sigma + O(|z_k/z_{k+1}|^N) + O(|z_k|^N)),
\]

where \( \gamma, \delta \) and \( \sigma \) are constants independent of \( N \). In particular, one has:

\[
\gamma = y_0 + e_i^T B_1^{-1} (y_0 z_k w_{k-1} - y_i),
\]

which depends only on \( y_0, \ldots, y_{k-1} \). Finally, one has

\[
y_n = z_k^N (\gamma + O(|z_k/z_{k+1}|^N) + O(|z_k/z_{k+1}|^{N-n}) + O(|z_k+1|^{-N})
\]

\[
+ O(|z_k+1|^{-N-n})).
\]

**Corollary 2.** Suppose that the roots of the characteristic polynomial \( p(z) \) satisfy the conditions of Theorem 1 and, moreover, \( |z_{k,-1}| < 1 \). Then

\[
y_n = z_k^N (\gamma + O(|z_k/z_{k+1}|^{N-n}) + O(|z_k+1|^{-N})
\]

\[
+ O(|z_{k,-1}|^n) + O(|z_k+1|^{-N-n}),
\]

where \( \gamma \), which is given by (4), depends only on \( y_0, \ldots, y_{k-1} \).

### 3. Boundary value methods

From now on, for any given matrix \( A = (a_{ij}) \), we shall denote by \( |A| \) the matrix whose entries are \( |a_{ij}| \). Moreover, to give the main results concerning BVMs, we need the following definitions.

**Definition 3.** We say that a polynomial \( p(z) \) of degree \( k = k_1 + k_2 \) is a \( S_{k_1,k_2} \)-polynomial if its roots are such that

\[
|z_1| \leq |z_2| \leq \cdots \leq |z_{k_1}| < 1 < |z_{k_1+1}| \leq \cdots \leq |z_k|,
\]
whereas it is a \( N_{k_1, k_2} \)-polynomial if
\[
|z_1| \leq |z_2| \leq \cdots \leq |z_k| \leq 1 < |z_{k+1}| \leq \cdots \leq |z_N|
\]
with simple roots of unit modulus.

We observe that for \( k_1 = k \) and \( k_2 = 0 \) a \( N_{k_1, k_2} \)-polynomial reduces to a Von Neumann polynomial and a \( S_{k_1, k_2} \)-polynomial reduces to a Schur polynomial.

Moreover, the convergence theorem for BVMs will use some results concerning the inverse of a Toeplitz band matrix like
\[
T_N = \begin{pmatrix}
  a_{k_1} & \cdots & a_k \\
  \vdots & \ddots & \vdots \\
  a_0 & \cdots & a_k \\
  \vdots & \ddots & \vdots \\
  a_0 & \cdots & a_{k_1}
\end{pmatrix}_{N \times N}
\]

where \( a_0 a_k \neq 0 \) and \( k_1 + k_2 = k \). For this purpose, let us consider the polynomial:
\[
p(z) = \sum_{i=0}^{k} a_i z^i.
\]

Then, the following result holds true.

**Lemma 4.** If the polynomial \( p(z) \) associated with the matrix \( T_N \) defined in (5) is a \( N_{k_1, k_2} \)-polynomial, then for \( N \) sufficiently large \( T_N^{-1} \) exists and has entries \( t_{ij}^{(-1)} \) such that:
1. \( |t_{ij}^{(-1)}| \leq \gamma \), for \( i \geq j \);
2. \( |t_{ij}^{(-1)}| \leq \nu \xi^{j-i} \), for \( i < j \), where \( 0 < \xi < 1 \).

In the above relations, the constants \( \gamma \), \( \nu \) and \( \xi \) can be chosen independent of \( N \). In particular, \( \xi \propto |z_{k_1+1}|^{-1} \), if \( |z_1| \leq \cdots \leq |z_{k_1}| \leq 1 < |z_{k_1+1}| \leq \cdots \leq |z_k| \) are the roots of \( p(z) \).

**Proof.** See [1]. \( \square \)

The results of the previous lemma can be recasted in matrix form as follows:
\[
|T_N^{-1}| \leq \gamma C_N + \nu D_N,
\]
where \( C_N \) is the \( N \times N \) lower triangular matrix having all unit entries and \( D_N \) is the upper triangular Toeplitz matrix having the entries on the last column given by:
\[
(\xi^{N-1}, \xi^{N-2}, \ldots, \xi^2, \xi, 0)^T.
\]

We are now in a position to state the convergence theorem for BVMs.

**Theorem 5.** Disregarding the effect of round-off errors, a BVM with \((k_1, k_2)\)-boundary conditions is convergent if it is consistent and the polynomial \( p(z) \) is a \( N_{k_1, k_2} \)-polynomial.
Proof. If the LMF (2) is used to approximate the solution of problem (1) by fixing the values $y_0, \ldots, y_{k-1}, y_N, \ldots, y_{N+k2-1}$, it is not difficult to see that the error equation can be written as:

$$A_N e = hB_N \delta f + \tau + g,$$

where

$$e = (e_{k_1}, \ldots, e_{N-1})^T, \quad e_i = y(t_i) - y_i,$$

$$\delta f = (f(t_{k_1}, y(t_{k_1})), \ldots, f(t_{N-1}, y(t_{N-1})) - f_{N-1})^T,$$

$$A_N = \begin{pmatrix}
    \alpha_{k_1} & \ldots & \alpha_k \\
    \ldots & \ddots & \ldots \\
    \alpha_0 & \ldots & \alpha_k
  \end{pmatrix}_{(N-k_1) \times (N-k_1)},$$

$$B_N = \begin{pmatrix}
    \beta_{k_1} & \ldots & \beta_k \\
    \ldots & \ddots & \ldots \\
    \beta_0 & \ldots & \beta_k
  \end{pmatrix}_{(N-k_1) \times (N-k_1)}.$$

$\tau$ is the vector whose entries are the local errors (which are $O(h^{p+1})$, $p \geq 1$, since the method is assumed to be consistent) and $g$ is the vector whose entries represent the errors on the boundary conditions, which we shall suppose to behave at least as $O(h^p)$:

$$g = -\begin{pmatrix}
    \sum_{i=0}^{k_1-1} (\alpha_i e_i - h\beta_i \delta f_i) \\
    \sum_{i=0}^{k_1-1} (\alpha_{k_i} e_{k_i-1} - h\beta_0 \delta f_{k_i-1}) \\
    0 \\
    \sum_{i=1}^{k_2} (\alpha_{i+k_1} e_{N-1+i} - h\beta_{i+k_1} \delta f_{N-1+i}) \\
    \sum_{i=0}^{k_2} (\alpha_0 e_{N-1+i} - h\beta_{k_2} \delta f_{N-1+i})
  \end{pmatrix}.$$

Let $L$ be the Lipschitz constant of $f$. Then, since for $N$ sufficiently large the matrix $A_N$ is always nonsingular (see Lemma 4), one has:

$$|e| \leq hL |A_N^{-1} B_N| |e| + |A_N^{-1}||\tau| + |g|.$$
From Lemma 4 and relation (6) it follows that
\[ \tilde{\tau} := |A_N^{-1}|(|\tau| + |g|) \leq (\gamma C_N + \nu \Delta_N)(|\tau| + |g|), \] (7)
for some \( \gamma, \nu > 0 \) and \( \xi \in (0, 1) \) which are independent of \( N \) (for brevity, we have used \( C_N \) and \( \Delta_N \) in place of \( C_{N-k} \) and \( \Delta_{N-k} \), respectively). It follows that the vector \( \tilde{\tau} \) has entries which are \( O(h^p) \), if the \( k \) entries of \( g \) are at least \( O(h^p) \). We have now
\[ (I - hL|A_N^{-1}B_N|)|e| \leq \tilde{\tau}. \]

Let us define the \((N - k_1) \times (N - k_1)\) matrices:
\[
G_N = \begin{pmatrix}
1 & \cdots & 1 \\
\vdots & \ddots & \vdots \\
1 & \cdots & 1
\end{pmatrix}, \quad Q_N = \begin{pmatrix}
0 & 1 & \cdots & 1 \\
1 & \vdots & \ddots & \vdots \\
\vdots & \ddots & \ddots & 1 \\
1 & \cdots & 1 & 0
\end{pmatrix},
\]
where \( G_N \) has \( k_1 \) lower and \( k_2 \) upper off-diagonals, and \( Q_N \) has \( k_2 < k + 1 \) upper off-diagonals. Moreover, let \( \alpha = \max \{\gamma, \nu\} \), \( \beta = \sum_{i=0}^{k} |\beta_i| \). One then obtains
\[
|A_N^{-1}B_N| \leq (\gamma C_N + \nu \Delta_N)\beta G_N
\leq \alpha(k + 1)\beta(C_N + Q_N + \Delta_N G_N).
\]

By posing \( \eta = \alpha(k + 1)\beta L \), it follows that
\[
(I - h\eta(C_N + Q_N + \Delta_N G_N))|e| \leq \tilde{\tau}. \] (8)

If \( h = (T - t_0)/(N + k_2 - 1) \) is sufficiently small, it is possible to show (see [5]) that the matrix \( M_N = (I - h\eta C_N) \) is an \( M \)-matrix, and moreover \( \|M_N^{-1}\|_\infty \) is smaller than \( 2e^{2\eta(T - t_0)} \), for \( h < (2\eta)^{-1} \). It follows that (8) can be written as
\[
M_N^{(1)}|e| := (I - h\eta M_N^{-1}(Q_N + \Delta_N G_N))|e| \leq M_N^{-1}\tilde{\tau}.
\]

Moreover, we have that
\[
\|Q_N + \Delta_N G_N\|_\infty \leq \|Q_N\|_\infty + \|\Delta_N\|_\infty \|G\|_\infty
\leq (k + 1)(1 + \xi(1 - \xi)^{-1}) = \frac{k + 1}{1 - \xi},
\]
which implies that, for \( h \) sufficiently small, the matrix \( M_N^{(1)} \) is also an \( M \)-matrix. Moreover, by posing
\[
\phi = 2\eta e^{2\eta(T - t_0)}\frac{k + 1}{1 - \xi},
\]

for \( h < (2\phi)^{-1} \) one obtains
\[
\| (M_N^{(1)})^{-1} \|_\infty \leq \sum_{n=0}^{\infty} \| hN M_N^{-1} (Q_N + A_N G_N) \|_\infty^2
\]
\[
\leq \sum_{n=0}^{\infty} (h\phi)^n = (1 - h\phi)^{-1} < 2.
\]
Finally, one then obtains:
\[
\| e \|_\infty \leq 4e^{2\pi (T - t_0)} \| \hat{\tau} \|_\infty,
\]
that is, the method is convergent and the global error is \( O(h^p) \). \( \square \)

By using the usual definitions for the polynomials \( \rho(z) \) and \( \sigma(z) \) associated with a given LMF, the above result leads naturally to define 0-stability for BVMs as follows.

**Definition 6.** A BVM with \((k_1, k_2)\)-boundary conditions is \( 0_{k_1, k_2} \)-stable if \( \rho(z) \) is a \( N_{k_1, k_2} \)-polynomial.

We observe that \( 0_{k, k_2} \)-stability reduces to the usual 0-stability, when \( k_1 = k \) and \( k_2 = 0 \).

The next step is to analyse the behavior of a BVM with \((k_1, k_2)\)-boundary conditions on the test equation
\[
y' = \lambda y, \quad \Re(\lambda) < 0. \tag{9}
\]
In this case, taking \( q = h\lambda \), one obtains the discrete problem:
\[
\pi(E, q) y_n := (\rho(E) - q\sigma(E)) y_n = 0,
\]
\[
y_0, \ldots, y_{k_1-1}, \quad y_N, \ldots, y_{N+k_2-1} \text{ fixed.}
\]
The characteristic polynomial of the difference equation is \( \pi(z, q) \). From the result of Corollary 2, it follows that the discrete solution is bounded if the polynomial \( \pi(z, q) \) is a \( S_{k_1, k_2} \)-polynomial. Therefore, we shall give the following definition.

**Definition 7.** For a given \( q \in \mathbb{C} \), a BVM with \((k_1, k_2)\)-boundary conditions is \((k_1, k_2)\)-absolutely stable if \( \pi(z, q) \) is a \( S_{k_1, k_2} \)-polynomial.

Again, \((k_1, k_2)\)-absolute stability reduces to the usual notion of absolute stability for \( k_1 = k \) and \( k_2 = 0 \). Similarly, one defines the region of \((k_1, k_2)\)-absolute stability of the method as follows:
\[
D_{k_1, k_2} = \{ q \in \mathbb{C} : \pi(z, q) \text{ is a } S_{k_1, k_2} \text{-polynomial} \}.
\]
Finally, a BVM with \((k_1, k_2)\)-boundary conditions is said to be \( A_{k_1, k_2} \)-stable if \( \mathbb{C} = D_{k_1, k_2} \). We observe that for BVMs there are no barriers concerning the maximum order for methods which are \( 0_{k, k_2} \)-stable and/or \( A_{k, k_2} \)-stable. In fact, in the next section we shall briefly examine a class of \( k \)-step BVMs which provides \( 0_{k_1, k_2} \)-stable and \( A_{k_1, k_2} \)-stable BVMs of order \( k \), for all \( k \geq 1 \). Other classes of methods which contains \( 0_{k_1, k_2} \)-stable and \( A_{k_1, k_2} \)-stable methods of order up to \( 2k \) can be found in [2, 3, 5].
4. The generalized backward differentiation formulae

Consider the particular class of \( k \)-step LMF having the polynomial \( \sigma(z) \) in its simplest form:
\[
\sigma(z) = z^j, \tag{10}
\]
for a given \( j \in \{0, 1, \ldots, k\} \). The methods of order \( k \) obtained with the choice \( j = k \) are widely used as IVMs and are usually called backward differentiation formulae (BDF). The BDF provide 0-stable methods until \( k = 6 \). It is in fact known that the BDF of order 7 is 0-unstable (see [9]). This is no more case, when \( j \) is not restricted to assume the particular value \( j = k \). In fact, in this case one can choose the value of \( j \) which originates the method with the best stability properties.

Having chosen \( \sigma(z) \) as in (10), the methods in this class can be written as:
\[
\sum_{i=0}^{k} \alpha_i y_{n+i} = h f_{n+j}. \tag{11}
\]
We have then \( k + 1 \) independent parameters left which permit us to obtain methods of maximum order \( k \). Moreover, for \( j = v \) chosen as follows:
\[
v = \begin{cases} 
(k + 1)/2 & \text{for odd } k, \\
k/2 + 1 & \text{for even } k,
\end{cases} \tag{12}
\]
the obtained formulae result to be both \( 0, k - v \)-stable and \( A_{v,k-v} \)-stable for all \( k \geq 1 \). In Figs. 1 and 2 the boundaries \( \Gamma_k \) of the corresponding regions \( D_{v,k-v} \) are plotted for odd \( k \) and even \( k \), respectively, up to \( k = 30 \). For each considered value of \( k \), the stability polynomial
\[
\pi(z, q) = \rho(z) - q z^v
\]
is of type \( (v, 0, k - v) \) in the region outside \( \Gamma_k \), and of type \( (v - 1, 0, k - v + 1) \) inside. It follows that the \( (v, k - v) \)-absolute stability region of the method is the one outside the corresponding boundary \( \Gamma_k \).

The linear multistep formulae with \( \sigma(z) = z^v \), \( v \) given by (12), will be called generalized backward differentiation formulae (GBDF). They must be used with \( (v, k - v) \)-boundary conditions.

We observe that the GBDF provide \( A_{v,k-v} \)-stable methods of order \( k \) for all \( k \geq 1 \), while the usual BDF are not \( A \)-stable, for \( k > 2 \). In Table 1, the coefficients of the GBDF are reported for \( k = 1, \ldots, 10 \). For brevity, for each value of \( k \) we report the normalized coefficients \( \hat{\alpha}_i = \alpha_i / \delta_k \).

Let us now rewrite the generic GBDF as follows:
\[
\sum_{i=-v}^{k-v} \alpha_{i+v} y_{i+v} = h f_n.
\]
This formula can be used for \( n = v, \ldots, N - 1 \), since the additional conditions consist in fixing the values
\[
y_0, \ldots, y_{v-1}, \quad y_N, \ldots, y_{N+k-v-1}.
\]
If these values are really known, one has then a set of \( N - v \) equations and an equal number of unknowns \( (y_v, \ldots, y_{N-1}) \). However, only the value \( y_0 \) is provided by the continuous problem. The values \( y_1, \ldots, y_{v-1} \) can also be obtained in standard ways (e.g., by Taylor expansions or by using a suitable IVM). This is obviously no more the case for the \( k - v \) final values \( y_N, \ldots, y_{N+k-v-1} \).
Fig. 1. Boundaries of the \((v, k - v)\)-absolute stability regions of the GBDF of order \(k, k = 1, 3, 5, \ldots, 29\).

Fig. 2. Boundaries of the \((v, k - v)\)-absolute stability regions of the GBDF of order \(k, k = 2, 4, 6, \ldots, 30\).
Table 1
Normalized coefficients of GBDF

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Table 2
Results for GBDF of order 3, 4, 5, 6

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<th>Error</th>
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Table 3
Results for GBDF of order 7, 8, 9, 10

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which must be treated as unknowns. This requires that an equal number of additional independent equations must be added. To preserve the order \( k \) of the method, these equations can be conveniently derived by methods of order \( k - 1 \). In our case, they can be chosen as follows:

\[
\sum_{i=0}^{k-1} x_{i,r} y_{N-v+i} = hf_{N+r}, \quad r = 0, \ldots, k - v - 1,
\]

where the coefficients \( \{x_{i,r}\} \) are uniquely determined so that each formula has order \( k - 1 \).

5. Numerical tests

In this section we examine the behavior of GBDF on two stiff test problems. The first problem is linear:

\[
y' = \begin{pmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},
\]

whose solution is

\[
y(t) = \frac{1}{2} \begin{pmatrix} e^{-2t} + e^{-40t}(\sin(t) + \cos(t)) \\ e^{-2t} - e^{-40t}(\sin(t) + \cos(t)) \\ e^{-40t}(\sin(t) - \cos(t)) \end{pmatrix}.
\]

Even if there is an initial transient where the solution varies very rapidly, by using a constant stepsize \( h \) over the interval \([0, 0.4]\) we obtain the maximum errors reported in Tables 2 and 3, for the GBDF of order 3, \ldots, 10. Observe that in Table 3 the last rate value for the GBDF of order 10 is far from the expected one since we used double precision and the errors are near the unit roundoff.

The second example is given by the Robertson's equations:

\[
y_1' = -0.04y_1 + 10^4y_2y_3, \quad y_1(0) = 1,
\]

\[
y_2' = 0.04y_1 - 10^4y_2y_3 - 3 \times 10^7y_2^2, \quad y_2(0) = 0,
\]

\[
y_3' = 3 \times 10^7y_2^2, \quad y_3(0) = 0.
\]

In this case, it is known \([7]\) that the second component \( y_2 \) reaches in a point \( \tilde{t} \) near \( t = 0 \) a quasi-stationary position, where \( y_2(\tilde{t}) \approx 3.65 \times 10^{-5} \). Then, this component again goes to zero very slowly. We consider the following mesh:

\[
t_i = t_{i-1} + h_i, \quad h_i = 1.2h_{i-1}, \quad i = 1, 2, \ldots, \quad h_0 = 6.6 \times 10^{-6}.
\]

In Fig. 3 we report the computed solution only in the interval \([0, 0.3]\), in order to observe the above described behavior of \( y_2(t) \). The solution obtained with the GBDF of order 10 is shown by a solid line. For comparison we also report the result provided by LSODE (dashed line) on the same mesh. The parameters used for LSODE, are: \( mf = 21, \ atol = rtol = 1e-14 \). As one can see, the solution computed by the GBDF has a more regular behavior than that computed by LSODE.
Fig. 3. Computed solution with the GBDF of order 10 (solid line) and with LSODE (dashed line).

References