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Convergence and stability of boundary value methods for ordinary differential equations[1]

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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

$$y' = f(t, y), \qquad t \in [t_0, T], \quad y(t_0) = y_0, \tag{1}$$

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

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \tag{2}$$

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over the partition

$$t_i = t_0 + ih, \qquad i = 0, \dots, N + k_2 - 1, \quad h = (T - t_0)/(N + k_2 - 1).$$

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 $y_0, \dots, y_{k-1}$ of the discrete solution. Since only y_0 is provided by the continuous problem, the remaining values $y_1, \dots, y_{k-1}$ 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

$$y_0, \dots, y_{k_1 - 1}, \qquad y_N, \dots, y_{N+k_2-1}, \quad k_1 + k_2 = k,$$

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

$$\sum_{i=0}^{k} p_i y_{n+i} = 0, \quad n = 0, \dots, N - k_1 - 1,$$

$$y_0, \dots, y_{k_1-1}, \quad y_N, \dots, y_{N+k_2-1} \text{ fixed,} \tag{3}$$

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

$$|z_1| \leqslant \cdots \leqslant |z_k|.$$

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*

$$y_n = z_{k_1}^n(\gamma + \mathrm{O}(|z_{k_1-1}/z_{k_1}|^n) + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^{N-n}) + \mathrm{O}(|z_{k_1+1}|^{-N})) + \mathrm{O}(|z_{k_1+1}|^{-(N-n)}),$$

where γ *depends only on* $y_0, \dots, y_{k_1-1}$.

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

$$y_n = \boldsymbol{e}_i^{\mathrm{T}} D_i^n \boldsymbol{c}_i + c_{k_1} z_{k_1}^n + \boldsymbol{e}_f^{\mathrm{T}} D_f^n \boldsymbol{c}_f,$$

where

$$D_i = \mathrm{diag}(z_1, \dots, z_{k_1 - 1}), \qquad D_f = \mathrm{diag}(z_{k_1+1}, \dots, z_k),$$
$$\boldsymbol{e}_i = (1, \dots, 1)^{\mathrm{T}} \in \mathbb{R}^{k_1 - 1}, \qquad \boldsymbol{e}_f = (1, \dots, 1)^{\mathrm{T}} \in \mathbb{R}^{k_2}.$$

The entries of the two vectors $\boldsymbol{c}_i$ and $\boldsymbol{c}_f$ and the scalar c_{k_1} must be determined in order to satisfy the boundary conditions. In matrix form they are:

$$\begin{pmatrix} 1 & \boldsymbol{e}_i^{\mathrm{T}} & \boldsymbol{e}_f^{\mathrm{T}} \\ \boldsymbol{w}_{k_1-1} z_{k_1} & U_{k_1-1} D_i & V_{k_1-1} D_f \\ \boldsymbol{w}_{k_2} z_{k_1} & U_{k_2} D_i^N & V_{k_2} D_f^N \end{pmatrix} \begin{pmatrix} c_{k_1} \\ \boldsymbol{c}_i \\ \boldsymbol{c}_f \end{pmatrix} = \begin{pmatrix} y_0 \\ \boldsymbol{y}_i \\ \boldsymbol{y}_f \end{pmatrix},$$

where

$$U_j = \begin{pmatrix} 1 & \cdots & 1 \\ z_1 & \cdots & z_{k_1-1} \\ \vdots & & \vdots \\ z_1^{j-1} & \cdots & z_{k_1-1}^{j-1} \end{pmatrix}, \qquad V_j = \begin{pmatrix} 1 & \cdots & 1 \\ z_{k_1+1} & \cdots & z_k \\ \vdots & & \vdots \\ z_{k_1+1}^{j-1} & \cdots & z_k^{j-1} \end{pmatrix},$$

$\boldsymbol{w}_j = (1, z_{k_1}, \dots, z_{k_1}^{j-1})^{\mathrm{T}}$, $\boldsymbol{y}_i = (y_1, \dots, y_{k_1-1})^{\mathrm{T}}$, and $\boldsymbol{y}_f = (y_N, \dots, y_{N+k_2-1})^{\mathrm{T}}$. The coefficient matrix G can be factored as follows:

$$G = \begin{pmatrix} 1 & \boldsymbol{e}_i^{\mathrm{T}} & \boldsymbol{e}_f^{\mathrm{T}} \\ \boldsymbol{w}_{k_1-1} z_{k_1} & U_{k_1-1} D_i & V_{k_1-1} D_f \\ \boldsymbol{w}_{k_2} z_{k_1}^N & U_{k_2} D_i^N & V_{k_2} D_f^N \end{pmatrix}$$
$$= \begin{pmatrix} 1 & & \\ \boldsymbol{w}_{k_1-1} z_{k_1} & I_i & \\ \boldsymbol{w}_{k_2} z_{k_1}^N & H & I_f \end{pmatrix} \begin{pmatrix} 1 & \boldsymbol{e}_i^{\mathrm{T}} & \boldsymbol{e}_f^{\mathrm{T}} \\ & B_1 & B_2 \\ & & C \end{pmatrix},$$

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

$$B_1 = U_{k_1-1} D_i - z_{k_1} \boldsymbol{w}_{k_1-1} \boldsymbol{e}_i^{\mathrm{T}}, \quad B_2 = V_{k_1-1} D_f - z_{k_1} \boldsymbol{w}_{k_1-1} \boldsymbol{e}_f^{\mathrm{T}},$$
$$H = (U_{k_2} D_i^N - z_{k_1}^N \boldsymbol{w}_{k_2} \boldsymbol{e}_i^{\mathrm{T}}) B_1^{-1}$$
$$= -z_{k_1}^N (\boldsymbol{w}_{k_2} \boldsymbol{e}_i^{\mathrm{T}} + \mathrm{O}(|z_{k_1-1}/z_{k_1}|^N)) B_1^{-1} = \mathrm{O}(|z_{k_1}|^N),$$
$$C = V_{k_2} D_f^N - z_{k_1}^N \boldsymbol{w}_{k_2} \boldsymbol{e}_f^{\mathrm{T}} - H B_2 = (V_{k_2} + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N)) D_f^N.$$

From the above relations, it follows that

$$G^{-1} = \begin{pmatrix} 1 + z_{k_1} e_i^{\mathrm{T}} B_1^{-1} w_{k_1-1} + w^{\mathrm{T}} C^{-1} v & w^{\mathrm{T}} C^{-1} H - e_i^{\mathrm{T}} B_1^{-1} & -w^{\mathrm{T}} C^{-1} \\ B_1^{-1}(B_2 C^{-1} v - z_{k_1} w_{k_1-1}) & B_1^{-1}(I_i + B_2 C^{-1} H) & -B_1^{-1} B_2 C^{-1} \\ -C^{-1} v & -C^{-1} H & C^{-1} \end{pmatrix},$$

where $w^{\mathrm{T}} = e_f^{\mathrm{T}} - e_i^{\mathrm{T}} B_1^{-1} B_2$ and $v = z_{k_1}^N w_{k_2} - z_{k_1} H w_{k_1-1} = \mathrm{O}(|z_{k_1}|^N)$. Then, one verifies that

$$\begin{aligned} c_{k_1} &= (1 + z_{k_1} e_i^{\mathrm{T}} B_1^{-1} w_{k_1-1} + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N)) y_0 \\ &\quad -(e_i^{\mathrm{T}} B_1^{-1} + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N)) y_i + \mathrm{O}(|z_{k_1+1}|^{-N}) \\ &=: \gamma + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N) + \mathrm{O}(|z_{k_1+1}|^{-N}), \\ c_i &= -B_1^{-1}((z_{k_1} w_{k_1-1} + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N)) y_0 - (I_i + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N)) y_i + \mathrm{O}(|z_{k_1+1}|^{-N})) \\ &=: \delta + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N) + \mathrm{O}(|z_{k_1+1}|^{-N}), \\ c_f &= D_f^{-N}(V_{k_2}^{-1} + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^N))(y_f + \mathrm{O}(|z_{k_1}|^N)) \\ &=: D_f^{-N}(\sigma + \mathrm{O}(z_{k_1}/z_{k_1+1}|^N) + \mathrm{O}(|z_{k_1}|^N)), \end{aligned}$$

where γ, δ and σ are constants independent of N. In particular, one has:

$$\gamma = y_0 + e_i^{\mathrm{T}} B_1^{-1}(y_0 z_{k_1} w_{k_1-1} - y_i), \tag{4}$$

which depends only on $y_0, \ldots, y_{k_1-1}$. Finally, one has

$$\begin{aligned} y_n &= z_{k_1}^n (\gamma + \mathrm{O}(|z_{k_1-1}/z_{k_1}|^n) + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^{N-n}) + \mathrm{O}(|z_{k_1+1}|^{-N})) \\ &\quad + \mathrm{O}(|z_{k_1+1}|^{-(N-n)}). \quad \square \end{aligned}$$

Corollary 2. *Suppose that the roots of the characteristic polynomial $p(z)$ satisfy the conditions of Theorem* 1 *and, moreover,* $|z_{k_1-1}| < 1$. *Then*

$$\begin{aligned} y_n &= z_{k_1}^n (\gamma + \mathrm{O}(|z_{k_1}/z_{k_1+1}|^{N-n}) + \mathrm{O}(|z_{k_1+1}|^{-N})) \\ &\quad + \mathrm{O}(|z_{k_1-1}|^n) + \mathrm{O}(|z_{k_1+1}|^{-(N-n)}), \end{aligned}$$

where γ, which is given by (4), *depends only on $y_0, \ldots, y_{k_1-1}$.*

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

$$|z_1| \leqslant |z_2| \leqslant \cdots \leqslant |z_{k_1}| < 1 < |z_{k_1+1}| \leqslant \cdots \leqslant |z_k|,$$

whereas it is a $N_{k_1k_2}$*-polynomial* if

$$|z_1| \leqslant |z_2| \leqslant \cdots \leqslant |z_{k_1}| \leqslant 1 < |z_{k_1+1}| \leqslant \cdots \leqslant |z_k|,$$

with simple roots of unit modulus.

We observe that for $k_1 = k$ and $k_2 = 0$ a $N_{k_1k_2}$-polynomial reduces to a Von Neumann polynomial and a $S_{k_1k_2}$-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

$$T_N = \begin{pmatrix} a_{k_1} & \cdots & a_k & & & \\ \vdots & \ddots & & \ddots & & \\ a_0 & & \ddots & & \ddots & \\ & \ddots & & \ddots & & a_k \\ & & \ddots & & \ddots & \vdots \\ & & & a_0 & \cdots & a_{k_1} \end{pmatrix}_{N\times N}, \tag{5}$$

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 $N_{k_1k_2}$-polynomial, then for N sufficiently large T_N^{-1} exists and has entries $t_{ij}^{(-1)}$ such that:*

(1) $|t_{ij}^{(-1)}| \leqslant \gamma$, *for $i \geqslant j$;*

(2) $|t_{ij}^{(-1)}| \leqslant \nu\xi^{j-i}$, *for $i < j$, where $0 < \xi < 1$.*

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

Proof. See [1]. □

The results of the previous lemma can be recasted in matrix form as follows:

$$|T_N^{-1}| \leqslant \gamma C_N + \nu \Delta_N, \tag{6}$$

where C_N is the $N \times N$ lower triangular matrix having all unit entries and Δ_N is the upper triangular Toeplitz matrix having the entries on the last column given by:

$$(\xi^{N-1}, \xi^{N-2}, \ldots, \xi^2, \xi, 0)^{\mathrm{T}}.$$

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 $\rho(z)$ is a $N_{k_1k_2}$-polynomial.*

Proof. If the LMF (2) is used to approximate the solution of problem (1) by fixing the values $y_0, \ldots, y_{k_1-1}, y_N, \ldots, y_{N+k_2-1}$, it is not difficult to see that the error equation can be written as:

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

where

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

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

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

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

τ is the vector whose entries are the local errors (which are $\mathrm{O}(h^{p+1})$, $p \geqslant 1$, 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 $\mathrm{O}(h^p)$:

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

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:

$$|e| \leqslant hL|A_N^{-1}B_N||e| + |A_N^{-1}|(|\tau| + |g|).$$

From Lemma 4 and relation (6) it follows that

$$\hat{\tau} := |A_N^{-N}|(|\tau| + |g|) \leqslant (\gamma C_N + \nu \Delta_N)(|\tau| + |g|), \tag{7}$$

for some γ, $\nu > 0$ and $\xi \in (0, 1)$ which are independent of N (for brevity, we have used C_N and Δ_N in place of C_{N-k_1} and Δ_{N-k_1}, respectively). It follows that the vector $\hat{\tau}$ has entries which are $\mathrm{O}(h^p)$, if the k entries of g are at least $\mathrm{O}(h^p)$. We have now

$$(I - hL|A_N^{-1}B_N|)|e| \leqslant \hat{\tau}.$$

Let us define the $(N-k_1) \times (N-k_1)$ matrices:

$$G_N = \begin{pmatrix} 1 & \cdots & 1 & & \\ \vdots & \ddots & & \ddots & \\ 1 & & \ddots & & 1 \\ & \ddots & & \ddots & \vdots \\ & & 1 & \cdots & 1 \end{pmatrix}, \qquad Q_N = \begin{pmatrix} 0 & 1 & \cdots & 1 & & \\ & \ddots & \ddots & & \ddots & \\ & & \ddots & \ddots & & 1 \\ & & & \ddots & \ddots & \vdots \\ & & & & \ddots & 1 \\ & & & & & 0 \end{pmatrix},$$

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

$$\begin{aligned} |A_N^{-1}B_N| &\leqslant (\gamma C_N + \nu \Delta_N)\beta G_N \\ &\leqslant \alpha(k+1)\beta(C_N + Q_N + \Delta_N G_N). \end{aligned}$$

By posing $\eta = \alpha(k+1)\beta L$, it follows that

$$(I - h\eta(C_N + Q_N + \Delta_N G_N))|e| \leqslant \hat{\tau}. \tag{8}$$

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

$$M_N^{(1)}|e| := (I - h\eta M_N^{-1}(Q_N + \Delta_N G_N))|e| \leqslant M_N^{-1}\hat{\tau}.$$

Moreover, we have that

$$\begin{aligned} \| Q_N + \Delta_N G_N \|_\infty &\leqslant \| Q_N \|_\infty + \| \Delta_N \|_\infty \| G \|_\infty \\ &< (k+1)(1 + \xi(1-\xi)^{-1}) = \frac{k+1}{1-\xi}, \end{aligned}$$

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

$$\|(M_N^{(1)})^{-1}\|_\infty \leqslant \sum_{n=0}^{\infty} \|h\eta M_N^{-1}(Q_N + \Delta_N G_N)\|_\infty^n$$

$$\leqslant \sum_{n=0}^{\infty} (h\phi)^n = (1 - h\phi)^{-1} < 2.$$

Finally, one then obtains:

$$\|e\|_\infty \leqslant 4e^{2\eta(T-t_0)}\|\hat{\tau}\|_\infty,$$

that is, the method is convergent and the global error is $\mathrm{O}(h^p)$. □

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 $0_{k_1k_2}$-*stable* if $\rho(z)$ is a $N_{k_1k_2}$-polynomial.

We observe that $0_{k_1k_2}$-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

$$y' = \lambda y, \qquad \Re(\lambda) < 0. \tag{9}$$

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 $S_{k_1k_2}$-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 $S_{k_1k_2}$-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:

$$D_{k_1k_2} = \{q \in \mathbb{C} : \pi(z, q) \text{ is a } S_{k_1k_2}\text{-polynomial}\}.$$

Finally, a BVM with (k_1, k_2)-boundary conditions is said to be $A_{k_1k_2}$-*stable* if $\mathbb{C}^- \subseteq D_{k_1k_2}$. We observe that for BVMs there are no barriers concerning the maximum order for methods which are $0_{k_1k_2}$-stable and/or $A_{k_1k_2}$-stable. In fact, in the next section we shall briefly examine a class of k-step BVMs which provides $0_{k_1k_2}$-stable and $A_{k_1k_2}$-stable BVMs of order k, for all $k \geqslant 1$. Other classes of methods which contains $0_{k_1k_2}$-stable and $A_{k_1k_2}$-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 $0_{v,k-v}$-stable and $A_{v,k-v}$-stable for all $k \geqslant 1$. In Figs. 1 and 2 the boundaries Γ_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 Γ_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 Γ_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 $k \geqslant 1$, 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

$$y_0, \ldots, y_{v-1}, \qquad y_N, \ldots, y_{N+k-v-1}.$$

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 $y_N, \ldots, y_{N+k-v-1}$,

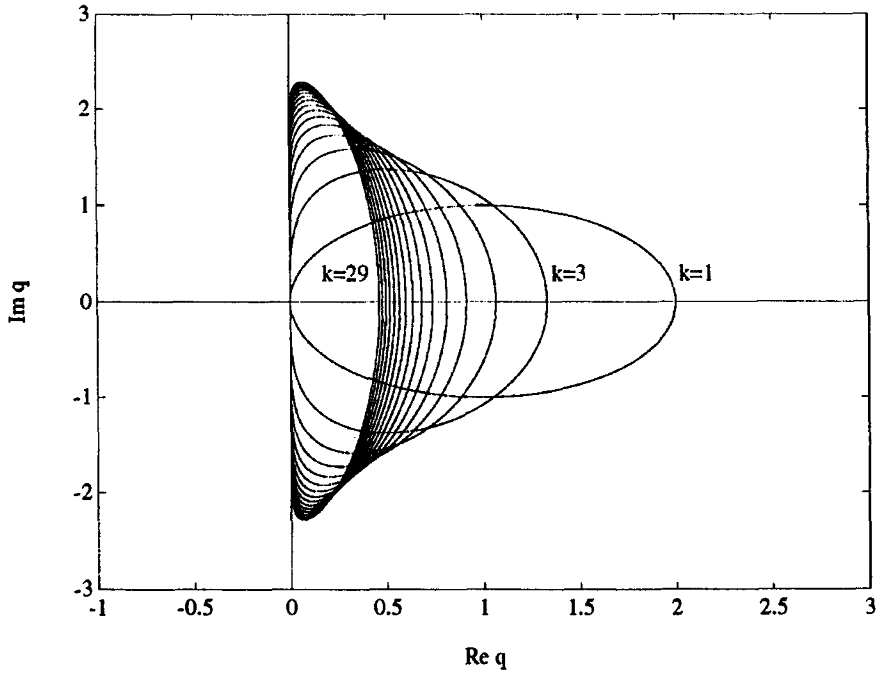

Fig. 1. Boundaries of the $(\nu, k-\nu)$-absolute stability regions of the GBDF of order k, $k = 1, 3, 5, \dots, 29$.

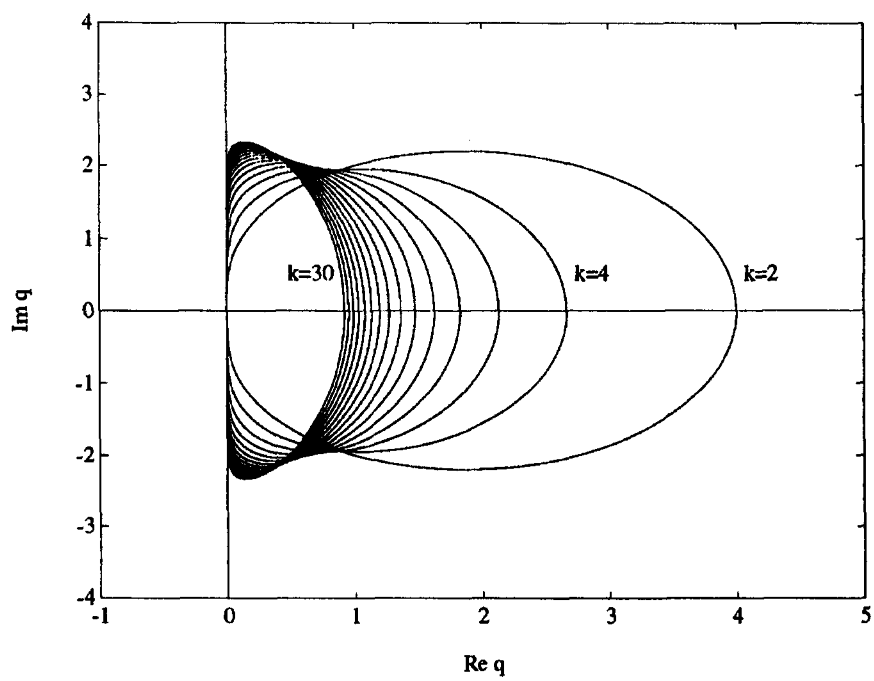

Fig. 2. Boundaries of the $(\nu, k-\nu)$-absolute stability regions of the GBDF of order k, $k = 2, 4, 6, \dots, 30$.

Table 1
Normalized coefficients of GBDF

k	v	δ_k	$\hat{\alpha}_0$	$\hat{\alpha}_1$	$\hat{\alpha}_2$	$\hat{\alpha}_3$	$\hat{\alpha}_4$	$\hat{\alpha}_5$	$\hat{\alpha}_6$	$\hat{\alpha}_7$	$\hat{\alpha}_8$	$\hat{\alpha}_9$	$\hat{\alpha}_{10}$
1	1	1	−1	1									
2	2	2	1	−4	3								
3	2	6	1	−6	3	2							
4	3	12	−1	6	−18	10	3						
5	3	60	−2	15	−60	20	30	−3					
6	4	60	1	−8	30	−80	35	24	−2				
7	4	420	3	−28	126	−420	105	252	−42	4			
8	5	840	−3	30	−140	420	−1050	378	420	−60	5		
9	5	2520	−4	45	−240	840	−2520	504	1680	−360	60	−5	
10	6	2520	2	−24	135	−480	1260	−3024	924	1440	−270	40	−3

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

h	Error	Rate	Error	Rate	Error	Rate	Error	Rate
1e −2	2.528e −02	—	8.002e −03	—	2.820e −03	—	2.517e −03	—
5e −3	3.623e −03	2.80	8.023e −04	3.32	2.922e −04	3.27	9.095e −05	4.79
2.5e −3	4.905e −04	2.88	6.930e −05	3.53	1.364e −05	4.42	1.815e −06	5.65
1.25e −3	7.219e −05	2.76	5.832e −06	3.57	5.044e −07	4.76	3.044e −08	5.90
6.25e −4	9.718e −06	2.89	4.164e −07	3.81	1.702e −08	4.89	4.851e −10	5.97

Table 3
Results for GBDF of order 7, 8, 9, 10

1e −2	1.187e −03	—	4.494e −04	—	1.153e −04	—	4.672e −05	—
5e −3	1.389e −05	6.42	2.683e −06	7.39	7.185e −07	7.33	3.155e −07	7.21
2.5e −3	1.079e −07	7.00	1.538e −08	7.45	3.494e −09	7.68	5.342e −10	9.21
1.25e −3	1.079e −09	6.64	8.543e −11	7.49	9.519e −12	8.52	6.072e −13	9.78
6.25e −4	9.409e −12	6.84	4.431e −13	7.59	2.176e −14	8.77	3.730e −14	4.02

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:

$$\sum_{i=0}^{k-1} \alpha_{i,r} y_{N-\nu+i} = h f_{N+r}, \quad r = 0, \dots, k-\nu-1,$$

where the coefficients $\{\alpha_{i,r}\}$ 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:

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

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 $3, \dots, 10$. 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:

$$\begin{aligned} y_1' &= -0.04 y_1 + 10^4 y_2 y_3, & y_1(0) &= 1, \\ y_2' &= 0.04 y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2, & y_2(0) &= 0, \\ y_3' &= 3 \times 10^7 y_2^2, & y_3(0) &= 0. \end{aligned}$$

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:

$$t_i = t_{i-1} + h_i, \qquad h_i = 1.2 h_{i-1}, \quad i = 1, 2, \dots, \qquad h_0 = 6.6 \times 10^{-6}.$$

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: $mf = 21$, $atol = rtol = 1\text{e}{-14}$. As one can see, the solution computed by the GBDF has a more regular behavior than that computed by LSODE.

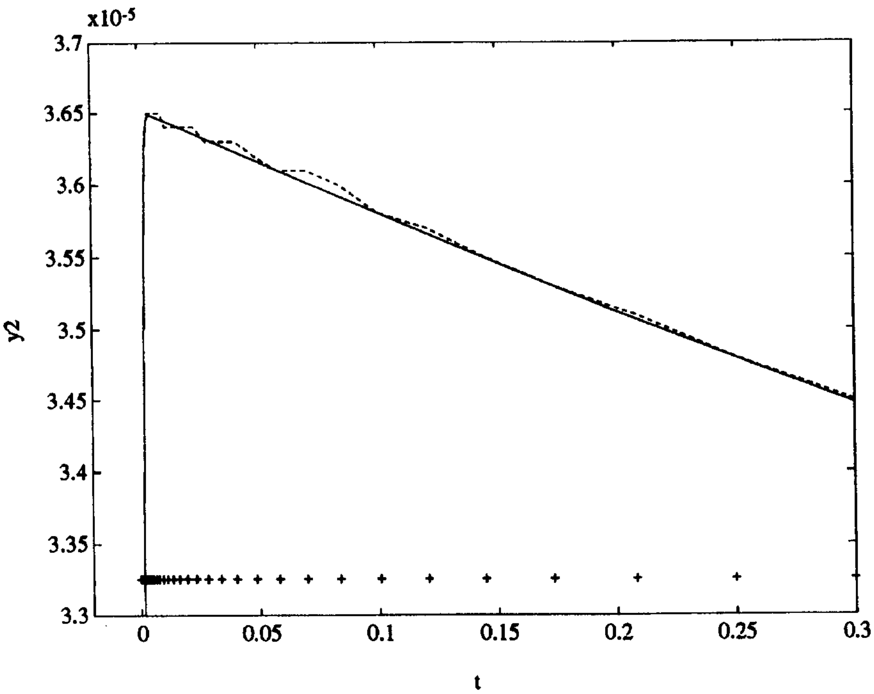

Fig. 3. Computed solution with the GBDF of order 10 (solid line) and with LSODE (dashed line).

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