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On the three term recurrence relation and BDF methods

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Abstract. In this paper, we propose to investigate important properties of the characteristic polynomials related to the backward differential formulas (BDF). We show that the BDF characteristic polynomials satisfy a three term recurrence relation that allows us to provide the location of their zeros.

Keywords. Three term recurrence relation, BDF methods, Numerical Stability, Zeros.

1 Introduction

A large development in the stability and convergence analysis of various numerical methods for solving differential equations based on numerical approximation has been observed in recent years. Numerical analysis and mathematical modeling are essential in many areas of modern life.

Most mathematical models used in the natural sciences and engineering are based on ordinary differential equations. Problems involving rapidly decaying transient solutions, for example, occur naturally in a wide variety of applications, including the study of spring and damping systems the analysis of control systems and problems in chemical kinetics. Most of these examples belong to a class of problems called stiff (mathematical stiffness) systems of differential equations:

$$y' = Ay + \phi(x),$$

where the matrix $A \in \mathbb{M}_m$ has different eigenvalues λ_i, $i = 1, \dots, m$, and $\phi(x)$ is a m-dimensional vector. More details of these problems can be found in [3].

This paper deals with important properties of the characteristic polynomial related to the backward differential formulas (or BDF methods). These were the first numerical

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methods to be proposed for stiff differential equations (Curtis and Hirschfelder [3]). We intend to prove that the characteristic polynomials of the BDF methods satisfy a three term recurrence relation and also show the behavior of their zeros.

2 Preliminary Results

In this section we provide a brief review literature related results.

2.1 Brown (K, L) methods

For the differential equation $y' = f(x, y)$, $y = y(x)$, and fixed integers, K and L, the *Brown* (K, L) *methods* [2] are defined by

$$\sum_{i=0}^{K} \alpha_i y_{n+i} = \sum_{j=1}^{L} h^j \beta_j f_{n+K}^{(j-1)}, \tag{1}$$

where the constants α_i and β_j are chosen so as to obtain the highest order possible for the method. Here, $f_{n+K}^{(j)}$ denotes the $j-$derivative of the function f with respect to x at the point x_{n+K}, and h represents the mesh spacing.

Jeltsch and Kratz [5] proved that the coefficients α_i and β_j are given by

$$\begin{aligned} \alpha_i &= (-1)^{K-i} \binom{K}{i} (K-i)^{-L}, \; i = 0, \ldots, K-1, \\ \alpha_K &= -\sum_{i=0}^{K-1} \alpha_i, \\ \beta_j &= \frac{(-1)^j}{j!} \sum_{i=0}^{K-1} (-1)^{K-i} \binom{K}{i} (K-i)^{j-L}, \; j = 1, \ldots, L. \end{aligned}$$

The Brown (K, L) methods may be represented by their characteristic polynomials

$$\rho(z) = \sum_{i=0}^{K} \alpha_i z^i \quad \text{and} \quad \sigma_j(z) = \beta_j z^K, \; j = 1, 2, ..., L.$$

It is known that a method is *zero-stable* if the zeros of the polynomial $\rho(z)$ are in the unit disc ($|z| \leq 1$) and the zeros of modulus one are simple. Further, a method is said to be *zero-unstable* if it is not zero-stable.

2.1.1 BDF methods

Considering $L = 1$, Brown (K, L) methods reduce to the Backward Differentiation Formulae known as *BDF methods.*

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In this case, from the Newton interpolation formula, we can represent the BDF methods by

$$\sum_{j=1}^{K} \frac{1}{j} \nabla^j y_{n+1} = h f_{n+1}, \tag{2}$$

and from [4] we can see that the characteristic polynomial of (2) is

$$\rho(\zeta) = \sum_{j=1}^{K} \frac{1}{j} \zeta^{K-j} (\zeta - 1)^j. \tag{3}$$

2.2 Zero location result

In [1] we can see the following result:

Theorem 2.1. *Let* $P(z) = \sum_{k=0}^{n} a_k z^k$ *be a polynomial such that* $n \geq 1$ *and* $a_k > 0$, $k = 0, \dots, n$. *Considering*

$$\lambda' = \min_{0 \leq k < n} \left\{ \frac{a_k}{a_{k+1}} \right\} \quad e \quad \lambda'' = \max_{0 \leq k < n} \left\{ \frac{a_k}{a_{k+1}} \right\},$$

then all zeros of $P(z)$ *lie in the region defined by* $\lambda' \leq |z| \leq \lambda''$.

3 Main results

3.1 The three term recurrence relation

In this subsection we analyze an important property of the characteristic polynomial of BDF methods, $\rho(\zeta)$, defined in subsection 2.1.1.

From the transformation $\zeta = \dfrac{1}{1-z}$ in the Eq. (3), we have

$$P(z) = (1-z)^K \rho(\zeta) = \sum_{j=1}^{K} \frac{z^j}{j}. \tag{4}$$

Hence, by definition of stability, the BDF method defined by formula (2) is stable if all zeros of (4) are outside the disk

$$C \doteq \{z; |z-1| \leq 1\},$$

with simple zeros allowed on the boundary.

We can rewrite the polynomial $P(z)$ defined in Eq. (4) as

$$P(z) = \frac{1}{K} z R_{K-1}(z), \tag{5}$$

where

$$R_{K-1}(z) = \sum_{j=1}^{K} \frac{K}{j} z^{j-1}, \; K \geq 1. \tag{6}$$

It is easy to see that the sequence of polynomials $\{R_m\}$, related to polynomial defined in Eq. (6), satisfies the three term recurrence relation

$$R_{m+1}(z) = (z + \beta_{m+1})R_m(z) - \alpha_{m+1} z R_{m-1}(z), \; m \geq 1, \tag{7}$$

where

$$R_0(z) = 1, \; R_1(z) = z + 2, \; \beta_m = \frac{m+1}{m}, \text{ and } \alpha_m = \frac{m}{m-1}, \; m = 2, 3, \ldots. \tag{8}$$

Interestingly, it is observed that $\beta_m = \alpha_{m+1}$, $m = 2, 3, \ldots$.

The three term recurrence relation of the form (7) was studied in [6]. This reference has many results related to the behavior of the zeros of this class of polynomials as, for example, the followings:

Lemma 3.1. *For any $m \geq 1$, the two consecutive polynomials R_m and R_{m+1} do not have common zeros.*

Theorem 3.1. *The zeros of R_m are the eigenvalues of the lower Hessenberg matrix*

$$\boldsymbol{H}_m = \begin{bmatrix} \eta_1 & \alpha_2 & 0 & \ldots & 0 & 0 \\ \eta_1 & \eta_2 & \alpha_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ \eta_1 & \eta_2 & \eta_3 & \ldots & \alpha_{m-1} & 0 \\ \eta_1 & \eta_2 & \eta_3 & \ldots & \eta_{m-1} & \alpha_m \\ \eta_1 & \eta_2 & \eta_3 & \ldots & \eta_{m-1} & \eta_m \end{bmatrix},$$

where $\eta_j = \alpha_j - \beta_j$, $j = 1, 2, \ldots, m$, with $\alpha_1 = 0$.

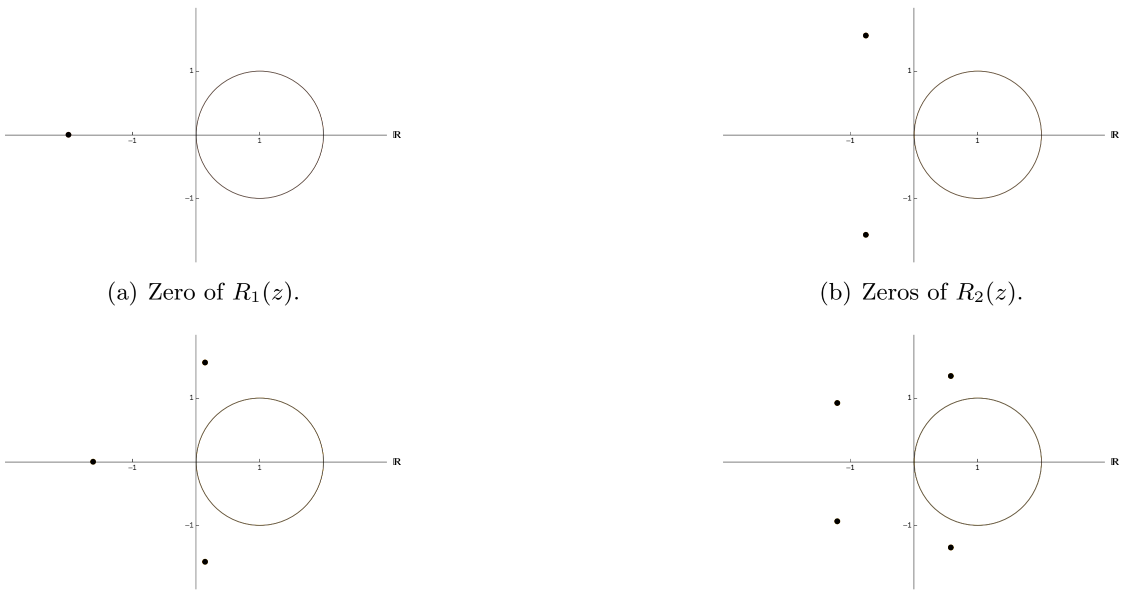
In this case, considering the three term recurrence relation (7) with the conditions presented in (8), we have

$$\mathbf{H}_m = \begin{bmatrix} -2 & 2 & 0 & \ldots & 0 & 0 \\ -2 & \frac{1}{2} & \frac{3}{2} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ -2 & \frac{1}{2} & \frac{1}{6} & \ldots & \frac{m-1}{m-2} & 0 \\ -2 & \frac{1}{2} & \frac{1}{6} & \ldots & \frac{1}{(m-1)(m-2)} & \frac{m}{m-1} \\ -2 & \frac{1}{2} & \frac{1}{6} & \ldots & \frac{1}{(m-1)(m-2)} & \frac{1}{m(m-1)} \end{bmatrix}.$$

3.2 On the location of the zeros of $R_m(z)$

In [4], Hairer and Wanner have showed that the BDF methods are unstable for $K \geq 7$. So, the polynomials $R_6, R_7, \ldots$ has zeros in the region $|z-1| \leq 1$. Furthermore, from Theorem 2.1, the zeros of polynomials $R_m(z)$, $m = 0, 1, \ldots$, defined by conditions (7) and (8), lie in the region $1 < |z| \leq 2$.

Figures 1 and 2 display the zeros of R_{K-1} for some values of K.



(a) Zero of $R_1(z)$. (b) Zeros of $R_2(z)$.

(c) Zeros of $R_3(z)$. (d) Zeros of $R_4(z)$.

Figure 1: Zeros of $R_{K-1}(z)$ for $K = 2, 3, 4$ and $K = 5$.

4 Conclusions

In this work we present an important property of the characteristic polynomials of the BDF methods: from the transformation $\zeta = \dfrac{1}{1-z}$, the polynomial $\rho(\zeta)$ satisfies the relation (4), where $P(z) = \dfrac{1}{K} z R_{K-1}(z) = \dfrac{1}{K} z \sum_{j=1}^{K} \dfrac{K}{j} z^{j-1}$. We show that the sequence of polynomials $\{R_m\}$, related to polynomial defined in equation (6), satisfies the three term recurrence relation (7) under the conditions (8). Furthermore, we explore some results on the behavior of the zeros of the polynomials $R_m(z)$, $m = 1, \ldots$.

Considering that the present study is in the initial phase of its development, it is intended in the next investigations to explore a similar relation (4) in order to generalize for Brown (K, L) methods that is to obtain a three term recurrence relation.

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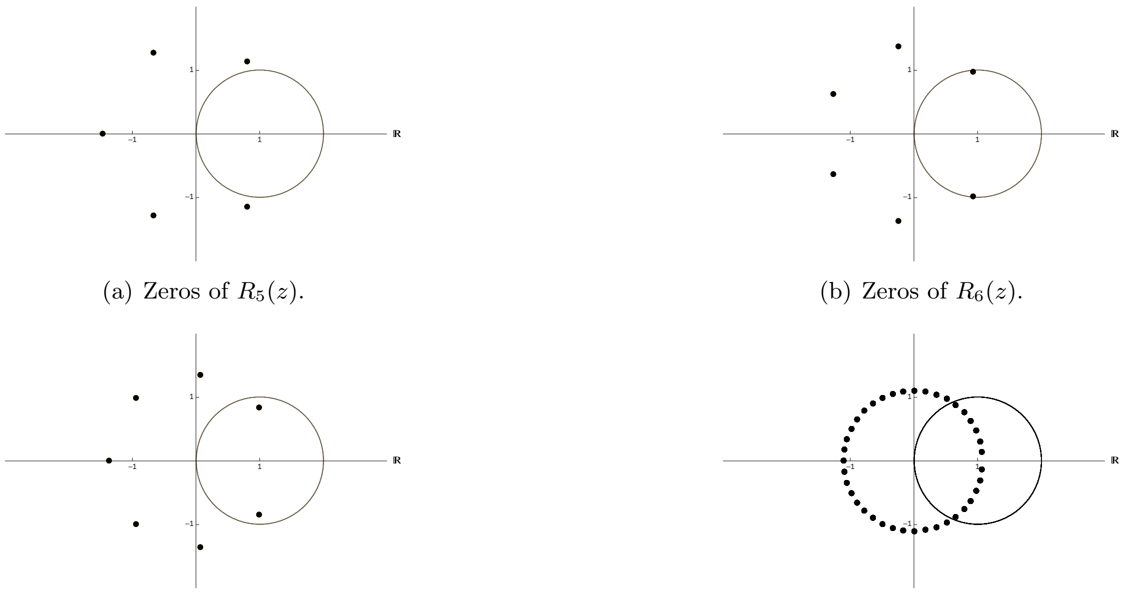

(a) Zeros of $R_5(z)$.

(b) Zeros of $R_6(z)$.

(c) Zeros of $R_7(z)$.

(d) Zeros of $R_{39}(z)$.

Figure 2: Zeros of $R_{K-1}(z)$ for $K = 6, 7, 8$ and $K = 40$.

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References

[1] N. Anderson, E. B. Saff and R. S. Varga. On the Eneström-Kakeya theorem and its sharpness, *Linear Algebra Appl.*, 28: 5–16, 1979.

[2] R. L. Brown. Some characteristics of implicit multistep-multiderivative integration formulas, *SIAM J. Numer. Anal.*, 14: 982–993, 1977.

[3] C. F. Curtis and J. O. Hirschfelder (1952). Integration of stiff problems, *Proc. Nat. Acad. Soc.*, 38: 235–243, 1952.

[4] E. Hairer and G. Wanner. On the instability of the BDF formulas, *SIAM J. Numer. Anal.*, 20: 1206–1209, 1983.

[5] R. Jeltsch and L. Kratz. On the stability properties of Brown's multistep multiderivative methods, *Numer. Math.,* 30: 25–38, 1978.

[6] A. P. da Silva and A. Sri Ranga. Polynomials generated by a three term recurrence relation: bounds for complex zeros. *Linear Algebra Appl.*, 397: 299–324, 2005.

