Strathprints Institutional Repository

Progress in Applied Mathematics **ISSN 1925-251X [Print]**
Vol. 1, No. 1, 2011, pp. 122-130 **ISSN 1925-2528 [Online]**
www.cscanada.org **www.cscanada.net**

Theoretical Results of One Class of Multiderivative Methods through Order Stars

Vanessa A. Botta[1,*]

Messias Meneguette[1]

José A. Cuminato[2]

Sean McKee[3]

Abstract: Order stars are applied to Brown (K, L) methods. They are displayed pictorially for a selection of methods and are used to provide succinct proofs of existing results. Asymptotic results concerning their stability are also presented.

Key Words: Brown (K, L) Methods; Stability; Characteristic Polynomials; Order Stars

1. BROWN METHODS

For the differential equation $y' = f(x, y)$, $y = y(x)$, and fixed integers, K and L, the Brown (K, L) methods[1] 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 ($f_{n+K}^{(j)}$ denotes the j−derivative of the function f with respect to x at the point x_{n+K}). Here h denotes the mesh spacing. Jeltsch and Kratz[2] proved that the coefficients are given by

$$\alpha_i = (-1)^{K-i} \begin{pmatrix} K \\ i \end{pmatrix} (K-i)^{-L},\ i = 0, \ldots, K-1,\ \alpha_K = -\sum_{i=0}^{K-1} \alpha_i, \tag{2}$$

$$\beta_j = \frac{(-1)^j}{j!} \sum_{i=0}^{K-1} (-1)^{K-i} \begin{pmatrix} K \\ i \end{pmatrix} (K-i)^{j-L},\ j = 1, \ldots, L. \tag{3}$$

For $L = 1$, Brown (K, L) methods reduce to the Backward Differentiation Formulae known as BDF methods; these were the first numerical methods to be proposed for stiff differential equations[3].

---

[1]Faculdade de Ciências e Tecnologia, Univ Estadual Paulista, Brazil. E-mail addresses: botta@fct.unesp.br (Vanessa A. Botta); messias@fct.unesp.br (Messias Meneguette).
[2]Instituto de Ciências Matemáticas e de Computação, Universidade de São Paulo, Brazil. E-mail address: jacumina@icmc.usp.br.
[3]Department of Mathematics, Strathclyde University, Glasgow, Scotland. E-mail address: smck@maths.strath.ac.uk.
*Corresponding author.
†Received 20 December 2010; accepted 17 January 2011.

The addition of derivatives in numerical methods gives more scope for better stability characteristics, such as larger regions of absolute stability[4]. Even though the computation of derivatives is expensive, the combination of the use of higher derivatives and other methods can produce new and improved methods[5]. For this reason, we study the stability of Brown methods through the theory of order stars; although little used in the literature, this new tool enables the stability of numerical methods to be analysed in a more concise and, arguably, more elegant way.

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

$$\rho(z) = \sum_{i=0}^{K} \alpha_i z^i \text{ and } \sigma_j(z) = \beta_j z^K, \;\; j = 1, 2, ..., L. \tag{4}$$

A method is zero-stable if the zeros of the polynomial $\rho(z)$ are in the unit disc and the zeros of modulus one are simple. Further, a method is said to be zero-unstable if it is not zero-stable. Here we have been essentially concerned with stability as the mesh spacing h tends to zero. Stability is also of interest in a practical situation when h is fixed, but when we would like the solution to remain bounded or tend to zero as n, the number of steps, increases indefinitely. To study "fixed step" stability the difference equation is often applied to the linear test equation $y' = \lambda y$ resulting in, for linear multistep methods, the characteristic polynomial

$$\pi(w, z) = \rho(z) - z\sigma(z), \;\; z = h\lambda. \tag{5}$$

For multiderivative methods the corresponding characteristic polynomial is

$$\pi(w, z) = \rho(z) - \sum_{j=1}^{L} z^j \sigma_j(w), \;\; z = h\lambda. \tag{6}$$

The stability of multistep multiderivative methods depends on the roots $w_i(z),\; 1 \leq i \leq k$ of $\pi(w, z) = 0$. Note that $\pi(w, z) \to \rho(z)$ as $h \to 0$ and $w_i(h) \to w_i,\; 1 \leq i \leq k$, where $\{w_i\}$ are the zeros of $\rho(w)$. For a multiderivative method to be consistent, $\rho(1) = 0$ is required. This zero, represented by $w_1(h)$), may be regarded as the principal branch of $\pi(w, z) = 0$ since $w_1(h) \to w_1$ as $h \to 0$.

Definition 1.1 *The set* $D = \{z \in \overline{\mathbb{C}} \;/\; |w_i(z)| \leq 1, 1 \leq i \leq k\}$ *is called region of absolute stability of the method, where* $\overline{\mathbb{C}} = \mathbb{C} \cup \infty$.

Definition 1.2 *If the set D consists of the whole of the left hand complex plane, then the method is said to be A-stable.*

More details about stability of multiderivative methods can be found in Ref. [6]. The following results are known about Brown (K, L) methods.

Theorem 1.3 (Jeltsch and Kratz[2]) *The Brown* (K, L) *methods have order of consistency* $p = K + L - 1$.

Theorem 1.4 (Iserles and Norsett[7]) *The Brown* (K, L) *method of order* p *is A-stable only if* $p \leq 2L$. *(Clearly this implies* $K \leq L + 1$*).*

Theorem 1.5 (Jeltsch and Kratz[2]) *Let L be fixed. The Brown* (K, L) *methods become zero-unstable for sufficiently large K.*

Theorem 1.6 (Jeltsch and Kratz[2]) *Let K be fixed. The Brown* (K, L) *methods become zero-stable for L sufficiently large.*

The purpose of this note is to introduce order stars for Brown (K, L) methods, compute the order stars for a number of Brown methods and then to re-prove Theorems 1.5 and 1.6 succinctly using order stars.

2. ORDER STARS

There are two types of order stars: order stars of the first kind and of the second kind and they have been shown to be related[7]. Wanner *et al.*[8] were the first to describe them and a comprehensive account may be found in Ref. [7]. For our purposes we shall only require order stars of the second kind and will therefore only focus on these.

For the Brown (K, L) methods, let

$$R(z) = \frac{\sum_{j=1}^{L} \sigma_j(e^z) z^{j-1}}{\rho(e^z)}, \quad F(z) = \frac{1}{z}, \tag{7}$$

and

$$\mu(z) = \frac{\sum_{j=1}^{L} \sigma_j(e^z) z^{j-1}}{\rho(e^z)} - \frac{1}{z}, \quad z \in \mathbb{C}. \tag{8}$$

Furthermore define

$$A_+ := \{z | \operatorname{Re}(\mu(z)) > 0\}, \tag{9}$$

$$A_0 := \{z | \operatorname{Re}(\mu(z)) = 0\}, \tag{10}$$

$$A_- := \{z | \operatorname{Re}(\mu(z)) < 0\}. \tag{11}$$

An order star $\mu(z)$ of the second kind for a Brown (K, L) method is the partition of the complex plane into the triplet $\{A_+, A_0, A_-\}$.

Let D be the stability region of the numerical method, according Definition 1.1. Then we say that R is A-acceptable and the related method is A-stable if $\{z \in \mathbb{C} | \operatorname{Re}(z) < 0\} \subset D$.

Definition 2.1 *The index $\iota(z)$ of a point $z \in A_0$ is defined as the number of sectors of A_- adjoining z.*

Let $z \in A_0$ and $p = \iota(z) > 0$. If μ is analytic at z and the point is approached by precisely p sectors of A_- and p sectors of A_+, each of asymptotic angle $\frac{\pi}{p}$, then we say that z is regular.

The next result relates the order of the method to the number of sectors forming the regions A_+ and A_-.

Lemma 2.2 *If the Brown (K, L) method has order p, then the origin is adjoined by $p - 1$ sectors of A_+ and separated by $p - 1$ sectors of A_-. All these sectors approach the origin with asymptotic angle $\frac{\pi}{p-1}$.*

The proof can be found in Ref. [9].

The next result establishes the zero-stability of a (K, L) method through order stars.

Lemma 2.3 *Brown methods are zero-stable if, and only if, all the poles of $\mu(z)$ reside in the closed left half-plane and the poles along the imaginary axis are simple.*

It is important to remember that, for the proofs of the above results, the use of the transformation $z \to \ln z$ is required. This maps, of course, the unit disk onto the left half-plane and the unit circle onto the imaginary axis.

The A-stability of a method or, equivalently, the A-acceptability of the approximation μ is given in the following result:

Lemma 2.4 *The approximation μ is A-acceptable if, and only if $A_- \cap \{i\mathbb{R}\} = \emptyset$.*

The proof can be found in Ref. [7].

The function $\mu(z)$ involves e^z, which is periodic in the complex plane. Hence, both zeros and poles are replicated by multiples of $2\pi i$, and this creates obvious difficulties for zero and pole counting arguments. It is therefore, necessary to restrict our attention to the region

$$J = \{z \in \mathbb{C} : |\,\mathrm{Im}(z)| \le \pi\}. \tag{12}$$

Let us define the sets

$$J^+ = \{z \in J : \mathrm{Re}(z) > 0\} \text{ and } J^- = \{z \in J : \mathrm{Re}(z) < 0\}. \tag{13}$$

Finally, a closed curve in A_0 will be called a loop.

Lemma 2.5 *There exists $\epsilon \in \mathbb{R}$ such that the set $\{z|\,\mathrm{Re}(z) \ge \epsilon\} \cap J$ is contained in one of the sets A_+ or A_-: if $\beta_L > 0$ then it belongs to A_+, otherwise it lies in A_-.*

The proof can be found in Ref. [10].

The next result defines the relative position between the zeros and poles of $\mu(z)$.

Lemma 2.6 *Let δ be a loop such that $\delta \cap \partial J = \emptyset$ and $\delta \cap J \ne \emptyset$. Then, there is on δ exactly one pole of μ between any two roots of $\mu(z) = 0$. Moreover, if $z_0 \in int(J)$ is a pole of μ of multiplicity m then it is approached by m sectors of A_+ and m sectors of A_- each with asymptotic angle of $\dfrac{\pi}{m}$.*

Lemma 2.7 *Let G be either a bounded A_+-region or A_--region such that $\{\mathbb{R} + i\pi\} \cap cl(G) \ne \emptyset$ and*

$$x_- = \min\{x \in \mathbb{R} : x + i\pi \in cl(G)\} > -\infty \tag{14}$$
$$x_+ = \max\{x \in \mathbb{R} : x + i\pi \in cl(G)\} < \infty. \tag{15}$$

Let $z_0 \in \partial G \cap int(J)$ be a zero of $\mu(z)$. Then

1. *if G is a A_--region then either $x_- + i\pi$ is a pole of μ or there is a pole of μ along the positively oriented portion of ∂G from $x_- + i\pi$ to z_0;*
2. *if G is a A_+-region then either $x_+ + i\pi$ is a pole of μ or there is a pole of μ along the positively oriented portion of ∂G from z_0 to $x_+ + i\pi$.*

Similar results are valid if $\mathbb{R} + i\pi$ is replaced by $\mathbb{R} - i\pi$.

Lemma 2.8 *Let z_0 be a pole of $\mu(z)$ with multiplicity m. Then $\iota(z_0) = m$ and z_0 is regular.*

Again, the proof of this result may be found in Ref. [7].

3. ORDER STARS FOR THE BROWN (K, L) METHODS

For the BDF methods, we have

$$\mu(z) = \frac{\sigma(e^z)}{\rho(e^z)} - \frac{1}{z} \text{ (equivalent to (8) with } L = 1). \tag{16}$$

For $K = 2$, this results in

$$\mu(z) = \frac{\left(\frac{2}{3}z - 1\right)e^{2z} + \frac{4}{3}e^z - \frac{1}{3}}{z\left(e^{2z} - \frac{4}{3}e^z + \frac{1}{3}\right)}, \tag{17}$$

and for $K = 4$,

$$\mu(z) = \frac{\left(\frac{12}{25}z - 1\right)e^{4z} + \frac{48}{25}e^{3z} - \frac{36}{25}e^{2z} + \frac{16}{25}e^z - \frac{3}{25}}{z\left(e^{4z} - \frac{48}{25}e^{3z} + \frac{36}{25}e^{2z} - \frac{16}{25}e^z + \frac{3}{25}\right)}. \tag{18}$$

Figures 1 and 2 display the order stars for the BDF methods with $K = 2, 3, 4, 6, 7$ and 9, respectively, in the interval $[-\pi, \pi]$. The dark region represents A_+ and the complementary area represents A_-. In each of these pictures the points in A_0 are the poles of $\mu(z)$ and the point at the origin represents the principal root of $\rho(z) = 0$, that is $z_0 = 1$.

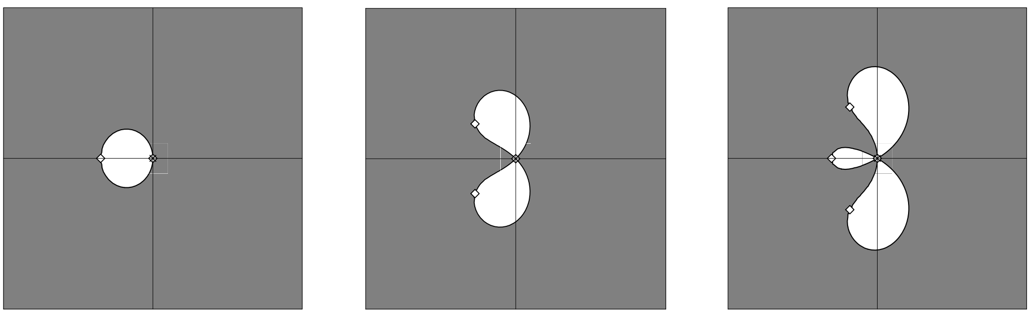

Figure 1: Order star of Brown (2,1), (3,1) and (4,1) methods, respectively

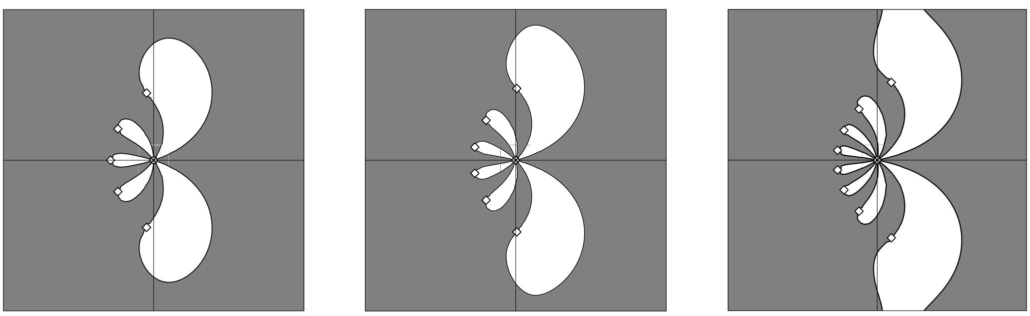

Figure 2: Order star of Brown (6,1), (7,1) and (9,1) methods, respectively

Observe that the order stars of each method has $p - 1 = K - 1$ sectors, where $p = K$ is the order of the method. For $K = 2$, $A_- \cap \{i\mathbb{R}\} = \emptyset$ and for $K \geq 3$, $A_- \cap \{i\mathbb{R}\} \neq \emptyset$. Then, the BDF methods are A-stable only if $K \leq 2$. For the point $z_0 = 0$ we have $\iota(0) = K - 1$, because $p = K - 1$ and $K - 1$ sectors of A_- approach $z_0 = 0$. So, from Lemma 2.8 it follows that $z_0 = 0$ is regular.

We know that the BDF methods are zero-stable only for $K \leq 6$ (see Hairer and Wanner[11]). This fact can be observed in Figures 1 and 2 by noting that the poles of $\mu(z)$, for $K = 1, 2, 3, 4, 5$ and 6, lie in the left half-plane. For $K = 7$ and $K = 9$, for example, the methods are zero-unstable.

In the general case, the order stars for the Brown (K, L) methods will have $K + L - 2$ sectors of A_- and $K + L - 2$ sectors of A_+ approaching the origin each with asymptotic angle of $\dfrac{\pi}{K + L - 2}$, as predicted by Lemma 2.2, because these methods have order $p = K + L - 1$.

From Ref. [12] we know that

$$\begin{aligned}
\mu\left(\frac{1}{\xi}\right) &= \frac{\sigma\left(e^{1/\xi}\right)}{\rho\left(e^{1/\xi}\right)} - \xi = \frac{\sigma\left(e^{1/\xi}\right) - \xi\rho\left(e^{1/\xi}\right)}{\rho\left(e^{1/\xi}\right)} \\
&= \frac{e^{K/\xi}\left(\beta_1 + \beta_2\left(\frac{1}{\xi}\right) + \ldots + \beta_L\left(\frac{1}{\xi}\right)^{L-1}\right) - \xi\left(\alpha_0 + \alpha_1 e^{1/\xi} + \ldots + \alpha_K e^{K/\xi}\right)}{\alpha_0 + \alpha_1 e^{1/\xi} + \ldots + \alpha_K e^{K/\xi}} \\
&= \frac{\beta_1 + \beta_2\left(\frac{1}{\xi}\right) + \ldots + \beta_L\left(\frac{1}{\xi}\right)^{L-1} - \xi\left(\frac{\alpha_0}{e^{K/\xi}} + \ldots + \alpha_K\right)}{\frac{\alpha_0}{e^{K/\xi}} + \ldots + \alpha_K}.
\end{aligned} \tag{19}$$

Then

$$\lim_{\xi \to 0} \xi^{L-1}\mu\left(\frac{1}{\xi}\right) = \frac{\beta_L}{\alpha_K}, \tag{20}$$

implying that 0 is a pole of order $L - 1$ of $\mu\left(\dfrac{1}{\xi}\right)$ and $z_0 = \infty$ is a pole of order $L - 1$ of $\mu(z)$.

So, from Lemma 2.8, $\iota(\infty) = L - 1$. Moreover,

$$\iota(0) = K + L - 2 = (K - 1) + (L - 1). \tag{21}$$

Then, $(K-1)+(L-1)$ sectors of A_- approach the origin, where $L-1$ sectors are obtained from $\iota(\infty) = L-1$ (by Lemma 2.5, these sectors reside in the right half-plane and are unbounded) and $K - 1$ sectors reside in the left half-plane, and contain the poles of the approximation $\mu(z)$ (by the Lemmas 2.6 and 2.7).

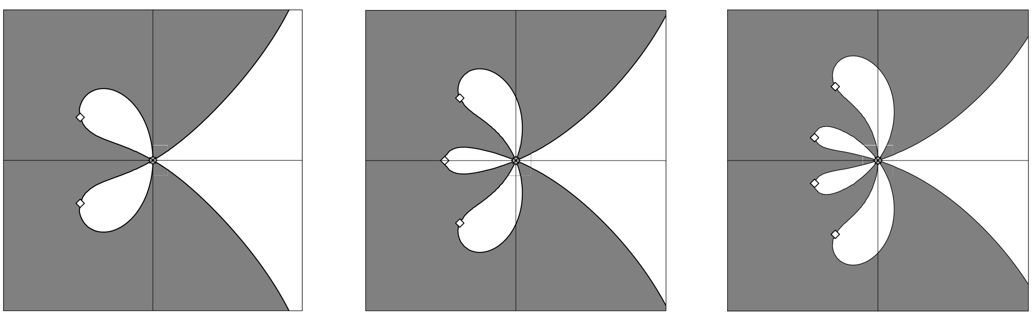

Figure 3: Order star of Brown (3,2), (4,2) and (5,2) methods, respectively

For example, in the case that $L = 2$, $p = K + 1$ and each order star has $p - 1 = K$ sectors we obtain the following. As $\iota(\infty) = 1$, there is one unbounded sector on the right half-plane. For $K = 3$, $A_- \cap \{i\mathbb{R}\} = \emptyset$ and for $K \geq 4$, $A_- \cap \{i\mathbb{R}\} \neq \emptyset$. Then, the $(K, 2)$ methods are A-stable only if $K \leq 3$. The point $z_0 = 0$ is an interpolation point of degree $p = K$ because K sectors of A_- approach $z_0 = 0$. Moreover, $\iota(0) = K - 1$. So, from Lemma 2.8 it follows that $z_0 = 0$ is regular. From Figures 3 and 4 it may be observed that the poles of $\mu(z)$, for $K = 3, 4, 5, 7$ and 10, lie in the left half-plane. Then, these methods are zero-stable. For $K = 11$, for example, the method is zero-unstable.

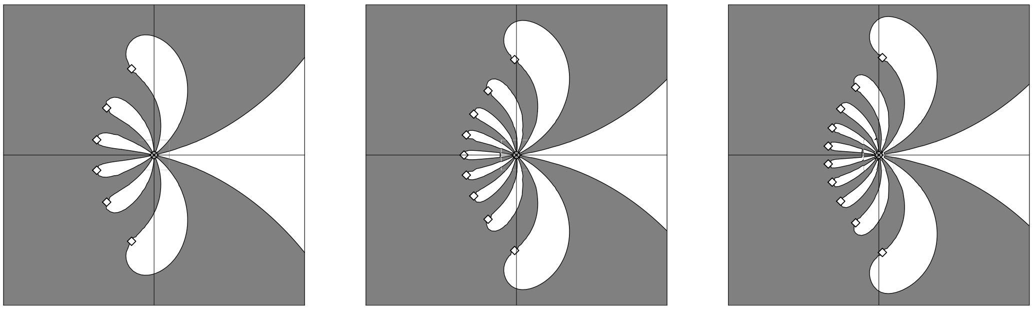

Figure 4: Order star of Brown (7,2), (10,2) and (11,2) methods, respectively

The Figure 5 show the order stars for other values of K and L.

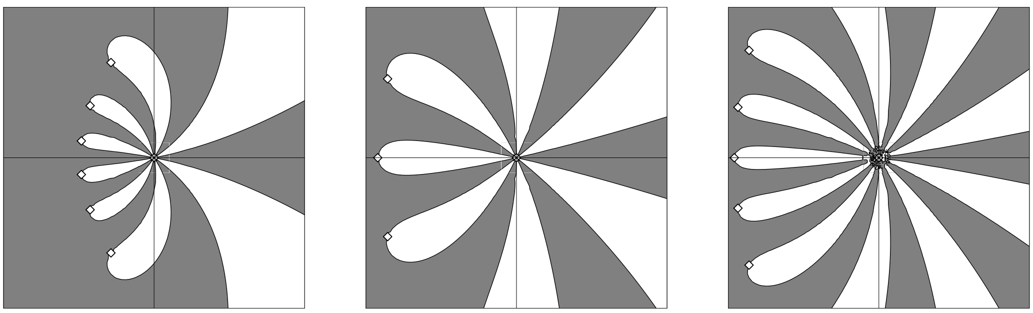

Figure 5: Order star of Brown (7,3), (4,5) and (6,7) methods, respectively

4. TWO ASYMPTOTIC RESULTS

Two asymptotic results concerning zero-stability will be given. Although these were previously discussed by Meneguette[4], order stars permit a much more concise proof.

Theorem 4.1 *Let L be fixed. Brown* (K, L) *methods become zero-unstable for K sufficiently large.*

Proof. Let

$$\mu(z) = \frac{\displaystyle\sum_{j=1}^{L} \sigma_j(e^z) z^{j-1}}{\rho(e^z)} - \frac{1}{z}, \tag{22}$$

be the generating function of the order stars for the Brown (K, L) methods. Observe that $\iota(\infty) = L - 1$. Then, for the (K, L) method,

$$\iota(0) = (K - 1) + (L - 1) \text{ and } \iota(\infty) = L - 1,$$

and for the $(K+1, L)$ method,

$$\iota(0) = K + (L-1) \text{ and } \iota(\infty) = L-1.$$

This means that, as K increases, the number of loops (which support the zeros of $\rho(z)$) increases with K and $\iota(\infty)$ remains constant. If the (K, L) method are to be zero-stable then, by Lemma 2.3, the loops of the order stars lie in the left half-plane. As the plane is divided by $K+L-2$ sectors of A_- and $K+L-2$ sectors of A_+ (by Lemma 2.2), for a sufficiently large K, the loops cross the imaginary axis and then at least one pole of $\mu(z)$ lies in the right half-plane. This characterizes a zero-unstable method.

If the loops in the right half-plane intersect with the left half-plane, when K increases, the loops cross the region $|\operatorname{Im}(z)| \leq \pi$; but the poles of $\mu(z)$ lie in this region (by the Lemmas 2.6 and 2.7) and, consequently, at least one pole lies in the right half-plane. □

Theorem 4.2 *Let K be fixed. The Brown* (K, L) *methods become zero-stable for L sufficiently large.*

Proof. Let K be fixed and L sufficiently large. As K is fixed then the number of sectors containing poles remains constant, because each one contains one distinct zero of $\rho(z)$. On the other hand for the (K, L) method,

$$\iota(0) = (K-1) + (L-1) \quad \text{and} \quad \iota(\infty) = L-1,$$

and for the $(K, L+1)$ method,

$$\iota(0) = (K-1) + L \quad \text{and} \quad \iota(\infty) = L.$$

Hence $\iota(\infty)$ increases with L. As the plane is divided by $K+L-2$ sectors of A_- and $K+L-2$ sectors of A_+ (by Lemma 2.2), then for sufficiently large L, the number of sectors from the positive x axis towards the y axis increases (because these sectors reside in the right half-plane). Then, by increasing the number of sectors related to the $\iota(\infty)$ sufficiently, the poles will lie in the left half-plane. This characterizes a zero-stable method.

If the loops in the left half-plane intersect with the right half-plane, when L increases, the loops cross the region $|\operatorname{Im}(z)| \leq \pi$; but the poles of $\mu(z)$ lie in this region and, consequently, for L sufficiently large, the poles will lie in the left half-plane. □

5. CONCLUSION

This article has introduced order stars as applied to the Brown (K, L) methods. The order stars of a number of Brown (K, L) methods have been computed and displayed pictorially. They then have been used to establish, in a succinct manner, two asymptotic results originally due to Ref. [2].

REFERENCES

[1] Brown, R. L. (1977). Some characteristics of implicit multistep multi-derivative integration formulas. *SIAM J. Numer. Anal.*, *14*(6), 982-993.

[2] Jeltsch, R., & Kratz, L. (1978). On the stability properties of Brown's multistep multiderivative methods. *Numer. Math., 30*(1), 25-38.

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

[4] Meneguette, M. (1987). Multistep multiderivative methods and related topics. (Doctoral dissertation, Oxford University, 1987).

[5] Butcher, J. C. (2003). *Numerical methods for ordinary differential equations*. New York: John Wiley & Sons.

[6] Jeltsch, R. (1977). Stiff stability of multistep multiderivative methods. *SIAM J. Numer. Anal., 14*(4), 760-772.

[7] Iserles, A., & Norsett, S. P. (1991). *Order stars*. London: Chapman and Hall.

[8] Wanner, G., Hairer, E., & Norsett, S. P. (1978). Order stars and stability theorems. *Bit, 18*(4), 475-489.

[9] Hairer, E., & Wanner, G. (1996). *Solving ordinary differential equations II - stiff and differential-algebraic problems*. New York: Springer-Verlag.

[10] Iserles, A., & Norsett, S. P. (1984). A proof of the first Dahlquist barrier by order stars. *Bit, 24*(4), 529-537.

[11] Hairer, E., & Wanner, G. (1983). On the instability of the BDF formulas. *SIAM J. Numer. Anal.*, *20*(6), 1206-1209.

[12] Botta, V. A. (2008). Zeros de polinômios característicos e estabilidade de métodos numéricos. (Doctoral dissertation, Universidade de São Paulo, 2008).