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# Theoretical Results of One Class of Multiderivative Methods through Order Stars

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**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 $\alpha_i$ and $\beta_j$ 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

$$\alpha_i = (-1)^{K-i} \binom{K}{i} (K-i)^{-L}, \; i = 0, \dots, K-1, \; \alpha_K = -\sum_{i=0}^{K-1} \alpha_i, \tag{2}$$

$$\beta_j = \frac{(-1)^j}{j!} \sum_{i=0}^{K-1} (-1)^{K-i} \binom{K}{i} (K-i)^{j-L}, \; j = 1, \dots, L. \tag{3}$$

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].

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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 $w_i(z),\ 1 \le i \le k$ of $\pi(w, z) = 0$. Note that $\pi(w, z) \to \rho(z)$ as $h \to 0$ and $w_i(h) \to w_i,\ 1 \le i \le k$, 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* $D = \{z \in \overline{\mathbb{C}}\ /\ |w_i(z)| \le 1, 1 \le i \le k\}$ *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* $p \le 2L$. *(Clearly this implies* $K \le L + 1$*).*

**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 $\mu$ 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 $\mu$ is given in the following result:

**Lemma 2.4** *The approximation $\mu$ 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

$$J = \{z \in \mathbb{C} : |\operatorname{Im}(z)| \leq \pi\}. \tag{12}$$

Let us define the sets

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

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 $\{z | \operatorname{Re}(z) \geq \epsilon\} \cap J$ 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 $\delta$ be a loop such that $\delta \cap \partial J = \emptyset$ and $\delta \cap J \neq \emptyset$. Then, there is on $\delta$ exactly one pole of $\mu$ between any two roots of $\mu(z) = 0$. Moreover, if $z_0 \in int(J)$ is a pole of $\mu$ 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 $\{\mathbb{R} + i\pi\} \cap cl(G) \neq \emptyset$ 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 $\mu$ or there is a pole of $\mu$ along the positively oriented portion of $\partial G$ from $x_- + i\pi$ to $z_0$;*

2. *if $G$ is a $A_+$-region then either $x_+ + i\pi$ is a pole of $\mu$ or there is a pole of $\mu$ along the positively oriented portion of $\partial G$ 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 $z_0 = 1$.

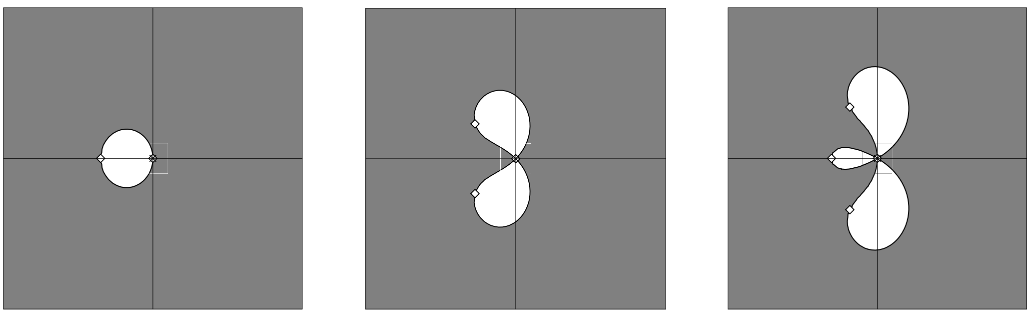

**Figure 1:** Order star of Brown (2,1), (3,1) and (4,1) methods, respectively

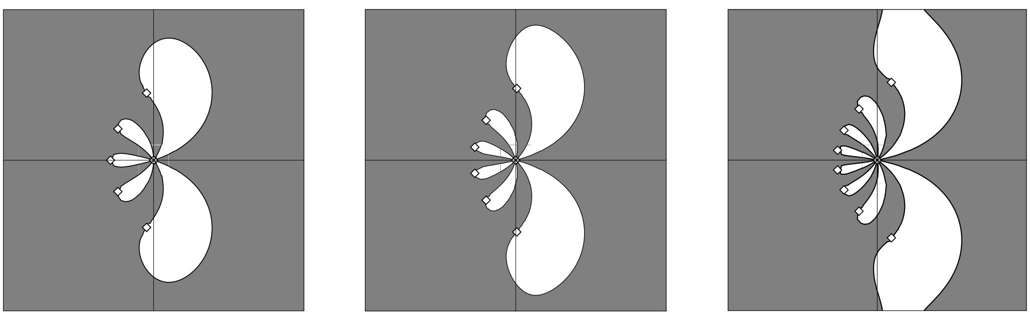

**Figure 2:** Order star of Brown (6,1), (7,1) and (9,1) methods, respectively

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

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

Then

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

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,

$$\iota(0) = K + L - 2 = (K - 1) + (L - 1). \qquad (21)$$

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).

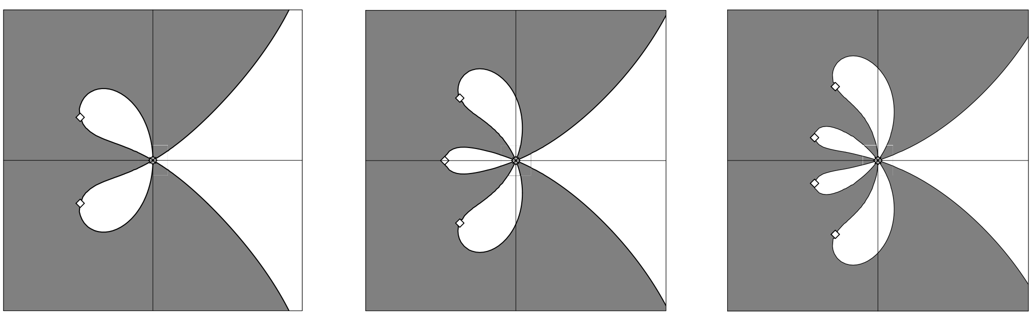

**Figure 3:** Order star of Brown (3,2), (4,2) and (5,2) methods, respectively

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.

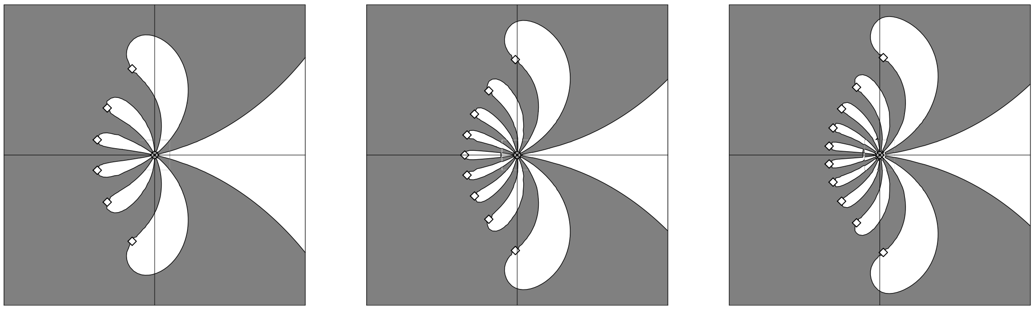

**Figure 4:** Order star of Brown (7,2), (10,2) and (11,2) methods, respectively

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

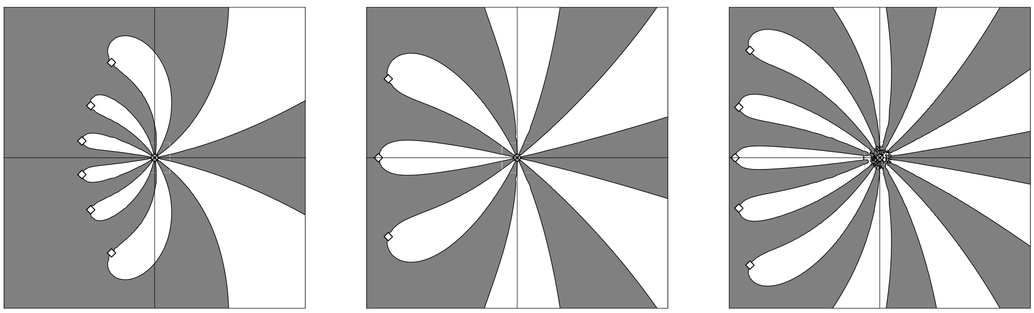

**Figure 5:** Order star of Brown (7,3), (4,5) and (6,7) methods, respectively

# 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

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

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].

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