Chapter 6

Bounding Clusters of Zeros of Analytic Functions

6.1 Introduction

In the previous chapter, we applied a verified method to calculate a validated polynomial factor of an analytic $f(z)$ which has a cluster of zeros around the origin. The number of zeros in the cluster and the radius of a disk which contains the cluster were assumed to be given in the computation. The purpose of this chapter is to present a method to determine the number of zeros in the cluster and compute a disk containing all the zeros in the cluster.

On locating the zeros of an analytic function in some regions of the complex plane, some methods based on numerical computation of contour integrals were proposed in [8, 11, 26, 29]. These methods reduce the problem to the easier problem of finding a polynomial having the same zeros as $f(z)$ in the given region. Sakurai and Sugiura [64, 65] proposed a verified factorization method to locate the cluster of zeros which are lie inside a small disk around the origin in the complex plane. In these papers, the number of zeros in the cluster and the radius of a small disk containing the cluster were supposed to be given by the user. Therefore, the results of this chapter can be used by these methods to further locate the zeros in the cluster.

On the other hand, a number of methods were proposed to detect and bound clusters of zeros of polynomials [21, 42, 60, 77]. Rump [60] proposed a hybrid method to compute an enclosing disk of the cluster of polynomials, and the quality of the radius of the disk can be of the order of the numerical sensitivity of the root cluster.

Since the zeros in a cluster of the n-degree Taylor polynomial of $f(z)$ converge to the zeros in a cluster of $f(z)$ as n tends to infinity, in this chapter, we present a method to bound the cluster of zeros of $f(z)$ by bounding the cluster of the Taylor polynomial of $f(z)$. First we perform a validated computation of the n-degree Taylor polynomial $p(z)$ of $f(z)$ using circular complex arithmetic, and get an interval coefficient polynomial $\boldsymbol{p}(z)$ which contains $p(z)$. Then we apply some well known formulae on bounding clusters of zeros of a polynomial to compute a disk containing the cluster of zeros of $p(z)$. Based on a validated computation of the upper bound of the remainder of the Taylor series of $f(z)$, a theorem based on Pellet's theorem [32] and Rouché's theorem is used to verify that the disk contains the cluster of zeros of $f(z)$. In this way we reduce the problem of bounding the cluster of zeros of an analytic function to the problem of bounding the cluster of zeros of a polynomial. Because of the efficiency of the methods used in bounding cluster of zeros of polynomials, the resulting disk is almost optimal. Numerical examples are presented to illustrate the effectiveness of the method.

6.2 A Method to Bound Zeros of Analytic Functions

Let $f(z)$ be analytic in a circular region $D = \{z : |z| \leq \rho\}$, where $\rho > 1$ is a positive real number smaller than the analytic radius of $f(z)$. Then $f(z)$ has the following Taylor expansion in D.

$$f(z) = \sum_{k=0}^{\infty} c_k z^k, \quad z \in D. \tag{6.1}$$

We assume that $f(z)$ has a cluster of m zeros around the origin and the cluster is distinctly separated from other zeros of $f(z)$. Let $p(z)$ be the n-degree Taylor polynomial of $f(z)$.

$$p(z) := \sum_{k=0}^{n} c_k z^k. \tag{6.2}$$

If n is large enough, then $p(z)$ also has a cluster of m zeros around the origin, the cluster is distinctly separated from other zeros of $p(z)$ and the zeros in the cluster converge to the zeros in the cluster of $f(z)$ as n tends to infinity. Now we consider the problem of bounding the cluster of zeros of $p(z)$. The following Pellet's theorem [32] can be used to calculate a disk containing the cluster of $p(z)$.

Theorem 6.2.1 (Pellet) *Let polynomial $p(z)$ be defined by (6.2), with $c_n c_0 \neq 0$. If the polynomial*

$$q(z) := \sum_{k=m+1}^{n} |c_k| z^k - |c_m| z^m + \sum_{k=0}^{m-1} |c_k| z^k \tag{6.3}$$

has two positive roots r and R, $r < R$, then $p(z)$ has exactly m zeros in or on the circle $A := \{z : |z| \leq r\}$ and no zeros in the annular ring $\{z : r < |z| < R\}$.

From Theorem 6.2.1 we see that given the Taylor polynomial $p(z)$ and the number m of zeros in the cluster of $f(z)$, we can obtain the disk A containing the cluster of $p(z)$ by calculating the smaller positive root of $q(z)$. If the cluster of $p(z)$ is sufficiently near the cluster of $f(z)$, then the disk A contains the cluster of $f(z)$. For two functions $P(z)$ and $Q(z)$, the following Rouché's theorem [32] can be used to verify whether they have the same number of zeros in a given region.

Theorem 6.2.2 (Rouché) *If $P(z)$ and $Q(z)$ are analytic interior to a simple closed Jordan curve C and if they are continuous on C and*

$$|P(z)| < |Q(z)|, \quad z \in C, \tag{6.4}$$

then the function $F(z) = P(z) + Q(z)$ has the same number of zeros interior to C as does $Q(z)$.

Using Theorem 6.2.2, we can calculate whether $f(z)$ and $p(z)$ have the same number of zeros in the disk A. In order to do this, we should take account of the influence of the remainder of the Taylor series of $f(z)$. From Theorem 6.2.1 and Theorem 6.2.2, we have the following theorem.

Theorem 6.2.3 *Let analytic function $f(z)$ be defined by (6.1), let $p(z)$ be the n-degree Taylor polynomial of $f(z)$ and be defined by (6.2). Let r be the smaller positive root of $q(z)$ defined by (6.3). If the following inequality*

$$\left| \sum_{k=n+1}^{\infty} c_k z^k \right| < |p(z)| \tag{6.5}$$

holds for $|z| = r$, then $f(z)$ has exactly m zeros in $A = \{z : |z| \le r\}$.

From Theorem 6.2.3, we see that if the inequality (6.5) holds, then the disk A calculated by Theorem 6.2.1 is an enclosing disk of the cluster of $f(z)$. In the next sections, we will first use the verified method proposed in the previous chapter to calculate the Taylor polynomial $p(z)$, then we use some existed methods to calculate a disk containing the cluster of $p(z)$, finally we perform a validated computation of the Taylor remainder of $f(z)$ and use Theorem 6.2.3 to verify that the disk contains the cluster of $f(z)$.

6.3 Validated Computation of $p(z)$

From the discussions in the previous section, first we consider the computation of the Taylor polynomial $p(z)$ of $f(z)$ in this section. Because of the roundoff errors in finite arithmetic computations, the exact Taylor polynomial of $f(z)$ can not be calculated. Therefore, we use the verified method proposed in the previous chapter to calculate an interval coefficient polynomial $\boldsymbol{p}(z)$ which contains $p(z)$. Circular complex arithmetic [50] is used in the computation.

Let interval coefficients polynomial $\boldsymbol{p}(z)$ be

$$\boldsymbol{p}(z) := \sum_{k=0}^{n} \boldsymbol{c}_k z^k, \tag{6.6}$$

where $\boldsymbol{c}_k$ are calculated by (5.33) and (5.34). Since $c_k \in \boldsymbol{c}_k$, $k = 0, \ldots, n$, we say that $p(z)$ is contained in $\boldsymbol{p}(z)$ and we denote this by $p(z) \in \boldsymbol{p}(z)$.

6.4 Bounding Cluster of Zeros of $p(z)$

6.4.1 Computation of the Number of Zeros in the Cluster

In this section, we use circular complex arithmetic to compute a validated bound for the cluster of zeros of $p(z)$. According to Theorem 6.2.1, given the number of zeros in the cluster, the bound for the cluster of $p(z)$ can be obtained by calculating the smaller positive root of $q(z)$. First we consider the problem of computing the number of zeros in the cluster of $p(z)$.

Several methods on determining the number of zeros in the cluster of a polynomial were discussed in [60]. A simple way is to evaluate the values $|c_k/c_{k+1}|$, $k = 0, \ldots, n-1$. If the cluster of $p(z)$ is distinctly separated from other zeros, then the value of $|c_m/c_{m+1}|$ will be much larger compared with $|c_k/c_{k+1}|$ for $k < m$ where m is the number of zeros in the cluster.

According to error analysis theory [71, 75], an arbitrary small change of the coefficients of a polynomial may lead to the disintegration of a multiple zero into a cluster of distinct zeros. On the other hand, the location and multiplicity of a cluster of zeros in a certain domain of $\mathbb{C}$ is a stable phenomenon: all sufficiently close polynomials have a zero cluster of the same multiplicity in that domain [25, 37].

Therefore, for interval coefficient polynomial $\boldsymbol{p}(z)$ which contains $p(z)$, if $p(z)$ has a cluster of zeros which is distinctly separated from other zeros and the radius of the coefficients of $\boldsymbol{p}(z)$ is sufficiently small, then any polynomial $p^*(z) \in \boldsymbol{p}(z)$ will have a cluster of zeros which is distinctly separated from the other zeros of $p^*(z)$ and the value $|c^*_m/c^*_{m+1}|$ will be much larger compared with $|c^*_k/c^*_{k+1}|$ for $k < m$ where c^*_k is the coefficients of $p^*(z)$. Therefore, from the fundamental property of interval arithmetic, we can calculate the number of zeros in the cluster of $p(z) \in \boldsymbol{p}(z)$ by evaluating the following inequalities.

$$|\boldsymbol{c}_k/\boldsymbol{c}_{k+1}| \gg |\boldsymbol{c}_{k-1}/\boldsymbol{c}_k|, \ k = 1, \ldots, n-1, \tag{6.7}$$

where $|\boldsymbol{a}| := \max_{a \in \boldsymbol{a}} |a|$ for a disk $\boldsymbol{a}$ in the complex plane. If (6.7) holds for $k = m$, then m will be the number of zeros in the cluster of $p(z)$.

6.4.2 Validated Computation of the Smaller Positive Root of $q(z)$

Let interval coefficient polynomial $\boldsymbol{q}(z)$ be

$$\boldsymbol{q}(z) := \sum_{k=m+1}^{n} \boldsymbol{b}_k z^k - \boldsymbol{b}_m z^m + \sum_{k=0}^{m-1} \boldsymbol{b}_k z^k, \tag{6.8}$$

where m is the number of zeros in the cluster of $p(z)$ and the coefficients $\boldsymbol{b}_k$ are calculated by

$$\begin{aligned} \mathrm{mid}(\boldsymbol{b}_k) &= |\mathrm{mid}(\boldsymbol{c}_k)|, \ k = 0, \dots, n, \ k \neq m, \\ \mathrm{mid}(\boldsymbol{b}_m) &= -|\mathrm{mid}(\boldsymbol{c}_m)|, \\ \mathrm{rad}(\boldsymbol{b}_k) &= \mathrm{rad}(\boldsymbol{c}_k), \ k = 0, \dots, n. \end{aligned} \tag{6.9}$$

Then from the fundamental property of interval arithmetic, if the radius of $\boldsymbol{b}_k$ is sufficiently small, then $|c_k| \in \boldsymbol{b}_k, \ k = 0, \dots, n$, i.e., $q(z) \in \boldsymbol{q}(z)$.

In the following, we consider the problem of computing an upper bound of the smaller positive root r of $q(z)$. For an interval coefficient polynomial $\boldsymbol{v}(z)$, in the case that each polynomial $v^*(z) \in \boldsymbol{v}(z)$ has only simple zeros, Petković [51] proposed an iterative method to calculate some pair-wise disjoint intervals $Z_1, \dots, Z_n$ with the property that any $v^*(z) \in \boldsymbol{v}(z)$ has exactly one zero in Z_j for $j = 1, \dots, n$. In this chapter, we apply interval Newton method [19] on $\boldsymbol{q}(z)$ to compute a sequence of disks $\boldsymbol{r}^{(k)}$ such that any $q^*(z) \in \boldsymbol{q}(z)$ has its smaller positive root in $\boldsymbol{r}^{(k)}$. Since $q(z) < 0$ for $r < z < R$, therefore, if the following inequality

$$\mathrm{mid}(\boldsymbol{q}(\boldsymbol{r}^{(k)})) + \mathrm{rad}(\boldsymbol{q}(\boldsymbol{r}^{(k)})) < 0 \tag{6.10}$$

holds, then an upper bound δ for r can be calculated by

$$\delta = |\mathrm{mid}(\boldsymbol{r}^{(k)})| + \mathrm{rad}(\boldsymbol{r}^{(k)}). \tag{6.11}$$

6.4.3 Computation of Initial Value

In the computation of δ, one problem is how to choose initial approximation. Since the unique positive root of the following Cauchy polynomial

$$s(z) = -c_m z^m + \sum_{k=0}^{m-1} c_k z^k. \tag{6.12}$$

is a good approximation of r, we apply interval Newton method on the following interval coefficient polynomial $\boldsymbol{s}(z)$ which contains $s(z)$ to compute a disk $\tilde{\boldsymbol{r}}$ which contains an approximation of r.

$$\boldsymbol{s}(z) = -\boldsymbol{b}_m z^m + \sum_{k=0}^{m-1} \boldsymbol{b}_k z^k, \tag{6.13}$$

where $\boldsymbol{b}_k$ are calculated by (6.9). The initial value used in the calculation can be calculated by

$$\tilde{r} = 2 \max_{1 \le k \le m} |\boldsymbol{b}_{m-k}/\boldsymbol{b}_m|^{1/k}. \tag{6.14}$$

6.5 Validated Computation of the Bound of Remainder of the Taylor Series of $f(z)$

For the upper bound δ of r, according to Theorem 6.2.3, if the inequality (6.5) holds for $|z| = \delta$, then the disk $\Omega = \{0\,;\delta\}$ contains the cluster of $f(z)$. In this section, we use circular complex arithmetic to perform a validated computation of the upper bound of remainder of the Taylor series of $f(z)$ on the boundary $\Gamma : \{z : |z| = \delta\}$ of Ω.

Since

$$\left| \sum_{k=n+1}^{\infty} c_k z^k \right| \le \sum_{k=n+1}^{\infty} |c_k||z|^k = \sum_{k=n+1}^{\infty} |c_k|\delta^k, \; z \in \partial\Omega. \tag{6.15}$$

From Cauchy's theorem (Theorem 5.3.4), we have

$$\left| \sum_{k=n+1}^{\infty} c_k z^k \right| \le M_\rho \frac{(\delta/\rho)^{n+1}}{1-\delta/\rho}, \quad z \in \partial\Omega, \tag{6.16}$$

where $\rho > 1$ is a real number smaller than the analytic radius of $f(z)$, $M_\rho := \max\limits_{|z|=\rho} |f(z)|$.

Next we consider the problem of computing ρ and the maximum value M_ρ of $|f(z)|$ on Γ. Using circular complex arithmetic and from the fundamental property of interval arithmetic, we can calculate a real number smaller than the analytic radius of $f(z)$ by computing the interval extension of $f(z)$ for some input disks. In this section we use Cdomain circular arithmetic system [72] to determine the analyticity of functions in input disks.

Eble [13] and Neher [39, 40] proposed a method based on global optimization methods [57] to calculate the maximum value of $|f(z)|$ on Γ with rectangular complex arithmetic. In this section, we use circular complex arithmetic. We use the method proposed in the previous chapter to calculate the maximum value of $|f(z)|$ on Γ.

Using a similar method as above, we also perform a computation of the lower bound of the minimum value of $|p(z)|$ on Γ. Based on these results, it is possible to perform a verification of the inequality (6.5).

6.6 Algorithm

From the discussions in the last sections, we give the following algorithm to calculate the number of zeros in the cluster of $f(z)$ and compute a disk containing the cluster. We assume that $f(z)$ is analytic in the unit disk, this condition can be satisfied by scaling $f(z)$.

Algorithm :

Input: $f(z)$, j, k.

Output: m, number of zeros in the cluster.

δ, radius of the enclosing disk of the cluster.

1. Compute a real number $\rho > 1$ such that $f(z)$ is analytic in $\{0\,;\rho\}$.
2. Compute the maximum value M_ρ of $|f(z)|$ on $|z| = \rho$.
3. Compute $\mathbf{c}_k$ by (5.33) and (5.34).
4. Compute the number m of zeros in the cluster by (6.7).
5. Compute an initial value $\tilde{r}$ by (6.14).

6. Perform j iterations by interval Newton method on $s(z)$ with initial value $\tilde{r}$ to get a disk $\tilde{r}^{(j)}$.
7. Perform k iterations by interval Newton method on $q(z)$ with initial value $\tilde{r}^{(j)}$ to get a disk $r^{(k)}$.
8. If $|\text{mid}(q(r^{(k)}))| - \text{rad}(q(r^{(k)})) < 0$ then compute δ by (6.11).
9. Compute the upper bound of $\left|\sum_{k=n+1}^{\infty} c_k z^k\right|$ on $|z| = \delta$ by (6.16).
10. Compute the lower bound of the minimum value of $|p(z)|$ on $|z| = \delta$.
11. If the result of step 9 is smaller than the result of step 10, then stop, else goto step1.

Where j and k are the number of iterations in step 6 and step 7, respectively.

6.7 Numerical Examples

Numerical examples were carried out in Matlab Ver. 6.5 with interval arithmetic package INTLAB [61, 62]. The determination of the analyticity of $f(z)$ was performed by using the Cdomain circular complex arithmetic system [72].

Example 6.1. Suppose that

$$\begin{aligned} f_1(z) &= (z^6 - 27.04z^5 + 208.0805z^4 - 413.293502z^3 + 16.303554z^2 - 0.202914z + 0.00081) \\ &\quad \times \exp(\frac{1}{3}z^2 + 2). \end{aligned}$$

Note that $f_1(z)$ has a cluster of 3 zeros: $0.01, 0.01, 0.02$. The maximum value of $|f_1(z)|$ on the boundary of the disk $\{0\,;\rho\}$ and the analyticity of $f_1(z)$ in the disk are calculated, the results are shown in Table 6.1, where $\tilde{M} = M_\rho/n$.

Table 6.1 Maximum value of $|f_1(z)|$ and analyticity of $f_1(z)$.

ρ	M_ρ	$\tilde{M}(n=14)$	$\tilde{M}(n=20)$	Analyticity
2	2.1×10^5	1.3×10^1	2.0×10^{-1}	yes
4	1.7×10^8	6.3×10^{-1}	1.5×10^{-4}	yes
6	7.4×10^{11}	9.4×10^0	2.0×10^{-4}	yes
8	3.0×10^{16}	6.8×10^3	2.6×10^{-2}	yes
16	5.1×10^{45}	7.1×10^{28}	4.2×10^{21}	yes

The center mid(c_k) and radius rad(c_k) of the validated Taylor coefficient c_k of $f_1(z)$ are shown in Table 6.2. The underline shows the different digits of the results compared with the results calculated by Mathematica with multiple precision arithmetic, N is the number of sampling points of FFT.

Table 6.2 Taylor coefficients of $f_1(z)$. ($N = 32$)

k	mid(c_k)	rad(c_k)
0	$5.985135440\underline{393919} \times 10^{-3}$	1.1×10^{-11}
1	$-1.499342929258\underline{345} \times 10^{0}$	5.4×10^{-12}
2	$1.2046987016309\underline{26} \times 10^{2}$	2.2×10^{-12}
3	$-3.054348652577926 \times 10^{3}$	8.0×10^{-12}
4	$1.57767477847371\underline{3} \times 10^{3}$	4.0×10^{-12}
$\vdots$	$\vdots$	$\vdots$
20	$6.499284\underline{877224497} \times 10^{-6}$	3.8×10^{-12}

From Table 6.1, when ρ is large, $\tilde{M}$ is also large, we take $\rho = 4$ and $n = 20$ so that $\tilde{M}$ is small. The calculated results are shown below.

$$m = 3,$$

$$\delta = 0.051,$$

$$M_\rho \frac{(\delta/\rho)^{n+1}}{1-\delta/\rho} = 1.1 \times 10^{-24},$$

$$|p(z)| \geq 0.15, \ |z| = \delta.$$

Since $1.1 \times 10^{-24} < 0.15$, it implies that the disk $\{0\,;0.051\}$ contains 3 zeros of $f_1(z)$.

Example 6.2. Suppose that

$$f_2(z) \ = \ (z^3 - 7.5 \times 10^{-4}z^2 - 3.75 \times 10^{-7}z + 1.25 \times 10^{-10}) \times \prod_{k=1}^{5}(z-k)\log(z+6).$$

Note that $f_2(z)$ has a cluster of 3 zeros: $0.001, 0.0005, 0.00025$. The maximum value of $|f_2(z)|$ on the boundary of the disk $\{0\,;\rho\}$ and the analyticity of $f_2(z)$ in the disk are shown in Table 6.3. The center $\mathrm{mid}(\boldsymbol{c}_k)$ and radius $\mathrm{rad}(\boldsymbol{c}_k)$ of the validated Taylor coefficient $\boldsymbol{c}_k$ of $f_2(z)$ are shown in Table 6.4.

Table 6.3 Maximum value of $|f_2(z)|$ and analyticity of $f_2(z)$.

ρ	M_ρ	$\tilde{M}(n=14)$	$\tilde{M}(n=20)$	Analyticity
2	2.8×10^4	1.7×10^0	2.7×10^{-2}	yes
3	2.1×10^5	4.4×10^{-2}	6.0×10^{-5}	yes
4	1.1×10^6	4.1×10^{-3}	1.0×10^{-6}	yes
5	4.9×10^6	8.0×10^{-4}	5.1×10^{-8}	yes
6	–	–	–	no

Table 6.4 Taylor coefficients of $f_2(z)$. $(N = 32)$

k	$\mathrm{mid}(\boldsymbol{c}_k)$	$\mathrm{rad}(\boldsymbol{c}_k)$
0	$-2.687639\underline{766296704} \times 10^{-8}$	4.4×10^{-13}
1	$8.0688043\underline{91208366} \times 10^{-5}$	5.4×10^{-13}
2	$1.61081704468\underline{5495} \times 10^{-1}$	3.4×10^{-13}
3	$-2.15364209434736\underline{8} \times 10^{2}$	6.8×10^{-13}
4	$4.7120891242447\underline{20} \times 10^{2}$	9.4×10^{-13}
$\vdots$	$\vdots$	$\vdots$
20	$-2.424\underline{940248602070} \times 10^{-10}$	9.4×10^{-13}

The calculated results for $\rho = 5$ and $n = 20$ are shown below.

$$m = 3,$$

$$\delta = 0.00116,$$

$$M_\rho \frac{(\delta/\rho)^{n+1}}{1 - \delta/\rho} = 2.3 \times 10^{-70},$$

$$|p(z)| \geq 5.2 \times 10^{-8}, \ |z| = \delta.$$

Since $2.3 \times 10^{-70} < 5.2 \times 10^{-8}$, it implies that the disk $\{0\,; 0.00116\}$ contains 3 zeros of $f_2(z)$.

6.8 Conclusion

A validated computation of the n-degree Taylor polynomial $p(z)$ for analytic function $f(z)$ is performed using circular complex arithmetic. A disk containing a cluster of zeros of $p(z)$ is found by a method based on Pellet's theorem. By a validated computation of the Taylor reminder series on the boundary of the disk, Rouche's theorem is able to be used to verify that the resulting disk contains a cluster of zeros of $f(z)$. Numerical examples show the applicability of this method.