ON EFFICIENT COMPUTATION
AND ASYMPTOTIC SHARPNESS OF KALANTARI'S BOUNDS
FOR ZEROS OF POLYNOMIALS

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ABSTRACT. We study an infinite family of lower and upper bounds on the
modulus of zeros of complex polynomials derived by Kalantari. We first give a
simple characterization of these bounds which leads to an efficient algorithm for
their computation. For a polynomial of degree n our algorithm computes the
first m bounds in Kalantari's family in $O(mn)$ operations. We further prove
that for every complex polynomial these lower and upper bounds converge to
the tightest annulus containing the roots, and thus settle a problem raised in
Kalantari's paper.

1. INTRODUCTION

In [3], Kalantari derives an infinite family of lower and upper bounds on the
modulus of zeros of analytic functions. When applied to complex polynomials,
these bounds can be computed in polynomial time.

Let

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0, \ a_0, \ldots, a_n \in \mathbb{C}, \ a_n a_0 \neq 0,$$

and

$$F(z) = f(z)z.$$

Then from an expansion formula of a fundamental family of root-finding iteration
functions applied to $F(z)$ at $z = 0$ (see (2.4) in [3]), we get

$$(1.1) \qquad 1 + \sum_{i=1+k}^{n+k} (-1)^{k+2} \frac{\hat{D}_{k+1,i+1}(0)}{D_{k+1}(0)} \theta^i = 0$$

for $k = 0, 1, 2, \ldots$, where θ is a zero of $f(z)$, and

$$D_m(z) = \det \begin{pmatrix} F'(z) & \frac{F''(z)}{2!} & \cdots & \frac{F^{(m-1)}(z)}{(m-1)!} & \frac{F^{(m)}(z)}{(m)!} \\ F(z) & F'(z) & \cdots & \ddots & \frac{F^{(m-1)}(z)}{(m-1)!} \\ 0 & F(z) & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{F''(z)}{2!} \\ 0 & 0 & \cdots & F(z) & F'(z) \end{pmatrix},$$

$$\hat{D}_{m,j}(z) = \det \begin{pmatrix} \frac{F''(z)}{2!} & \frac{F'''(z)}{3!} & \cdots & \frac{F^{(m)}(z)}{(m)!} & \frac{F^{(j)}(z)}{j!} \\ F'(z) & \frac{F''(z)}{2!} & \ddots & \frac{F^{(m-1)}(z)}{(m-1)!} & \frac{F^{(j-1)}(z)}{(j-1)!} \\ F(z) & F'(z) & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \frac{F''(z)}{2!} & \frac{F^{(j-m+2)}(z)}{(j-m+2)!} \\ 0 & 0 & \cdots & F'(z) & \frac{F^{(j-m+1)}(z)}{(j-m+1)!} \end{pmatrix},$$

and "det" denotes determinant.

Let

$$\hat{c}_{k,i} = (-1)^{k+2} \frac{\hat{D}_{k+1,i+1}(0)}{D_{k+1}(0)};$$

then (1.1) becomes

$$(1.2) \qquad\qquad 1 + \sum_{i=1+k}^{n+k} \hat{c}_{k,i} \theta^i = 0.$$

Now define

$$\gamma_k = \max \left\{ |\hat{c}_{k,i}|^{1/i} : \ i = 1+k, \ldots, n+k \right\} \quad \text{and} \quad u_k = \gamma_k |\theta|.$$

Then $u_k^i \geq |\hat{c}_{k,i} \theta^i|$ and

$$(1.3) \qquad\qquad \sum_{i=1+k}^{n+k} u_k^i \geq \sum_{i=1+k}^{n+k} |\hat{c}_{k,i} \theta^i| \geq 1.$$

Proposition 1.1. *Inequality* (1.3) *implies* $u_k > r_k$, *where* $r_k < 1$ *is the unique positive zero of the polynomial* $t^{k+1} + t - 1$.

Proof. The following proof was given by Kalantari [3].

First, the polynomial $q(t) = t^{k+1} + t - 1$ has a unique positive zero $r_k < 1$. This follows from the inequalities $q(0) < 0$, $q(1) > 0$, and $q'(t) > 0$ for $t \geq 0$.

Now assume $u_k \leq r_k < 1$. Note by definition that $u_k > 0$. So we have

$$\frac{u_k^{k+1}}{1 - u_k} > u_k^{k+1} \frac{1 - u_k^n}{1 - u_k} = \sum_{i=1+k}^{n+k} u_k^i \geq 1,$$

or equivalently $u_k^{k+1} + u_k - 1 > 0$. But by strict upward monotonicity of $q(t)$ for $t \geq 0$, $0 < u_k \leq r_k$ implies $u_k^{k+1} + u_k - 1 \leq 0$, a contradiction. $\qquad\square$

Plugging $u_k = \gamma_k|\theta|$ into $u_k > r_k$, we obtain an infinite family of lower bounds on zeros of $f(z)$:

$$|\theta| > \frac{r_k}{\gamma_k} = L_k, \quad k = 0, 1, 2, 3, \ldots.$$

The quantity L_k is called the $(k+2)$-th order lower bound (and denoted by L_{k+2}) in [3].

To obtain upper bounds on zeros of $f(z)$, we apply the above lower bounds to $g(z) = a_0 z^n + a_1 z^{n-1} + \cdots + a_{n-1}z + a_n$. Since the reciprocals of zeros of $g(z)$ are zeros of $f(z)$, the reciprocal of the lower bound L_k on zeros of $g(z)$ is the upper bound U_k on zeros of $f(z)$, which is called the $(k+2)$-th order upper bound (and denoted by U_{k+2}) in [3].

The first bounds L_0 and U_0 of this family also appear in Henrici [1] as Theorem 6.4b and Corollary 6.4k, respectively.

Remark 1.2. A straightforward computation of the lower bound L_m on zeros of $f(z)$ takes $O(m^3 n)$ operations.

In Section 2, we give a simple characterization of Kalantari's bounds which leads to an efficient algorithm that computes the first m bounds on zeros of $f(z)$ in $O(mn)$ operations. In Section 3, we prove that for every complex polynomial the upper and lower bounds converge to the tightest annulus containing the roots, and thus settle a problem raised in [3].

2. THE ALGORITHM

The key element in our algorithm is the efficient computation of $\hat{c}_{k,i}$. We start with an alternative interpretation of $\hat{c}_{k,i}$.

For each integer $k \geq 0$, define

$$\Omega(k) = \{1 + \sum_{i=1+k}^{n+k} \alpha_i z^i : \alpha_i \in \mathbb{C}\}.$$

That is, $\Omega(k)$ is the set of complex polynomials of degree $n+k$ whose constant term is 1, and the coefficients of z^i, $i = 1, \ldots, k$ are 0.

Then for each integer $k \geq 0$, there exists a unique polynomial $q_k(z)$ of degree k, such that

$$f(z)q_k(z) \in \Omega(k).$$

Moreover, the coefficient of z^i, $i \geq 0$, in $q_k(z)$ is independent of k, so we can write

$$q_k(z) = \sum_{i=0}^{k} b_i z^i.$$

The existence and uniqueness of b_i, $i = 0, 1, 2, \ldots$, and hence the existence and uniqueness of $q_k(z)$, $k = 0, 1, 2, \ldots$, are implied by recurrence (2.2) shown below.

For each integer $k \geq 0$, let

(2.1) $$h_{n+k}(z) \equiv f(z)q_k(z) = f(z)\sum_{i=0}^{k} b_i z^i = 1 + \sum_{i=1+k}^{n+k} c_{k,i} z^i.$$

That is, $c_{k,i}$ is defined as the coefficient of z^i in $h_{n+k}(z)$.

It is easy to see that b_i and $h_{n+i}(z)$, $i = 0, 1, 2, \ldots$, satisfy the following recurrence:

(2.2a) $b_0 = 1/a_0, \quad h_n(z) = b_0 f(z),$

(2.2b) $b_i = -c_{i-1,i}/a_0, \quad h_{n+i}(z) = h_{n+i-1}(z) + b_i z^i f(z), \quad i = 1, 2, \ldots.$

Proposition 2.1. *For each integer $k \geq 0$, define*

$$\hat{h}_{n+k}(z) \equiv 1 + \sum_{i=1+k}^{n+k} \hat{c}_{k,i} z^i.$$

Then

$$\hat{h}_{n+k}(z) \equiv h_{n+k}(z),$$

or equivalently $\hat{c}_{k,i} = c_{k,i}$ for $i = 1 + k, \ldots, n + k$.

Proof. From (1.2) the zeros of $f(z)$ are also zeros of $\hat{h}_{n+k}(z)$. Thus, if the zeros of $f(z)$ are all simple, we can factor $f(z)$ out of $\hat{h}_{n+k}(z)$. That is, $\hat{h}_{n+k}(z) = f(z)\hat{g}_k(z)$, where $\hat{g}_k(z)$ is a polynomial of degree k. Since $\hat{h}_{n+k}(z) \in \Omega(k)$, we have

$$\hat{g}_k(z) \equiv g_k(z), \quad \hat{h}_{n+k}(z) \equiv h_{n+k}(z),$$

hence the proof of the claim.

If $f(z)$ has root(s) of multiplicity greater than 1, we can view $f(z)$ as the limit of a sequence of polynomials of degree n whose roots are all simple. Since both $c_{k,i}$ and $\hat{c}_{k,i}$ are continuous functions of $a_0, \ldots, a_n$, we conclude that our claim holds in this case, too. □

Now we can write γ_k as a function of $c_{k,i}$, $i = 1 + k, \ldots, n + k$:

$$\gamma_k = \max \left\{ |c_{k,i}|^{1/i} : \ i = 1 + k, \ldots, n + k \right\}.$$

Our algorithm makes use of recurrence (2.2) to compute $h_{n+k}(z)$, from which the coefficients $c_{k,i}$ are extracted to compute γ_k and then the lower bounds L_k, $k = 0, \ldots, m - 1$. Observe that r_k is independent of the polynomial f whose roots we want to bound, so it can be precomputed and stored in a lookup table. We shall assume r_k is available to our algorithm.

Algorithm 1: Computing the first m lower bounds on zeros of $f(z)$ in $O(mn)$ operations.

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input : $f(z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0$, $a_n a_0 \neq 0$ and m.
output: The first m lower bounds on zeros of $f(z)$.

$b_0 = 1/a_0$;
$h_n(z) = b_0 f(z)$;
$\gamma_0 = \max \left\{ |c_{0,i}|^{1/i} : \ i = 1, \ldots, n \right\}$;
output $L_0 = r_0/\gamma_0$;
for k *from* 1 *to* $m - 1$ **do**
  $b_k = -c_{k-1,k}/a_0$;
  $h_{n+k}(z) = h_{n+k-1}(z) + b_k z^k f(z)$;
  $\gamma_k = \max \left\{ |c_{k,i}|^{1/i} : \ i = 1 + k, \ldots, n + k \right\}$;
  output $L_k = r_k/\gamma_k$;
end

Remark 2.2. We can scale $f(z)$ to make $a_0 = 1$, thus eliminating the division operation when computing b_i.

It is hard to believe that the lower bounds generated by such a simple scheme would be asymptotically sharp, not to mention that each L_k has to be a lower bound on zeros of $q_k(z) = \sum_{i=0}^{k} b_i z^i$ as well. Yet extensive numerical experiments suggest that this family is indeed asymptotically sharp.

Example 2.3. Let $f(z) = 3z^5 + 4z^4 + 4z^3 + 2z^2 + 2z + 1$. It has 5 distinct roots: $\theta_1 = -0.57478$, $\theta_2 = 0.27086 + 0.69254i$, $\theta_3 = 0.27086 - 0.69254i$, $\theta_4 = -0.65014 + 0.79124i$, $\theta_5 = -0.65014 - 0.79124i$, and the smallest and largest moduli of these roots are 0.57478 and 1.0241, respectively.

We now use Algorithm 1 to compute the first 7 lower bounds on zeros of $f(z)$:

k	b_k	$h_{5+k}(z)$	γ_k	r_k	L_k
0	1	$1 + 2z + 2z^2 + 4z^3 + 4z^4 + 3z^5$	2.	0.50000	0.25000
1	-2	$1 - 2z^2 - 4z^4 - 5z^5 - 6z^6$	1.4142	0.61803	0.43702
2	2	$1 + 4z^3 + 3z^5 + 2z^6 + 6z^7$	1.5874	0.68233	0.42984
3	-4	$1 - 8z^4 - 5z^5 - 14z^6 - 10z^7 - 12z^8$	1.6818	0.72449	0.43079
4	8	$1 + 11z^5 + 2z^6 + 22z^7 + 20z^8 + 24z^9$	1.6154	0.75488	0.46730
5	-11	$1 - 20z^6 - 24z^8 - 20z^9 - 33z^{10}$	1.6475	0.77809	0.47227
6	20	$1 + 40z^7 + 16z^8 + 60z^9 + 47z^{10} + 60z^{11}$	1.6938	0.79654	0.47027

As the above table shows, although the first few bounds are not monotonically improving, the trend is already set. As we explore higher order bounds, this trend toward convergence becomes very clear:

k	L_k	U_k	k	L_k	U_k	k	L_k	U_k
10	0.49680	1.2140	150	0.56178	1.0502	1000	0.57192	1.0295
50	0.54586	1.0838	200	0.56436	1.0449	4000	0.57389	1.0258
100	0.55717	1.0598	250	0.56602	1.0413	8000	0.57429	1.0249

Upper bounds for zeros of $f(z)$ given by the well-known formulas (i)–(viii) listed in Mignotte [6, Theorem 4.2, pp. 146–148] are (i) 4.3333, (ii) 2.3333, (iii, iv) 6.6667, (v) 2.6667, (vi) 1.6667, (vii) 1.3333, and (viii) 5.3985. The best bound is obtained by formula (vii), which only works for polynomials with positive real coefficients. The first 3 upper bounds in Kalantari's family are $U_0 = 2.6667, U_1 = 1.6759$, and $U_2 = 1.1774$. So in this particular instance, U_2 beats all the bounds in Theorem 4.2 of [6]. Moreover, Kalantari's bounds are applicable to all complex polynomials.

In general, the first members of Kalantari's family already exhibit superior performance as individual bounds. In an empirical study conducted by McNamee and Olhovsky [5], U_2 stands out as the best among a sample of upper bounds, outperforming 44 other bounds in the literature by a wide margin. However, the superiority of Kalantari's bounds are achieved at the price of high computational complexity.

A MAPLE program that implements Algorithm 1 and its upper bound counterpart is available online at `http://paul.rutgers.edu/~yjin/MAPLE/kbounds`.

3. Proof of convergence

In this section we shall prove the following result.

Theorem 3.1. *Let $\theta_1, \ldots, \theta_s$ be distinct zeros of $f(z)$ with multiplicities $d_1, \ldots, d_s$; then*

$$\lim_{k \to \infty} L_k = \min\{|\theta_1|, |\theta_2|, \ldots, |\theta_s|\}.$$

Remark 3.2. By symmetry, we also have

$$\lim_{k \to \infty} U_k = \max\{|\theta_1|, |\theta_2|, \ldots, |\theta_s|\}.$$

Thus, both the lower and upper bounds are asymptotically sharp.

Proof of Theorem 3.1. The key observation is that the sequence $\{b_i\}_{i=0}^{\infty}$ is generated by $\frac{1}{f(z)}$, i.e.,

$$\frac{1}{f(z)} = \frac{1}{a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0} = \sum_{i=0}^{\infty} b_i z^i.$$

To see this, note that (2.1) implies

(3.1a) $$a_0 b_0 = 1,$$

(3.1b) $$\sum_{j=0}^{i} a_j b_{i-j} = 0 \qquad \text{for } 1 \le i < n,$$

(3.1c) $$\sum_{j=0}^{n} a_j b_{i-j} = 0 \qquad \text{for } i \ge n,$$

so we have

$$f(z) \left(\sum_{i=0}^{\infty} b_i z^i \right) = \left(\sum_{i=0}^{n} a_i z^i \right) \left(\sum_{i=0}^{\infty} b_i z^i \right) = 1.$$

Remark 3.3. The above identity may be seen as the limiting case of (2.1) as k approaches infinity.

It is well known in the calculus of finite differences that

$$b_i = \sum_{j=1}^{s} P_j(i) \theta_j^{-i} \qquad \text{for } i \ge 0,$$

where

$$f(z) = a_0 + a_1 z + \cdots + a_{n-1} z^{n-1} + a_n z^n = a_0 \prod_{j=1}^{s} \left(1 - \theta_j^{-1} z \right)^{d_j},$$

and $P_j(x)$ is a polynomial of degree $d_j - 1$ (see Stanley [7, Theorem 4.1, p. 110]). This can be proved by expanding the rational function $\frac{1}{f(z)}$ into partial fractions, or by solving the linear homogeneous recurrence (3.1c).

Let $\rho_{\min} = \min\{|\theta_1|, |\theta_2|, \ldots, |\theta_s|\}$. First we bound b_i:

$$|b_i| \le \sum_{j=1}^{s} \left| P_j(i) \theta_j^{-i} \right| \le \sum_{j=1}^{s} |P_j(i)| \rho_{\min}^{-i} \le Q(i) \rho_{\min}^{-i},$$

where $Q(x)$ is a polynomial of degree $\max\{d_1, \ldots, d_s\} - 1$ with positive coefficients.

Next we bound $c_{k,i}$. We shall use the fact that $Q(x)$ is monotonically increasing when $x \geq 0$.

Let

$$\alpha = \max\{|a_0|, |a_1|, \ldots, |a_n|\} \quad \text{and} \quad \beta = \max\{1, \rho_{\min}^n\} \sum_{j=0}^{n-1} \rho_{\min}^j.$$

For $k \geq n, \ i = 1 + k, \ldots, n + k$, we have

$$|c_{k,i}| = \left| \sum_{j=i-n}^{k} a_{i-j} b_j \right| \leq \alpha Q(k) \sum_{j=i-n}^{k} \rho_{\min}^{-j} \leq \alpha Q(i) \rho_{\min}^{-i+(i-k)} \sum_{j=0}^{n-1} \rho_{\min}^j \leq \alpha \beta Q(i) \rho_{\min}^{-i}.$$

Thus,

$$\begin{aligned}
\gamma_k &= \max\left\{ |c_{k,i}|^{1/i} : \ i = 1 + k, \ldots, n + k \right\} \\
&\leq \max\left\{ [\alpha \beta Q(i)]^{1/i} : \ i = 1 + k, \ldots, n + k \right\} \rho_{\min}^{-1} = B_k.
\end{aligned}$$

On the other hand, $\gamma_k > r_k / \rho_{\min} = A_k$. It is easy to verify that

$$\lim_{i \to \infty} [\alpha \beta Q(i)]^{1/i} = 1 \qquad \text{and} \qquad \lim_{k \to \infty} r_k = 1.$$

So

$$\lim_{k \to \infty} A_k = \rho_{\min}^{-1} \qquad \text{and} \qquad \lim_{k \to \infty} B_k = \rho_{\min}^{-1}.$$

Since $A_k < \gamma_k \leq B_k$, we conclude that

$$\lim_{k \to \infty} \gamma_k = \rho_{\min}^{-1}.$$

Finally,

$$\lim_{k \to \infty} L_k = \lim_{k \to \infty} \frac{r_k}{\gamma_k} = \rho_{\min} = \min\{|\theta_1|, |\theta_2|, \ldots, |\theta_s|\}. \qquad \square$$

Remark 3.4. The linear recurrence (3.1c) with initial conditions (3.1a) and (3.1b) allows us to compute $b_0, b_1, \ldots, b_k$ directly. Together with identity (2.1), it gives rise to another efficient algorithm to compute $c_{k,i}, \ i = 1 + k, \ldots, n + k$:

Algorithm 2: Computing $c_{k,i}, \ i = 1 + k, \ldots, n + k$, in $O(kn)$ arithmetic operations using linear recurrence relation (3.1) and identity (2.1).

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input : $f(z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0, \ a_n \neq 0, a_0 = 1$ and k.
output: $c_{k,i}, \ i = 1 + k, \ldots, n + k$.

$b_0 = 1$;
for i *from* 1 *to* k **do**
  $b_i = -\sum_{j=1}^{\min\{n,i\}} a_j b_{i-j}$;
end
for i *from* $1 + k$ *to* $n + k$ **do**
  $c_{k,i} = \sum_{j=\max\{0, i-n\}}^{k} a_{i-j} b_j$;
end

Remark 3.5. While there are plenty of individual bounds on polynomial roots in the literature, families of such bounds are rare, and Kalantari's family is the only one we know of that is asymptotically sharp. For a bibliography on bounds of polynomial roots, see McNamee [4].

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