Error Bounds for Zeros of a Polynomial Based Upon Gerschgorin's Theorems

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ABSTRACT. Given N approximations to the zeros of an Nth-degree polynomial, N circular regions in the complex z-plane are determined whose union contains all the zeros, and each connected component of this union consisting of K such circular regions contains exactly K zeros. The bounds for the zeros provided by these circular regions are not excessively pessimistic; that is, whenever the approximations are sufficiently well separated and sufficiently close to the zeros of this polynomial, the radii of these circular regions are shown to overestimate the errors by at most a modest factor simply related to the configuration of the approximations. A few numerical examples are included.

KEY WORDS AND PHRASES: error bounds, polynomial zeros, Gerschgorin's theorems, a posteriori error analysis, approximate zeros

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1. *Introduction*

Suppose L distinct points $z_1, z_2, \cdots, z_L$ are given in the complex plane, and associated with each z_k is a positive integer M_k, the "multiplicity" of z_k; suppose $\sum_1^L M_k = N$. These points z_k, with their multiplicities M_k, are supposed to approximate the zeros $\xi_1, \xi_2, \cdots, \xi_N$ of a monic polynomial

$$P(z) \equiv z^N + \sum_{k=0}^{N-1} a_k z^k \equiv \prod_{k=1}^{N} (z - \xi_k)$$

of degree N with given coefficients $a_0, a_1, \cdots, a_{N-1}$. For example, we might assume that the set of zeros $\xi_1, \xi_2, \cdots, \xi_N$ can be partitioned into L disjoint subsets, with M_k zeros in the kth subset all close to z_k.

Our object is to determine how close the zeros of $P(z)$ are to the approximations z_k. Toward this goal we obtain circular regions containing all the zeros of $P(z)$ by applying Gerschgorin's theorems to a certain matrix R similar to the companion matrix of $P(z)$. The matrix R is dependent upon the polynomial and perhaps its derivatives at the points z_k. In case the points z_k are "sufficiently well separated" and "significantly close" to the zeros of $P(z)$, we bound the radii of these circular regions to show that the radius of the circle about z_k overestimates the absolute error of the approximation z_k by a factor near $M_k L$.

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2. *A Matrix R Similar to P(z)'s Companion Matrix C*

In this section we construct a certain $N \times N$ matrix R similar to the companion matrix

$$C \equiv \begin{pmatrix} 0 & & & & & -a_0 \\ 1 & 0 & & & & -a_1 \\ & 1 & \cdot & & & \cdot \\ & & \cdot & \cdot & & \cdot \\ & & & \cdot & \cdot & \cdot \\ & & & \cdot & 0 & -a_{N-2} \\ & & & & 1 & -a_{N-1} \end{pmatrix}$$

of the polynomial $P(z)$; the eigenvalues of C, and so of R, are the zeros of $P(z)$. In later sections we apply Gerschgorin's theorems (Taussky and Marcus [12]) to another matrix similar to R to obtain circular regions containing all the zeros of $P(z)$.

Let L distinct points z_k and L positive integers M_k be given such that $\sum_{k=1}^{L} M_k = N$. Then we have

LEMMA 1. *For each* $k = 1, 2, \cdots, L$ *and each* $j = 1, 2, \cdots, M_k$, *let*

$$(j-1)!p_{kj} \equiv \left(\frac{d}{dz}\right)^{j-1} P(z) \Big|_{z=z_k}$$

and

$$(M_k - j)!h_{kj} \equiv \left(\frac{d}{dz}\right)^{M_k-j} \prod_{i \neq k} (z - z_i)^{-M_i} \Big|_{z=z_k}.$$

In addition, let $\mathbf{p}^\tau$ *and* $\mathbf{h}^\tau$ *be the row vectors*

$$(p_{11}, p_{12}, \cdots, p_{1M_1}, p_{21}, \cdots, p_{LM_L}) \quad \text{and} \quad (h_{11}, h_{12}, \cdots, h_{1M_1}, h_{21}, \cdots, h_{LM_L}),$$

respectively, where the superscript τ *on a vector denotes the transpose of the vector. Then the companion matrix* C *is similar to the matrix*

$$R \equiv J - \mathbf{p}\mathbf{h}^\tau,$$

where

$$J \equiv \begin{pmatrix} J_1 & & & & \\ & J_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & J_L \end{pmatrix}_{N \times N} \quad \text{and} \quad J_k \equiv \begin{pmatrix} z_k & & & \\ 1 & z_k & & \\ & 1 & \cdot & \\ & & \cdot & \cdot \\ & & & 1 & z_k \end{pmatrix}_{M_k \times M_k}.$$

PROOF. We propose to demonstrate that $R = VCV^{-1}$, where V is the $N \times N$ confluent Vandermonde matrix (Aitken [2, p. 119]):

$$V \equiv \begin{pmatrix} 1 & z_1 & z_1^2 & \cdot & \cdot & \cdot & \cdot & z_1^{N-1} \\ 0 & 1 & 2z_1 & \cdot & \cdot & \cdot & \cdot & (N-1)z_1^{N-2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 1 & M_1 z_1 & \cdot & \cdot & \binom{N-1}{M_1-1} z_1^{N-M_1} \\ 1 & z_2 & z_2^2 & \cdot & \cdot & \cdot & \cdot & z_2^{N-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & 1 & M_L z_L & \cdot & \cdot & \binom{N-1}{M_L-1} z_L^{N-M_L} \end{pmatrix}.$$

For example, when $L = 2$, $z_1 = \alpha$, $M_1 = 3$, $z_2 = \beta$, $M_2 = 2$, and $N = 5$,

$$V \equiv \begin{bmatrix} 1 & \alpha & \alpha^2 & \alpha^3 & \alpha^4 \\ 0 & 1 & 2\alpha & 3\alpha^2 & 4\alpha^3 \\ 0 & 0 & 1 & 3\alpha & 6\alpha^2 \\ 1 & \beta & \beta^2 & \beta^3 & \beta^4 \\ 0 & 1 & 2\beta & 3\beta^2 & 4\beta^3 \end{bmatrix}.$$

First we can verify directly that

$$VC = JV - \mathbf{p}(0, 0, \cdots, 0, 1). \tag{1}$$

Next observe that the columns of V^{-1} are the coefficients of generalized Lagrange-Hermite interpolating polynomials and so, from the formulation of these polynomials given by Spitzbart [10], discover that the vector $\mathbf{h}^T$ is the final row of the inverse of V. Hence

$$RV = JV - \mathbf{p}(0, 0, \cdots, 0, 1). \tag{2}$$

Combining (1) and (2) shows that the matrix R is similar to the companion matrix C.

3. *Gerschgorin's Theorems and Circular Regions Containing the Zeros of* $P(z)$

For any $N \times N$ matrix $A \equiv (a_{ij})$, Gerschgorin's theorems applied to the columns of A say that all the eigenvalues of A lie in the union of the disks

$$|z - a_{kk}| \le \sum_{\substack{i=1 \\ i \ne k}}^{N} |a_{ik}|$$

in the complex z-plane, and that each connected component of this union consisting of K such disks contains exactly K eigenvalues of A. We apply this theorem to a matrix A diagonally similar to R.

THEOREM 1. *Let there be given L distinct points z_k approximating the zeros of $P(z)$, and associated with each z_k, a positive integer M_k representing the multiplicity of the approximation z_k; suppose $\sum_{k=1}^{L} M_k = N$. For $k = 1, 2, \cdots, L$ and $j = 1, 2, \cdots, M_k$, define the circles*

$$\Gamma_{kj}(e_k) : |z - z_k| \le \rho_{kj}(e_k) \equiv (1 - \delta_{jM_k})e_k + L\,|h_{kj}| \sum_{m=1}^{M_k} |p_{km}|\, e_k^{m-j},$$

where the e_k are arbitrary positive numbers, δ_{ij} is the Kronecker delta, and p_{kj} and h_{kj} are defined in Lemma 1. Then the union of the N circular regions $\Gamma_{kj}(e_k)$ contains all the zeros of $P(z)$. Any connected component of this union consisting of just K circles $\Gamma_{kj}(e_k)$ contains exactly K zeros of $P(z)$.

PROOF. Apply Gerschgorin's theorems to the columns of the matrix $E^{-1}RE$, where E is a block diagonal matrix with L blocks

$$E_k \equiv \pi_k \operatorname{diag}\,(e_k^{M_k-1}, e_k^{M_k-2}, \cdots, e_k, 1)$$

and

$$\pi_k \equiv \begin{cases} 1 & \text{if all } p_{kj} = 0 \text{ for } j = 1, 2, \cdots, M_k, \\ \sum_{m=1}^{M_k} |p_{km}|\, e_k^{m-M_k} & \text{otherwise.} \end{cases}$$

For the kth block, the jth Gerschgorin disk is

$$|z - z_k + p_{kj}h_{kj}| \le (1 - \delta_{jM_k})e_k + (L - \kappa)|h_{kj}| \sum_{m=1}^{M_k} |p_{km}| e_k^{m-j} - |p_{kj}h_{kj}|,$$

where κ is the number of values of k for which all $p_{kj} = 0$, $j = 1, 2, \cdots, M_k$. Now notice that this jth disk of the kth block is contained in $\Gamma_{kj}(e_k)$. This completes the proof of Theorem 1.

We state the special case $L = N$ of Theorem 1 as a corollary.

COROLLARY 1. *Suppose N distinct points $z_1, z_2, \cdots, z_N$ are given. Define*

$$\Gamma_{k1}: |z - z_k| \le N|P(z_k)| / \prod_{\substack{i=1 \\ i \ne k}}^{N} |z_i - z_k|.$$

Then the union of the circular regions Γ_{k1} contains all the zeros of $P(z)$. Any connected component of this consisting of just K circles Γ_{k1} contains exactly K zeros of $P(z)$.

We point out here that the N regions Γ_{k1} of Corollary 1 can be readily computed. To be more specific, if the N points z_k are distinct but otherwise arbitrary complex numbers, $N(2N - 1)$ complex multiplications, $N(3N - 1)/2$ complex additions, $2N$ complex absolute values, and $2N$ real multiplications or divisions are required to compute the N regions of Corollary 1.

Our problem now is to find an e_k which minimizes

$$R_k(e_k) \equiv \max_{1 \le j \le M_k} \rho_{kj}(e_k).$$

But before proceeding with the general case, we dispose of two special cases; first, when $p_{kj} = 0$ for $j = 1, 2, \cdots, M_k$, and second, when $M_k = 1$. When all the p_{kj} are zero, z_k is a zero of the polynomial of multiplicity M_k, and hence there is no need to consider $R_k(e_k)$. When $M_k = 1$, $R_k(e_k) = L|p_{k1}h_{k1}|$ is independent of e_k.

Hence, assume that $M_k > 1$ and at least one of the $p_{kj} \ne 0$ for $j = 1, 2, \cdots, M_k$. The functions $\rho_{kj}(e_k)$ are all convex over $(0, \infty)$. In addition, $\rho_{k1}(e_k)$ increases monotonically from $L|p_{k1}h_{k1}|$ to infinity over $(0, \infty)$ and $\rho_{kM_k}(e_k)$ decreases to $L|p_{kM_k}h_{kM_k}|$ over $(0, \infty)$. Hence the function $R_k(e_k)$ is convex. If all p_{kj} are zero except p_{kM_k} then $R_k(e_k) = L|h_{kM_k}p_{kM_k}|$. Otherwise $R_k(e_k)$ attains its minimum value at just one point, say at $e_k = e_k^*$. This e_k^* is the abscissa of a point where either two of the graphs $y = \rho_{kj}(e_k)$ intersect with slopes of opposite signs, or one of the graphs $y = \rho_{kj}(e_k)$ attains its minimum.

In case $M_k = 2$, this point e_k^* can be computed easily since e_k^* is the root of the simple equation $\rho_{k1}(e_k) = \rho_{k2}(e_k)$. However, for $M_k > 2$, the determination of e_k^* is costly. It will turn out that whenever the root g_k of the equation in g,

$$g^{M_k} = L|h_{kM_k}| \sum_{m=1}^{M_k} |p_{km}| g^{m-1}, \tag{3}$$

is small compared to the separation $\min_{i \ne k} |z_k - z_i|$ (which is the situation that we are most interested in), then the root will be a good approximation to e_k^*. For this choice of e_k, the radii $\rho_{kj}(e_k)$ are

$$\rho_{kj}(g_k) = g_k((1 - \delta_{jM_k}) + |h_{kj}/h_{kM_k}| g_k^{M_k - j}). \tag{4}$$

The proof of our next theorem shows more precisely when g_k is a good approximation to e_k^*.

When $M_k > 2$, we can determine iteratively an upper bound for the positive root of the polynomial eq. (3) by applying the Newton-Raphson method to the reciprocal polynomial of (3) computing its only real zero $1/g_k$. The Newton-Raphson iteration will converge to this zero $1/g_k$ provided only that the initial iterate is positive.

The calculation of g_k is considerably cheaper than the calculation of e_k^* since the calculation of e_k^* requires the solutions to at least one and perhaps several equations like (3). In addition, when we have good well-separated approximations to the zeros of $P(z)$, the advantage of the best value e_k^* over the estimate g_k of e_k^* is negligible. Hence, for most applications of Theorem 1, we believe that it is worthwhile to use g_k in place of e_k^*.

We comment here that if the points z_k are distinct but otherwise arbitrary complex numbers, we can compute each h_{kj} for $M_k > 1$ in fewer than N long complex operations ($\times$ or $/$) and N short complex operations ($+$ or $-$). To illustrate this point, we use the results of Burnside and Panton [4], who express the coefficients of a power series, representing the reciprocal of a polynomial, in terms of sums of powers of the polynomial's zeros. Since the quantities h_{kj} are derivatives of the reciprocal of the polynomial $\prod_{m=1;m\neq k}^{L} (z - z_m)^{M_m}$ evaluated at $z = z_k$, then we have from the results of Burnside and Panton [4], for $j = M_k - 1, M_k - 2, \cdots, 2, 1$,

$$h_{kj} = (M_k - j)^{-1} \sum_{m=j+1}^{M_k} S_{k,m-j} h_{km}, \tag{5}$$

where

$$S_{kj} \equiv \sum_{\substack{m=1\\ m\neq k}}^{L} \frac{M_m}{(z_m - z_k)^j} \quad \text{and} \quad h_{kM_k} \equiv \prod_{\substack{m=1\\ m\neq k}}^{L} (z_k - z_m)^{-M_m}.$$

Some experiments have been performed with the above techniques for computing the h_{kj}'s. So far, these techniques have not displayed numerical instability.

4. *Upper Bounds for the Radii of the Circular Regions of Theorem* 1

We now apply Theorem 1 to an Nth-degree polynomial $P(z)$ using L well-separated approximations $z_1, z_2, \cdots, z_L$ close to the zeros of $P(z)$. Our goal is to show that the regions $\Gamma_{kj}(g_k)$ of Theorem 1 are small and overestimate the error of the approximation z_k by at most a factor near $M_k L$, where M_k is the "multiplicity" of the kth approximation. Under certain circumstances it is shown that, if the radii of the regions of Theorem 1 about z_k are reduced by more than this factor near $M_k L$, these smaller circular regions are certain to contain fewer than M_k zeros of $P(z)$.

Before stating these results, let us define the expression "close well-separated approximation."

Let the zeros of the Nth-degree polynomial be grouped into L clusters such that for each k, the point z_k approximates the M_k zeros $\xi_{k1}, \xi_{k2}, \cdots, \xi_{kM_k}$ of the kth cluster. Suppose $\sum_{k=1}^{L} M_k = N$. Define for each $k = 1, 2, \cdots, L$,

$$\Theta_k \equiv \max_j |z_k - \xi_{kj}|, \quad \Delta_k \equiv \min_{i\neq k} |z_k - z_i|, \quad \Psi_k \equiv \Theta_k/\Delta_k, \quad \Phi_k \equiv \max_{i\neq k} \Theta_i/|z_k - z_i|.$$

Clearly the point z_k is close to a cluster of M_k zeros of $P(z)$ when Θ_k is small, and is well separated when Δ_k is large. Hence to the extent that Ψ_k is small, z_k is a close well-separated approximation. Also, to the extent that Φ_k is small, the remaining points

$z_1, z_2, \cdots, z_{k-1}, z_{k+1}, z_{k+2}, \cdots, z_L$ are close approximations well separated from the point z_k but not necessarily separated from each other.

We now give upper bounds for the radii of the regions $\Gamma_{kj}(g_k)$, $k = 1, 2, \cdots, M_k$ in terms of these measures Θ_k, Ψ_k, and Φ_k of close well-separated approximations.

LEMMA 2. *For any* k, *the radii* $\rho_{kj}(g_k)$ *of the circular regions* $\Gamma_{kj}(g_k)$ *for* $j = 1, 2, \cdots, M_k$ *cannot exceed*

$$\begin{cases} \lambda_k \max\limits_{1\le j\le M_k} \left((1-\delta_{jM_k}) + \binom{N-j-1}{M_k-j}\left(\frac{\lambda_k}{\Delta_k}\right)^{M_k-j}\right) & \text{for } M_k < N, \\ \lambda_k & \text{for } M_k = N, \end{cases}$$

where

$$\lambda_k \equiv \Theta_k/[\{1 + (N-M_k)\Psi_k\}\{(1+L^{-1} \times \{1+(N-M_k)\Psi_k\}^{-M_k}\{1+\Phi_k\}^{M_k-N})^{1/M_k} - 1\}]$$

and g_k *is the positive root of eq.* (3).

PROOF. Without loss of generality, assume $k = 1$. First we obtain upper bounds for $|h_{1M_1}p_{1j}|$, $j = 1, 2, \cdots, M_1$. Consider the product representation of both p_{11} and h_{1M_1}, namely

$$p_{11} \equiv \prod_{i=1}^{L}\prod_{m=1}^{M_i}(z_1 - \xi_{im}) \quad \text{and} \quad h_{1M_1} \equiv \sum_{i=2}^{L}\sum_{m=1}^{M_i}(z_1 - z_i)^{-1}.$$

Using the triangle inequality, an upper bound for the factor $(z_1 - \xi_{im})$ in p_{11} is $|z_1 - z_i| + \Theta_i$. Each factor $(z_1 - \xi_{im})$ for $i \ge 2$ in p_{11} has a corresponding factor $(z_1 - z_i)^{-1}$ in h_{1M_1}. Since $\Theta_i/|z_1 - z_i| \le \Phi_1$, we have $|h_{1M_1}p_{11}| \le \Theta_1^{M_1}(1+\Phi_1)^{N-M_1}$. To obtain upper bounds for $|h_{1M_1}p_{1j}|$ for $j \ge 2$, we differentiate the product representation of p_{11} with respect to z_1 and use the triangle inequality upon each factor $(z_1 - \xi_{im})$ as above. Hence terms in p_{1j} of the form $(z_1 - \xi_{im})$ for $i \ge 2$ can be bounded by $|z_1 - z_i|(1 + \Phi_1)$. Finally, each time an expression in p_{11} such as $(z_1 - \xi_{im})$ for $i \ge 2$ is differentiated, one of the factors $(z_1 - z_i)^{-1}$ in h_{1M_1} will not match with its corresponding expression $(z_1 - \xi_{im})$ in p_{1j}, and so $|z_1 - z_i|^{-1}$ is replaced by its upper bound Δ_1^{-1}. Combining the above steps, we see that the expression

$$\frac{1}{(j-1)!}\left(\frac{d}{dx}\right)^{j-1}(\Theta_1 + x)^{M_1}\left(1 + \Phi_1 + \frac{x}{\Delta_1}\right)^{N-M_1}\Bigg|_{x=0}$$

is an upper bound for $|h_{1M_1}p_{1j}|$. Applying Leibniz's rule for the $(j-1)$-th derivative of a product of two functions, we obtain

$$|h_{1M_1}p_{1j}| \le \binom{M_1}{j-1}\Theta_1^{M_1+1-j}\sum_{m=0}^{j-1}\binom{j-1}{m}\left(\frac{\Theta_1}{\Delta_1}\right)^m \cdot (1+\Phi_1)^{N-M_1-m}\prod_{i=0}^{m-1}\left(\frac{N-M_1-i}{M_1-j+2+i}\right).$$

But

$$\Theta_1/\Delta_1 \equiv \Psi_1, \qquad \prod_{i=0}^{m-1}\left(\frac{N-M_1-i}{M_1-j+2+i}\right) \le (N-M_1)^m$$

and

$$\sum_{m=0}^{j-1} \binom{j-1}{m} \left((N - M_1) \frac{\Theta_1}{\Delta_1} \right)^m = (1 + (N - M_1)\Psi_1)^{j-1}.$$

Hence

$$| h_{1M_1} p_{1j} | \le \binom{M_1}{j-1} \Theta_1^{M_1+1-j} (1 + \Phi_1)^{N-M_1} (1 + (N - M_1)\Psi_1)^{j-1}. \quad (6)$$

Now we bound the ratio $| h_{1j}/h_{1M_1} |$. First assume $M_k < N$. From the definition of h_{kj} in Lemma 1, this ratio $| h_{1j}/h_{1M_1} |$ involves sums of products of $(z_1 - z_i)^{-1}$, $i = 2, 3, \cdots, L$. Since an upper bound for the reciprocals $| z_1 - z_i |^{-1}$ is Δ_1^{-1}, an upper bound for $| h_{1j}/h_{1M_1} |$ is $\binom{N-j-1}{M_1-j} \Delta_1^{j-M_1}$. Now when $M_k = N$, $h_{1j} = \delta_{jM_1}$. Hence

$$\left| \frac{h_{1j}}{h_{1M_1}} \right| \le \begin{cases} \binom{N-j-1}{M_1-j} \Delta_1^{j-M_1} & \text{for } M_1 < N, \\ \delta_{jM_1} & \text{for } M_1 = N. \end{cases} \quad (7)$$

Now we are ready to place upper bounds on the radii $\rho_{1j}(g_1)$, where g_1 is the root of eq. (3). From eq. (4) using the upper bound (7) for $| h_{1j}/h_{1M_1} |$, the radii $\rho_{1j}(g_1)$ are bounded above by

$$\rho_{1j}(g_1) \le \begin{cases} g_1 \left(1 - \delta_{jM_1} + \binom{N-j-1}{M_1-j} \left(\frac{g_1}{\Delta_1} \right)^{M_1-j} \right) & \text{for } M_1 < N, \\ g_1 & \text{for } M_1 = N. \end{cases}$$

Now an upper bound for g_1 is the positive root of the equation

$$g^{M_1} = L(1 + \Phi_1)^{N-M_1} \Theta_1^{M_1} \sum_{m=1}^{M_1} \binom{M_1}{m-1} (1 + (N - M_1)\Psi_1)^{m-1} \left(\frac{g}{\Theta_1} \right)^{m-1}, \quad (8)$$

which is derived from eq. (3) by substituting the upper bounds (6) for the terms $| h_{1M_1} p_{1m} |$, $m = 1, 2, \cdots, M_1$.

Using the identity in x,

$$\sum_{m=1}^{M_1} \binom{M_1}{m-1} x^{m-1} = (1 + x)^{M_1} - x^{M_1}$$

with

$$x = \left(\frac{g}{\Theta_1} \right) (1 + (N - M_1)\Psi_1),$$

it can be verified that λ_1 is the positive root of eq. (8). Hence the radii $\rho_{1j}(g_1)$ are bounded above by

$$\rho_{1j}(g_1) \le \begin{cases} \lambda_1 \left(1 - \delta_{jM_1} + \binom{N-j-1}{M_1-j} \left(\frac{\lambda_1}{\Delta_1} \right)^{M_1-j} \right) & \text{for } M_1 < N, \\ \lambda_1 & \text{for } M_1 = N. \end{cases}$$

This completes the proof of Lemma 2.

Using Lemma 2, we now analyze the behavior of Theorem 1's regions as the parameters Θ_k and Φ_k decrease to zero.

As we expect, the regions $\Gamma_{kj}(g_k)$, $j = 1, 2, \cdots, M_k$ become small as Θ_k becomes small. In addition, when Ψ_k and Φ_k are small, $\rho_{kj}(g_k)$ is approximately

$$\frac{\Theta_k}{(1 + (1/L))^{1/M_k} - 1}.$$

In order to obtain this linear variation of $\rho_{kj}(g_k)$ with the error Θ_k, we must restrict the sizes of Ψ_k and Φ_k as follows:

$$\begin{array}{ll} \text{for } M_k = 1, & \Phi_k \ll (N-1)^{-1}, \\ \text{for } 1 < M_k < N, & \Phi_k \ll (N - M_k)^{-1} \text{ and} \\ & \Psi_k \ll \log_e (1 + (1/L))^L/(LM_k(N - M_k)), \\ \text{for } M_k = N, & \text{no restriction on } \Psi_k \text{ or } \Phi_k \text{ is necessary.} \end{array}$$

Notice that, in order to obtain small radii $\rho_{kj}(g_k)$, we seem to require a more accurate approximation z_k when $M_k > 1$ than when $M_k = 1$.

Finally, Lemma 2 gives the following theorem which indicates by how much the radii $\rho_{kj}(g_k)$ can overestimate the error Θ_k when none of the regions $\Gamma_{kj}(g_k)$ intersects the regions $\Gamma_{ij}(g_i)$, $i \neq k$.

THEOREM 2. *Suppose none of the regions* $\Gamma_{kj}(g_k)$, $j = 1, 2, \cdots, M_k$, *about* z_k *intersects the regions* $\Gamma_{ij}(g_i)$, $j = 1, 2, \cdots, M_i$ *for* $i \neq k$. *Define for each* $i = 1, 2, \cdots, L$,

$$\tilde{\Theta}_i \equiv \max \{|z - z_i| \mid z \in \textit{connected component of } \bigcup_{m,n} \Gamma_{mn}(g_m) \textit{ containing } z_i\},$$

$$\tilde{\Psi}_k \equiv \tilde{\Theta}_k/\Delta_k,$$

$$\tilde{\Phi}_k \equiv \max_{i \neq k} (\tilde{\Theta}_i/|z_k - z_i|),$$

$$\tilde{\lambda}_k \equiv \tilde{\Theta}_k \Big/ \left[\left(1 + \frac{(1 + \tilde{\Phi}_k)^{M_k - N}}{L(1 + (N - M_k)\tilde{\Psi}_k)^{M_k}}\right)^{1/M_k} - 1\right],$$

and

$$f_k \equiv \tilde{\Theta}_k \Big/ \tilde{\lambda}_k \max_{1 \le j \le M_k} \left(1 - \delta_{jM_k} + \binom{N - j - 1}{M_k - j}\left(\frac{\tilde{\lambda}_k}{\Delta_k}\right)^{M_k - j}\right).$$

Then at least one zero of $P(z)$ *lies in the annular region*

$$f_k \max_j \rho_{kj}(g_k) \le |z - z_k| \le \max_j \rho_{kj}(g_k).$$

PROOF. Clearly $\tilde{\Psi}_k$ and $\tilde{\Phi}_k$ are upper bounds for Ψ_k and Φ_k respectively. Hence $f_k \max_j \rho_{kj}(g_k)$ is a lower bound for Θ_k and so the annular region

$$f_k \max_j \rho_{kj}(g_k) \le |z - z_k| \le \max_j \rho_{kj}(g_k)$$

contains at least one zero of $P(z)$. This completes the proof of Theorem 2.

Notice for small $\tilde{\Psi}_k$ and $\tilde{\Phi}_k$, this factor f_k^{-1} is approximately $((1 + 1/L)^{1/M_k} - 1)^{-1}$, which is less than $LM_k/\log_e (1 + (1/L))^L$. Hence, if the radii of the regions $\Gamma_{kj}(g_k)$, $j = 1, 2, \cdots, M_k$ are reduced by a factor near LM_k for small $\tilde{\Psi}_k$ and $\tilde{\Phi}_k$, these smaller regions are certain to contain fewer than M_k zeros of $P(z)$.

In case an approximation z_k is close to a cluster of M_k zeros of the polynomial and well separated from the remaining approximations, we can prove that circular regions about z_k, smaller than those of Theorem 1 by a factor at most L and often near L, contain exactly M_k zeros of $P(z)$. These results appear elsewhere (Smith [9]).

We comment here that Cauchy's theorem (Marden [7, Th. 27.1]) concerning a circular region about the origin containing all the zeros of a polynomial is the special case $L = 1$, $M_1 = N$, and $z_1 = 0$ of Theorem 1. In addition, the lower bound for the zero of largest magnitude given by Birkoff [3] is the lower bound of Theorem 2 for the special case $L = 1$, $M_1 = N$, and $z_1 = 0$.

5. *Theorems* 1 *and* 2 *Applied to a Class of Polynomials*

In most applications, we need to locate the zeros of a polynomial for which the value of the polynomial and its derivatives at the points z_k are not primary data but are computed from some representation of the polynomial, involving primary data, in the presence of rounding errors. As a result, we often have only upper and lower bounds for the magnitudes of the polynomial and its derivatives; namely, for $k = 1, 2, \cdots, L$ and $j = 1, 2, \cdots, M_k$,

$$0 \le \mathbf{p}_{kj} \le \left| \left(\frac{d}{dz_k}\right)^{j-1} \frac{P(z_k)}{(j-1)!} \right| \le \bar{p}_{kj} .$$

(Such upper and lower bounds can be computed using Kahan's error analysis (Smith [8] or Adams [1]) or interval arithmetic). Hence, in order to locate the zeros of a particular polynomial $P(z)$, we must locate the zeros of all polynomials in a class $\mathcal{P}$ of polynomials of which $P(z)$ is a member.

We now restate the special case $e_k = g_k$ of Theorem 1 and Theorem 2 for a class $\mathcal{P}$ of polynomials.

THEOREM 1′. *Given the class $\mathcal{P}$ of polynomials*

$$\mathcal{P} \equiv \left\{ Q(z) \mid \mathbf{p}_{kj} \le \left| \left(\frac{d}{dz_k}\right)^{j-1} \frac{Q(z_k)}{(j-1)!} \right| \le \bar{p}_{kj} \quad \text{for } k = 1, 2, \cdots, L \text{ and } j = 1, 2, \cdots, M_k \right\},$$

let $\bar{g}_k$ be the root of eq. (3) *for which all the p_{kj} are replaced by $\bar{p}_{kj}$. Then the union of the N regions $\Gamma_{kj}(\bar{g}_k)$ contains the zeros of each polynomial in $\mathcal{P}$. Any connected component of this union consisting of just K circles $\Gamma_{kj}(\bar{g}_k)$ contains exactly K zeros of each polynomial in $\mathcal{P}$.*

PROOF. We need only note that g_k is an increasing function of each p_{kj} and $\rho_{kj}(g_k)$ is an increasing function of g_k.

THEOREM 2′. *Given the same class $\mathcal{P}$ of polynomials as above, let $\mathbf{g}_k$ be the root of eq.* (3) *with all the p_{kj} replaced by $\mathbf{p}_{kj}$, and let $\mathbf{f}_k$ be the f_k defined in Theorem 2 but computed from $\Gamma_{kj}(\bar{g}_k)$. Suppose none of the regions $\Gamma_{kj}(\bar{g}_k)$, $j = 1, 2, \cdots, M_k$ about z_k intersects the regions $\Gamma_{ij}(\bar{g}_i)$, $j = 1, 2, \cdots, M_i$ for $i \ne k$. Then at least one zero of each polynomial in $\mathcal{P}$ lies in the annular region*

$$\mathbf{f}_k \max_j \rho_{kj}(\mathbf{g}_k) \le |z - z_k| \le \max_j \rho_{kj}(\bar{g}_k).$$

PROOF. We need only note that f_k is a decreasing function of the radii $\rho_{kj}(g_k)$.

Theorems 1′ and 2′ show us how to apply and interpret our theorems in case of imprecise data. However, there is one other important interpretation of Theorem 2 which we give below.

Suppose Theorem 2′ is applicable about a point z_k to a class $\mathcal{P}$ of polynomials where for all k and j, $\mathbf{p}_{kj} = 0$. Then there exists a smallest region $\mathfrak{M}$ containing z_k and at the same time M_k zeros of every polynomial in $\mathcal{P}$. Now Theorem 2′ says that the largest circular region $\Gamma_{kj}(\bar{g}_k)$, $j = 1, 2, \cdots, M_k$ of Theorem 1′ centered at z_k is at most a factor $1/f_k \approx LM_k$ larger than the smallest possible circle centered at z_k containing $\mathfrak{M}$.

6. *Distinct Approximations* ($M_k = 1$) *Versus Confluent Approximations* ($M_k > 1$) *for a Multiple Zero*

Zero-finding algorithms such as ZERPOL (Smith [8]) usually give distinct approximations to the multiple zeros of a polynomial. The natural question is: If the distinct approximations to a multiple zero are replaced by a confluent approximation, say the average of the distinct approximations (Daniels [5]), will the union of the regions of Theorem 1 centered at this confluent approximation be smaller than the union of the regions of Theorem 1 centered at the distinct approximations to that multiple zero? A brief analysis of this question is impeded, first, by the uncertain effect of rounding errors when computing the polynomial and its derivatives, and second, by the unknown distribution of the distinct approximations given by the zero-finding algorithm. Hence, we leave the analysis of this question to our thesis (Smith [9]) and only summarize our experimental results below for this paper.

For these experiments, we use the subroutine ZERPOL to find the distinct approximations to the multiple zeros and use Kahan's error analysis (Smith [8] or Adams [1]) for the evaluation of a polynomial in order to obtain upper bounds for the magnitudes of a polynomial and its derivatives.

From our experiments, we find that the size of the regions $\Gamma_{kj}(g_k)$ obtained from the distinct approximations is very sensitive to the distribution of the distinct approximations and to the upper bound for the rounding errors which accumulate when computing the polynomial and its derivatives. On the other hand, the size of the regions $\Gamma_{kj}(g_k)$ obtained from this confluent approximation (that is, the average of the distinct approximations) is not nearly as sensitive to the distribution of the distinct approximations or to the upper bound for the rounding errors. In addition, the union of the regions $\Gamma_{kj}(g_k)$ obtained from the distinct approximations is, in all our experiments, larger than the union of the regions obtained from this confluent approximation.

A careful count of the number of arithmetic operations required to compute the h_{kj} using (5) and p_{kj} using Horner's scheme shows that $N^2 + (N - L)(L - 3) + L(L - 1)/2$ complex additions and subtractions, and $N^2 + (L - 1)(2N - L) + L$ complex multiplications and divisions, are required. Hence the number of operations required to compute the p_{kj} and h_{kj} for confluent approximations is less than the number of operations to compute the p_{kj} and h_{kj} for distinct approximations. However, to compute the regions of Theorem 1 for confluent approximations, we must determine upper bounds for the roots of eqs. (3) for $k = 1, 2, \cdots, L$. The computation of such upper bounds for the roots of these equations using Newton's method requires approximately $2N(n + 2)$ real multiplications and divisions and $2N(n + 2)$

real additions and subtractions, assuming n Newton iterations are required to solve each eq. (3). Thus, overall, the computations of the regions using confluent approximations cost slightly more than the computations for the regions using distinct approximations.

7. *Numerical Examples*

Before examining the numerical examples in Tables I and II, we explain in detail how the results are obtained. Our polynomial zero-finding routine ZERPOL (Programmer's Reference Manual [11] or Smith [8]) determines approximations with 27 binary bits in the fractional part to the zeros of our example polynomials. These approximations are expanded to 16 decimal digits and rounded to the number of places given in the tables. The discrepancy between an approximation accurate to 16 digits and the corresponding approximation given in the tables is added to the radii of Theorem 1 and the sum, rounded upward to 3 digits, appears in Table II under the column headed "Radii of Theorem 1."

The values of the polynomial and its derivatives at the approximations are computed using double precision arithmetic on the IBM 7094-II. We use Kahan's error analysis (Adams [1] or Smith [8]) to ensure that upper bounds for the magnitudes of the polynomial and its derivatives at the approximations are obtained. These upper bounds are used to compute the radii of Theorem 1, which implies that the radii of Theorem 1 displayed in the tables give regions containing the zeros of all polynomials in a certain class $\mathcal{P}$ (see Section 5) for which the polynomial given in the left column of the tables is a member.

Finally we remark here that a dagger (†) beside a radius indicates that the $\bar{p}_{kj}$'s used to compute the particular radii are dominated by rounding errors. In terms of the class $\mathcal{P}$, this implies that $\mathbf{p}_{kj}$'s equal zero.

Now we briefly comment on the results in Table I, which display the radii of Theorem 1 for a few polynomials taken from Henrici and Watkins [6].

The first polynomial illustrates the use of Theorem 1 when the approximations are reasonably well separated. As Theorem 2 indicates, the radii of the regions Γ_{k1} are approximately four times larger than the errors $|z_k - \xi_{k1}|$.

The second and third polynomials have multiple zeros. These polynomials show that in some cases the regions of Theorem 1 obtained from distinct approximations to multiple zeros do not overestimate excessively the errors $|z_k - \xi_{kj}|$. Notice that the region Γ_{31} for the third polynomial does not contain any zeros of this polynomial and yet as Theorem 2 states, the union of the regions Γ_{11}, Γ_{21}, Γ_{31} contains all the zeros of this polynomial.

The union of the regions $\Gamma_{kj}(g_k)$ for the fourth polynomial does not contain the zeros for this polynomial given by Henrici and Watkins nor the zeros given in the correction to their paper by Thomas [13]. The zeros given by Thomas are the exact zeros of the fifth polynomial which differs from the fourth polynomial at the coefficient a_5.

The large differences in the bounds between the fourth and fifth polynomial seem startling since the polynomials only differ by two units in the last place of the coefficient a_5. However, notice that the approximations of the fifth polynomial for which the bounds are vastly different in magnitude are the exact zeros of that polynomial. Hence the bounds for these approximations are small but not zero because

TABLE I. CIRCULAR REGIONS OF THEOREM 1 FOR SEVERAL POLYNOMIALS TAKEN FROM HENRICI AND WATKINS [6]

Polynomial $p(z) = \sum_{k=0}^{N} a_k z^k$		Exact zeros	*Approximations* z_k		Radii of Theorem 1
k	a_k		Real part	Imaginary part	
0	105105				
1	310205	−1.05	−1.0500001610	0.000000000000	$0.644_{10} - 6$
2	410100	−1	−0.9999998510	0.000000000000	$0.597_{10} - 6$
3	305000	$-0.5 + \sqrt{-0.751}$	−0.5000000000	0.866602562368	$0.255_{10} - 8$
4	100000	$-0.5 - \sqrt{-0.751}$	−0.5000000000	−0.866602562368	$0.255_{10} - 8$
0	18				
1	21	−3	−2.9999999702	$0.37000597_{10} - 3$	$0.556_{10} - 3$
2	8	−3	−2.9999999702	$-0.37000597_{10} - 3$	$0.556_{10} - 3$
3	1	−2	−2.0000000000	0.000000000000	†$0.167_{10} - 12$
0	100006				
1	300012	−1.00006	−1.0001358000	0.000000000000	$0.150_{10} - 3$
2	300006	−1	−0.9999177000	0.000000000000	$0.150_{10} - 3$
3	100000	−1	−1.0000065000	0.000000000000	†$0.175_{10} - 5$
0	−198000000				
1	−364800000		30.0000000000	0.000000000000	$0.104_{10} - 7$
2	−197170000		−10.0000000000	10.000000000000	$0.174_{10} - 6$
3	−37313000		−10.0000000000	−10.000000000000	$0.174_{10} - 6$
4	−53510400		−5.0000001790	0.000000000000	$0.185_{10} - 6$
5	−88653098		−1.0000000000	1.000000000000	$0.416_{10} - 7$
6	−50761800		−1.0000000000	−1.000000000000	$0.416_{10} - 7$
7	−9133400		−1.0000000000	1.095445156000	$0.508_{10} - 7$
8	−460800		−1.0000000000	−1.095445156000	$0.508_{10} - 7$
9	−2500		−1.4999998510	0.000000000000	$0.314_{10} - 7$
10	1000		−1.0000000300	0.000000000000	$0.119_{10} - 8$
0	−198000000				
1	−364800000	30	30.0000000000	0.000000000000	†$0.334_{10} - 12$
2	−197170000	$-10 + \sqrt{-100}$	−10.0000000000	10.000000000000	†$0.830_{10} - 12$
3	−37313000	$-10 - \sqrt{-100}$	−10.0000000000	−10.000000000000	†$0.830_{10} - 12$
4	−53510400	−5	−5.0000000000	0.000000000000	†$0.291_{10} - 12$
5	−88653100	$-1 + \sqrt{-1}$	−1.0000000000	1.000000000000	†$0.681_{10} - 13$
6	−50761800	$-1 - \sqrt{-1}$	−1.0000000000	−1.000000000000	†$0.681_{10} - 13$
7	−9133400	$-1 + \sqrt{-1.2}$	−1.0000000000	1.095445111400	$0.362_{10} - 7$
8	−460800	$-1 - \sqrt{-1.2}$	−1.0000000000	−1.095445111400	$0.362_{10} - 7$
9	−2500	−1.5	−1.5000000000	0.000000000000	†$0.168_{10} - 12$
10	1000	−1	−1.0000000000	0.000000000000	†$0.825_{10} - 13$

† The magnitude of p_{k1} is dominated by Kahan's upper bound for the rounding errors.

of rounding errors. On the other hand, the approximations given for the zeros of the fourth polynomial are not the exact zeros but only approximations which agree with the exact zeros to 7 or 8 digits.

Table II demonstrates how the regions of Theorem 1 can vary when we replace the distinct approximations to a cluster of zeros with the average of the distinct approximations to that cluster. For the confluent approximations in this table, we give only the radii of the largest region centered at the confluent approximation.

TABLE II. Distinct Approximations Versus Confluent Approximations to Clusters of Zeros

Polynomial	k	*Distant approximations*		*Radii of Theorem* 1, *distinct approximations*	k	*Confluent approximations*		*Radii of Theorem* 1, *confluent approximations*
		Real part	*Imaginary part*			*Approximations*	M_k	
$(z-1)^4(z-2)^2(z-3)$	1	1.00042820	0.000000000	†$0.445_{10}-2$	1	1.000000015	4	††$0.842_{10}-3$
	2	0.99999990	$0.42807_{10}-3$	†$0.794_{10}-2$				
	3	0.99999990	$-0.42807_{10}-3$	†$0.794_{10}-2$				
	4	0.99957200	0.000000000	†$0.431_{10}-2$				
	5	1.99999980	0.000000000	†$0.780_{10}-4$	2	1.999999985	2	††$0.337_{10}-5$
	6	2.00000010	0.000000000	†$0.794_{10}-4$				
	7	3.00000000	0.000000000	†$0.933_{10}-11$	3	3.000000000	1	†$0.400_{10}-11$
$(z-1)(z-2)^2(z-3)^4$	1	1.00000000	0.000000000	†$0.112_{10}-11$	1	1.000000000	1	†$0.480_{10}-12$
	2	2.00000130	0.000000000	†$0.491_{10}-4$	2	2.000000000	2	†$0.707_{10}-5$
	3	1.99999870	0.000000000	†$0.504_{10}-4$				
	4	2.99894860	0.000000000	†$0.560_{10}-1$	3	3.000000000	4	†$0.326_{10}-2$
	5	3.00105010	0.000000000	†$0.581_{10}-1$				
	6	3.00000070	$0.103425_{10}-2$	†0.114				
	7	3.00000070	$-0.103425_{10}-2$	†0.114				
$(z-1)^9$	1	0.99998184	$0.484111_{10}-3$	†$0.390_{10}15$	1	1.000000015	9	††$0.413_{10}-1$
	2	0.99998184	$-0.484111_{10}-3$	†$0.390_{10}15$				
	3	1.00040310	0.000000000	†$0.119_{10}16$				
	4	1.00012150	0.000000000	†$0.440_{10}21$				
	5	1.00012040	0.000000000	†$0.805_{10}21$				
	6	1.00011910	0.000000000	†$0.371_{10}21$				
	7	0.99970717	0.000000000	†$0.517_{10}16$				
	8	0.99958629	0.000000000	†$0.112_{10}16$				
	9	0.99997886	0.000000000	†$0.871_{10}17$				
$(z^2-1)^2$	1	−1.00000000	0.000000000	$0.155_{10}-6$	1	−1.000000000	2	†$0.472_{10}-7$
	2	−0.99999996	0.000000000	$0.122_{10}-6$				
	3	1.00000000	0.000000000	†$0.149_{10}-6$	2	1.000000000	2	†$0.472_{10}-7$
	4	0 99999998	0.000000000	†$0.173_{10}-6$				
$10^5(z+1)^2(z+1.00006)$	1	−1.00013580	0.000000000	$0.150_{10}-3$	1	−1.000020000	3	$0.413_{10}-4$
	2	−0.99991770	0.000000000	$0.150_{10}-3$				
	3	−1.00000650	0.000000000	†$0.175_{10}-5$				

† The magnitudes of p_{kj} for $j = 1,2,\cdots, M_k$ are dominated by Kahan's upper bound for the rounding errors.

†† The magnitudes of p_{kj} for $j = 1,2,\cdots, M_k - 1$ are dominated by Kahan's upper bound for the rounding errors.

These regions are determined from Theorem 1 by setting $e_k = g_k$ where g_k is the positive root of eq. (3).

The first three polynomials of this table illustrate large variations in the size of the regions $\Gamma_{kj}(g_k)$ when the distinct approximations to multiple zeros are replaced by the confluent approximation formed from the average of the distinct approximations. The largest variation which we have observed so far appears in the third polynomial and the smallest change appears in the fourth polynomial. The changes in the first two polynomials are typical for most of our experiments.

The fifth polynomial shows how the regions $\Gamma_{kj}(g_k)$ change when three distinct approximations are replaced by a confluent approximation of multiplicity three even though the polynomial does not have a zero of multiplicity three.

We comment now that some of the results in Tables I and II appear to contradict Theorem 2. For instance, the bound for the error of the confluent approximation z_1 of the first polynomial in Table II overestimates the actual error by a factor near 60,000, whereas Theorem 2 predicts that the bound of Theorem 1 does not overestimate the actual error by more than a factor near 12 ($LM_1 = 3 \times 4$). Remember, however, that for these results we have only upper bounds for the magnitude of the polynomials and their derivatives and not the exact magnitudes for these quantities.

8. *Conclusion*

Given N approximations to the zeros of an Nth-degree polynomial, we compute N circular regions whose union contains all the zeros of the polynomial. For these circular regions, there is no danger of misplacing any of the zeros whenever some of these regions overlap. In addition, if the approximations are well separated and close to the zeros, these circular regions are small. Finally, whenever these circular regions about different centers do not overlap, some of the zeros of the polynomial will certainly be misplaced if the radii of these regions are reduced by a modest factor simply related to the degree of the polynomial and the "multiplicities" of the approximations.

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