A Stopping criteria for polynomial root finders

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Abstract:
Finding adequate stopping criteria for polynomial root finders is not always easy. To aggressive stopping criteria and you will never convergence to an acceptable root or too lax and you find roots with a lesser degree of accuracy than possible by the actually limitation of the machine precision. Stopping criteria's are based on the round off errors when evaluation a polynomial at a given real or complex point x.

Introduction:
When locating the zeros of a polynomial, it is usually difficult to know just when to terminate the iteration process. It. is desirable to terminate the process when the zero is known to within round off accuracy. Various ad hoc stopping criteria have been used; however, such criteria do not take into account particular properties of the polynomial being evaluated. Such properties might include the condition of the polynomial, multiple zeros, or clusters of zeros. In this paper a stopping criterion is presented which requires that the value of the polynomial be smaller than a calculated bound for the round off error.

Evaluation of Polynomials:
To evaluate a polynomial P at z:

$$P(z) = a_n z^n + a_{n-1} z^{n-1} + ... + a_1 z + a_0$$

We generally use Horner recurrence given by:

$$b_n = a_n$$
$$b_k = b_{k-1} z + a_k \quad k = n-1,...,0$$

The last term of this recurrence b_0 is now P(z).

This evaluation of P(z) requires therefore n multiplications and additions for a total of 2n operations. The above mention recurrence works well for polynomial with real coefficients evaluated at a real point x, as well as for polynomials with complex coefficients evaluated at a complex point Z=x+*i*y in which case multiplication and addition is replaced with the complex multiplication and addition for complex arithmetic given by:

Complex multiplication: (a+*i*b)(c+*i*d) = (ac – bd) + *i*(ad+bc)
Complex addition: (a+ib)+(c+id) = ac + *i*bd

Since a Complex multiplication requires 4 'real' multiplications and 2 additions the total number of operations involving is 4n+2n or 6n 'real' operations for polynomials with complex coefficients evaluated at a complex point.

In the case of a polynomial *P* with real coefficients evaluated at a complex point Z we in general are using Horner recurrence but in a special version using only real arithmetic:

$$Z = x + iy$$
$$p = -2x$$
$$q = x^2 + y^2$$
$$b_n = a_n$$
$$b_{n-1} = a_{n-1} - pb_n$$
$$b_k = a_k - pb_{k+1} - qb_{k+2} \qquad k = n-2,...,1$$
$$b_0 = a_0 + xb_1 - qb_2$$
$$P(Z) = b_0 + iyb_1$$

It therefore requires 4n operation instead of 2n for the real case to evaluate a polynomial with real coefficients and a complex point Z.

Polynomial	Real coefficient	Complex coefficients
Number of operations:		
Real point	2n	4n
Complex point	4n	6n

Error in arithmetic's operations:

J.H.Wilkinson in "Rounding errors in algebraic processes" [3] has showed that the errors in performing algebraic operations are bound by:

$\varepsilon < \frac{1}{2}\beta^{1-t}$ $\quad \beta$ *is the base, and t is the precision* (Assuming round to nearest)

For the Intel microprocessor series and the IEE754 standard for floating point operations $\beta =$ 2 and t=53 for 64bit floating point arithmetic or 2^{-53}

A simple upper bound:

A simple upper bound can then be obtained using above information for a polynomial with degree n.

Polynomial		
Number of operations:	Real coefficient	Complex coefficients
Real point	$\lvert a_o \rvert \cdot 2n{\cdot}2^{-53}$	$\lvert a_o \rvert \cdot 4n{\cdot}2^{-53}$
Complex point	$\lvert a_o \rvert \cdot 4n{\cdot}2^{-53}$	$\lvert a_o \rvert \cdot 6n{\cdot}2^{-53}$

A more advanced error bound.

Polynomial root finders usually can handle polynomials with both real and complex coefficients evaluated at a real or complex number. So in principle we have 3 different scenarios (real coefficients at a real point, real coefficients at a complex point and complex coefficients at a complex point) that we must deal with in order to calculate a root to the limitations of the machine precision. Since the bound of the round off errors is different for these 3 scenarios we need to evaluated them individually.

Case 1: Polynomial with real coefficients a_n evaluated at a real point x, using Horners method:

$$b_n = a_n$$
$$b_k = b_{k-1}x + a_k \quad k = n-1,\ldots,0$$

And error bound can be computed using similar recurrence as follows:

$$e_n = |b_n|\frac{1}{2}$$
$$e_k = e_{k-1}|x| + |b_k| \quad k = n-1,\ldots,0$$
$$e = (4e_0 - 2b_0)\varepsilon \quad where\ \varepsilon = \frac{1}{2}\beta^{1-t}$$

Case 2: Polynomial with real coefficients a_n evaluated at a complex point z, using Horners.

$$Z = x + iy$$
$$p = -2x$$
$$q = x^2 + y^2$$
$$b_n = a_n$$
$$b_{n-1} = a_{n-1} - pb_n$$
$$b_k = a_k - pb_{k+1} - qb_{k+2} \qquad k = n-2,\ldots,1$$
$$b_0 = a_0 + xb_1 - qb_2$$
$$P(Z) = b_0 + iyb_1$$

Adams [1] has shown that a error bound can be computed using the following recurrence:

$$e_n = |b_n|\frac{7}{9}$$

$$e_k = e_{k-1}|Z| + |b_k| \quad k = n-1,...,0$$

$$e = (4.5e_0 - 3.5(|b_0| + |b_1||Z|) + |x||b_1|)\varepsilon \quad where\ \varepsilon = \frac{1}{2}\beta^{1-t}$$

To evaluate a polynomial P at x P(x) we generally used Horner recurrence given by:

Case 3: Polynomial with complex coefficients z_n evaluated at a complex point z, using Horner's method. This gets a little bit more complicated. Grant and Hitchins [2] derive an upper error bound for the errors in evaluating the polynomial as follows

$$P(Z) = (a_n + ib_n)z^n + (a_{n-1} + ib_{n-1})z^{n-1} + ... + (a_1 + ib_1)z + (a_0 + b_0)$$

Using the Horner's method and keeping track on the real component c_k and the imaginary component d_k separately we get:

$$c_n = a_n, \quad d_n = b_n$$

$$c_k = c_{k+1}x - yd_{k+1} + a_k \quad k = n-1,...,0$$

$$d_k = d_{k+1}x + yc_{k+1} + b_k \quad k = n-1,...,0$$

Using these values an error bound can now be calculated using the recurrence:

$$g_n = 1, \quad h_n = 1$$

$$g_k = |x|(g_{k+1} + |c_{k+1}|) + |y|(h_{k+1} + |d_{k+1}|) + |a_k| + 2|c_k| \quad k = n-1,...,0$$

$$h_k = |y|(g_{k+1} + |c_{k+1}|) + |x|(h_{k+1} + |d_{k+1}|) + |b_k| + 2|d_k|$$

A now the error is $(g_0+ih_0)\varepsilon$, where $\varepsilon = ½\ \beta^{1-t}$. Now since the recurrence in itself introduce error [2] safeguard the calculation by adding the upper bound for the rounding errors in the recurrence, so we have the bound for evaluating a complex polynomial in a complex point:

$$e = (g_0 + ih_0)\varepsilon(1+\varepsilon)^{5n} \quad where\ \varepsilon = \frac{1}{2}\beta^{1-t}$$

<u>Other methods:</u>

[4] Provide a comprehensive list of other methods to consider and is a good reference for what has be done in this field over the years.

Interval arithmetic is another obvious choice. They benefit is that if we use interval arithmetic in our evaluation we immediately have a bound for the error in our evaluation.

Reference

1. Adams, D A stopping criterion for polynomial root finding. Communication of the ACM Volume 10/Number 10/ October 1967 Page 655-658
2. Grant, J A & Hitchins, G D. Two algorithms for the solution of polynomial equations to limiting machine precision. The computer Journal volume 18 Number 3, page 258-264
3. Wilkinson, J H, Rounding errors in Algebraic Processes, Prentice-Hall Inc, Englewood cliffs, NJ 1963
4. McNamee, J.M., Numerical Methods for Roots of Polynomials, Part I, Elsevier, Kidlington, Oxford 2009