Roots of Polynomials

(Com S 477/577 Notes)

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A direct corollary of the fundamental theorem of algebra is that p(x) can be factorized over the complex domain into a product $a_n(x-r_1)(x-r_2)\cdots(x-r_n)$, where a_n is the leading coefficient and r_1, r_2, \ldots, r_n are all of its n complex roots. We will look at how to find roots, or zeros, of polynomials in one variable. The solution of multi-variate polynomials can often be transformed into a problem that requires the solution of single-variate polynomials.

1 Roots of Low Order Polynomials

We will start with the closed-form formulas for roots of polynomials of degree up to four. For polynomials of degrees more than four, no general formulas for their roots exist. Root finding will have to resort to numerical methods discussed later.

1.1 Quadratics

A quadratic equation

$$ax^2 + bx + c = 0, \qquad a \neq 0,$$

has two roots:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

If the coefficients a, b, c are real, it follows that

if $b^2 - 4ac > 0$ the roots are real and unequal;

if $b^2 - 4ac = 0$ the roots are real and equal;

if $b^2 - 4ac < 0$ the roots are imaginary.

1.2 Cubics

The cubic equation

$$x^3 + px^2 + qx + r = 0$$

can be reduced by the substitution

$$x = y - \frac{p}{3}$$

to the normal form

$$y^3 + ay + b = 0, (1)$$

where

$$a = \frac{1}{3}(3q - p^2),$$

 $b = \frac{1}{27}(2p^3 - 9pq + 27r).$

Equation (1) has three roots:

$$y_1 = A + B,$$

 $y_2 = -\frac{1}{2}(A+B) + \frac{i\sqrt{3}}{2}(A-B),$
 $y_3 = -\frac{1}{2}(A+B) - \frac{i\sqrt{3}}{2}(A-B),$

where $i^2 = -1$ and

$$A = \sqrt[3]{-\frac{b}{2} + \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}},$$

$$B = \sqrt[3]{-\frac{b}{2} - \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}}.$$

The three roots can be verified below:

$$(y - y_1)(y - y_2)(y - y_3) = (y - A - B)(y^2 + (A + B)y + A^2 - AB + B^2)$$

$$= y^3 - 3ABy - (A + B)(A^2 - AB + B^2)$$

$$= y^3 - 3ABy - A^3 - B^3$$

$$= y^3 + ay + b.$$

Suppose p, q, r are real (and hence a and b are real). Three cases exist:

- $\frac{b^2}{4} + \frac{a^3}{27} > 0$. There are one real root $y = y_1$ and two conjugate imaginary roots.
- $\frac{b^2}{4} + \frac{a^3}{27} = 0$. There are three real y roots of which at least two are equal:

$$-2\sqrt{-\frac{a}{3}}, \qquad \sqrt{-\frac{a}{3}}, \qquad \sqrt{-\frac{a}{3}} \quad \text{if } b > 0,$$

$$2\sqrt{-\frac{a}{3}}, \qquad -\sqrt{-\frac{a}{3}}, \qquad -\sqrt{-\frac{a}{3}} \quad \text{if } b < 0,$$

$$0, \quad 0, \quad 0 \quad \text{if } b = 0.$$

• $\frac{b^2}{4} + \frac{a^3}{27} < 0$. There are three real and unequal roots:

$$y_k = 2\sqrt{-\frac{a}{3}}\cos\left(\frac{\phi}{3} + \frac{2k\pi}{3}\right), \qquad k = 0, 1, 2,$$

where

$$\cos \phi = \begin{cases} -\sqrt{\frac{b^2/4}{-a^3/27}} & \text{if } b > 0; \\ \sqrt{\frac{b^2/4}{-a^3/27}} & \text{if } b < 0. \end{cases}$$

Every root y_k thus obtained corresponds to a root $x_k = y_k - p/3$ of the original cubic equation.

1.3 Quartics

The quartic equation

$$x^4 + px^3 + qx^2 + rx + s = 0$$

can be reduced to the form

$$y^4 + ay^2 + by + c = 0 (2)$$

by the substitution

$$x = y - \frac{p}{4},$$

where

$$a = q - \frac{3p^2}{8},$$

$$b = r + \frac{p^3}{8} - \frac{pq}{2},$$

$$c = s - \frac{3p^4}{256} + \frac{p^2q}{16} - \frac{pr}{4}.$$

The quartic (2) can be factorized under some condition. The equation that must be solved to make it factorizable is called the *resolvent cubic*:

$$z^{3} - qz^{2} + (pr - 4s)z + (4qs - r^{2} - p^{2}s) = 0.$$

Let z_1 be a real root of the above cubic. Then the four roots of the original quartic are

$$x_1 = -\frac{p}{4} + \frac{1}{2}(R+D),$$

$$x_2 = -\frac{p}{4} + \frac{1}{2}(R-D),$$

$$x_3 = -\frac{p}{4} - \frac{1}{2}(R-E),$$

$$x_4 = -\frac{p}{4} - \frac{1}{2}(R+E),$$

where

$$R = \sqrt{\frac{1}{4}p^2 - q + z_1},$$

$$D = \begin{cases} \sqrt{\frac{3}{4}p^2 - R^2 - 2q + \frac{1}{4}(4pq - 8r - p^3)R^{-1}} & \text{if } R \neq 0, \\ \sqrt{\frac{3}{4}p^2 - 2q + 2\sqrt{z_1^2 - 4s}} & \text{if } R = 0, \end{cases}$$

$$E = \begin{cases} \sqrt{\frac{3}{4}p^2 - R^2 - 2q - \frac{1}{4}(4pq - 8r - p^3)R^{-1}} & \text{if } R \neq 0; \\ \sqrt{\frac{3}{4}p^2 - 2q - 2\sqrt{z_1^2 - 4s}} & \text{if } R = 0. \end{cases}$$

For more details see [1] or [9].

2 Root Counting

Consider a polynomial of degree n:

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0, \qquad a_n \neq 0.$$

The fundamental theorem of algebra states that p has n real or complex roots, counting multiplicities. If the coefficients a_0, a_1, \ldots, a_n are all real, then the complex roots occur in conjugate pairs, that is, in the form $c \pm di$, where $c, d \in \mathbb{R}$ and $i^2 = -1$. If the coefficients are complex, the complex roots need not be related.

Using Descartes' rules of sign, we can count the number of real positive zeros that p(x) has. More specifically, let v be the number of variations in the sign of the coefficients $a_n, a_{n-1}, \ldots, a_0$ (ignoring coefficients that are zero). Let n_p be the number of real positive zeros. Then

- (i) $n_p \leq v$,
- (ii) $v n_p$ is an even integer.

A negative zero of p(x), if exists, is a positive zero of p(-x). The number of real negative zeros of p(x) is related to the number of sign changes in the coefficients of p(-x).

EXAMPLE 1. Consider the polynomial $p(x) = x^4 + 2x^2 - x - 1$. Then v = 1, so n_p is either 0 or 1 by rule (i). But by rule (ii) $v - n_p$ must be even. Hence $n_p = 1$.

Now look at $p(-x) = x^4 + 2x^2 + x - 1$. Again, the coefficients have one variation in sign, so p(-x) has one positive zero. In other words, p(x) has one negative zero.

To summarize, simply by looking at the coefficients, we conclude that p(x) has one positive real root, one negative real root, and two complex roots as a conjugate pair.

Descartes' rule of sign still leaves an uncertainty as to the exact number of real zeros of a polynomial with real coefficients. An exact test was given in 1829 by Sturm, who showed how to count the real roots within any given range of values.

Let f(x) be a real polynomial. Denote it by $f_0(x)$ and its derivative f'(x) by $f_1(x)$. Proceed as in Euclid's algorithm to find

$$f_0(x) = q_1(x) \cdot f_1(x) - f_2(x),$$

$$f_1(x) = q_2(x) \cdot f_2(x) - f_3(x),$$

$$\vdots$$

$$f_{k-2}(x) = q_{k-1}(x) \cdot f_{k-1}(x) - f_k(x),$$

$$f_{k-1}(x) = q_k(x)f_k(x),$$

where $deg(f_i(x)) < deg(f_{i-1}(x))$, for $1 \le i \le k$. The signs of the remainders are negated from those in the Euclid algorithm.

Note that the divisor f_k that yields zero remainder is a greatest common divisor of f(x) and f'(x). The sequence f_0, f_1, \ldots, f_k is called a *Sturm sequence* for the polynomial f.

Theorem 1 (Sturm's Theorem) The number of distinct real zeros of a polynomial f(x) with real coefficients in (a,b) is equal to the excess of the number of changes of sign in the sequence $f_0(a), \ldots, f_{k-1}(a), f_k(a)$ over the number of changes of sign in the sequence $f_0(b), \ldots, f_{k-1}(b), f_k(b)$.

In fact, we can multiply f by a positive constant, or a factor involving x, provided that the factor remains positive throughout (a, b), and the modified function can be used for computing all further terms f_i of the sequence.

EXAMPLE 2. Use Sturm's theorem to isolate the real roots of

$$x^5 + 5x^4 - 20x^2 - 10x + 2 = 0.$$

We first compute the Sturm functions:

$$f_0(x) = x^5 + 5x^4 - 20x^2 - 10x + 2,$$

$$f_1(x) = x^4 + 4x^3 - 8x - 2,$$

$$f_2(x) = x^3 + 3x^2 - 1,$$

$$f_3(x) = 3x^2 + 7x + 1,$$

$$f_4(x) = 17x + 11,$$

$$f_5(x) = 1.$$

By setting $x = -\infty, 0, \infty$, we see that there are 3 negative roots and 2 positive roots. All roots lie between -10 and 10, in fact, between -5 and 5. We then try all integral values between -5 and 5. The following table records the work:

	$-\infty$	-10	-5	-4	-3	-2	-1	0	1	2	5	10	∞
f_0	_	_	_		+	_	_	+	_	+	+	+	+
f_1	+	+	+	+	_	_	_	_	_	+	+	+	+
f_2	_	_	_		_	+	+	_	+	+	+	+	+
f_3	+	+	+	+	+	_	_	+	+	+	+	+	+
f_4	_	_	_	1	_	_	_	+	+	+	+	+	+
f_5	+	+	+	+	+	+	+	+	+	+	+	+	+
var.	5	5	5	5	4	3	3	2	1	0	0	0	0

Thus, there is a root in (-4, -3), a root in (-3, -2), a root in (-1, 0), a root in (0, 1), and a root in (1, 2).

3 More Bounds on Roots

It is known that p(x) must have at least one root, real or complex, inside the circle of radius ρ_1 about the origin of the complex plane, where

$$\rho_1 = \min \left\{ n \left| \frac{a_0}{a_1} \right|, \sqrt[n]{\left| \frac{a_0}{a_n} \right|} \right\}. \tag{3}$$

In the case $a_1 = 0$, we have $\left| \frac{a_0}{a_1} \right| = \infty$ and $\rho_1 = \sqrt[n]{\left| \frac{a_0}{a_n} \right|}$. Meanwhile, if we let

$$\rho_2 = 1 + \max_{0 \le k \le n-1} \left| \frac{a_k}{a_n} \right|,\tag{4}$$

then all zeros of p(x) must lie inside the circle of radius ρ_2 about the origin.

Theorem 2 (Cauchy's Theorem) Given a polynomial $p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_0$, $a_n \neq 0$, define the polynomials

$$P(x) = |a_n|x^n + |a_{n-1}|x^{n-1} + \dots + |a_1|x - |a_0|,$$

$$Q(x) = |a_n|x^n - |a_{n-1}|x^{n-1} - \dots - |a_0|.$$

By Descartes' rules, P(x) has exactly one real positive zero r_1 and Q(x) has exactly one real positive zero r_2 . Then all zeros z of p(x) lie in the annular region

$$r_1 \le |z| \le r_2. \tag{5}$$

EXAMPLE 3. Let $p(x) = x^5 - 3.7x^4 + 7.4x^3 - 10.8x^2 + 10.8x - 6.8$. Applying bound (3), we know that at least one zero of p is inside the circle $|x| \le \rho_1$, where

$$\rho_1 = \min \left\{ 5 \cdot \frac{6.8}{10.8}, \sqrt[5]{\frac{6.8}{1}} \right\}$$
$$= \min \left\{ 3.14815, 1.46724 \right\}$$
$$= 1.46724.$$

Applying bound (4), all zeros lie inside the circle $|x| \leq \rho_2$, where

$$\rho_2 = 1 + \max\{3.7, 7.4, 10.8, 10.8, 6.8\} = 11.8.$$

Let us try to apply Cauchy's theorem. First, we have that

$$P(x) = x^5 - 3.7x^4 - 7.4x^3 - 10.8x^2 - 10.8x - 6.8,$$

$$Q(x) = x^5 + 3.7x^4 + 7.4x^3 + 10.8x^2 + 10.8x - 6.8,$$

whose positive zeros are

$$r_1 = 0.63 \cdots,$$

$$r_2 = 5.6 \cdots.$$

Therefore all zeros of p(x) lie in the region $0.63 \cdots \le |x| \le 5.6 \cdots$.

How does one use the above root bounds? Use them as heuristics to give us a way of localizing the possible zeros of a polynomial. By localizing the zeros, we can guide the initial guesses of our numerical root finders.

4 Deflation

The effort of root finding can be significantly reduced by the use of deflation. Once you have found a root r of a polynomial p(x), consider next the deflated polynomial q(x) which satisfies

$$p(x) = (x - r)q(x).$$

The roots of q are exactly the remaining roots of p(x). Because the degree decreases, the effort of finding the remaining roots decreases. More importantly, with deflation we can avoid the blunder

of having our iterative method converge twice to the same root instead of separately to two different roots.

We can obtain q(x) by evaluating p(x) at x = r using Horner scheme. Recall the intermediate quantities b_0, \ldots, b_n from the evaluation, where $b_n = a_n$, and $b_{i-1} = a_{i-1} + rb_i$, for $i = n, \ldots, 1$. We know that

$$p(x) = b_0 + (x - r)(b_n x^{n-1} + \dots + b_2 x + b_1).$$
(6)

Since $b_0 = p(r) = 0$, we obtain

$$q(x) = b_n x^{n-1} + \dots + b_2 x + b_1. \tag{7}$$

Deflation can also be carried out by synthetic division of p(x) by q(x) which acts on the array of polynomial coefficients. It must, however, be utilized with care. Because each root is known with only finite accuracy, errors can build up in the roots as the polynomials are deflated. The order in which roots are found can affect the stability of the deflated coefficients. For example, suppose the new polynomial coefficients are computed in the decreasing order of the corresponding powers of x. The method is stable if the root of smallest absolute value is divided out at each stage.

Roots of deflated polynomials are really just "good suggestions" of the roots of p. Often we need to use the original polynomial p(x) to polish the roots in the end.

5 Newton's Method

The first method we introduce on polynomial root finding is Newton's method. Suppose we have an estimate x_k of a root at iteration step k. Newton's method yields the estimate at step k + 1:

$$x_{k+1} = x_k - \frac{p(x_k)}{p'(x_k)}. (8)$$

Recall that we can evaluate p(t) and p'(t) together efficiently using Horner scheme, generating intermediate quantities $b_n, b_{n-1}, \ldots, b_0 = p(t)$ (and thus the polynomial q(x) in (7)). Equations (6) and (7) are combined into

$$p(x) = p(t) + (x - t)q(x),$$
 (9)

which implies p'(t) = q(t). If t is actually a root of p(x), it follows from equation (9) that

$$q(x) = \frac{p(x)}{x - t}$$

is already the deflated polynomial, which can be viewed as a byproduct of the Newton's method.

To find a zero of p(x), Newton's method takes an initial guess x_0 of a root and iterates according to (8) until some termination condition is satisfied, for instance, until $p(x_i)$ or $|x_{i+1} - x_i|$ is close enough to zero.

One situation that Newton's method does not work well is when the polynomial p(x) has a double root r, that is, when

$$p(x) = (x - r)^2 h(x).$$

In this case p(x) shares a factor with its derivative which is of the form

$$p'(x) = 2(x - r)h(x) + (x - r)^{2}h'(x).$$

As x approaches r, both p and p' approach zero. In applying Newton's method, machine imprecision will dominate evaluation of the term $\frac{p(x)}{p'(x)}$ as x tends to r. In this case one tiny number is divided by one very small number.

One can avoid the double-root problem by seeking quadratic factors directly in deflation. This is also useful when looking for a pair of complex conjugate roots of a polynomial with real coefficients. For higher order roots, one can detect their possibilities to some extent and apply special techniques to either find or rule out them.

Polynomials are often sensitive to variations in their coefficients. Consequently, after several deflations, the remaining roots may be very inaccurate. One solution is to polish the roots using a very accurate method, once approximations to these roots have been found from deflated polynomials. Newton's method is generally good for polishing both real and complex roots.

6 Müller's Method

Newton's method is a *local* method, that is, it may fail to converge if the initial estimate is too far from a root. Now we introduce a global root finding technique. After the roots are found, we can polish them as we desire (often using Newton's method).

Müller's method can find any number of zeros, real or complex, often with global convergence. Since it is also applicable to functions other than polynomials, we here present it for finding a zero of a general function f(x), not necessarily a polynomial.

The method makes use of quadratic interpolation. Suppose the three prior estimates of a zero of f(x) in the current iteration are the points x_{k-2}, x_{k-1}, x_k . To compute the next estimate we will construct the polynomial of degree ≤ 2 that interpolates f(x) at x_{k-2}, x_{k-1}, x_k , then find one of its roots. We begin with the interpolating polynomial in the Newton form

$$p(x) = f(x_k) + f[x_{k-1}, x_k](x - x_k) + f[x_{k-2}, x_{k-1}, x_k](x - x_k)(x - x_{k-1}),$$

where $f[x_{k-1}, x_k]$ and $f[x_{k-2}, x_{k-1}, x_k]$ are divided differences. Using the equality

$$(x - x_k)(x - x_{k-1}) = (x - x_k)^2 + (x - x_k)(x_k - x_{k-1}),$$

we can rewrite p(x) as

$$p(x) = f(x_k) + b(x - x_k) + a(x - x_k)^2,$$

where

$$a = f[x_{k-2}, x_{k-1}, x_k],$$

$$b = f[x_{k-1}, x_k] + f[x_{k-2}, x_{k-1}, x_k](x_k - x_{k-1})$$

Now let p(x) = 0 and solve for x as the next approximation

$$x_{k+1} = x_k - \frac{2f(x_k)}{b \pm \sqrt{b^2 - 4af(x_k)}}.$$

In the above we choose the form of zeros of the quadratic $ax^2 + bx + c$ to be

$$x = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$
 instead of $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

for numerical stability. This is mainly because $c = f(x_k)$ gets very small near a root of f. Also for numerical stability, the '±' sign in the denominator $b \pm \sqrt{b^2 - 4ac}$, is chosen so as to maximize the magnitude of the denominator. Note that complex estimates are introduced automatically due to the square-root operation.

Algorithm 1 finds all roots, with or without multiplicities, of a polynomial that has only real coefficients, by combining Müller's method with deflation and root polishing (using Newton's method).

Algorithm 1 Müller's method

```
Input: p(x) = a_n x^n + \cdots + a_1 x + a_0, where a_i \in \mathbb{R} for 0 \le i \le n and a_n \ne 0
Output: its roots r_0, r_1, \ldots, r_{n-1}
  if deg(p) \le 4 then
     use the correponding closed forms in Section 1
  else
     p_0(x) \leftarrow p(x)
     l \leftarrow 0
     while deg(p_l) \geq 5 do
        one root of p_l must lie inside the circle of radius \rho_1 in (3) in Section 3
        generate three root estimates within the circle.
        use Müller's method to find one root r_l of p_l(x)
        if r_l is real then
           p_{l+1}(x) \leftarrow p_l/(x-r_l) (apply Horner scheme for deflation)
           l \leftarrow l + 1
           while p_l(r_{l-1}) = 0 (a multiple root) do
              p_{l+1}(x) \leftarrow p_l/(x-r_l)
              l \leftarrow l + 1
           end while
        else
           r_l = a_l + ib_l and its complex conjugate \overline{r_l} = a_l - ib_l are two roots
           p_{l+2}(x) \leftarrow p_l/((x-r_l)(x-\overline{r_l})) = p_l/(x^2-2a_lx+a_l^2+b_l^2)
           l \leftarrow l + 2
           while p_l(r_{l-2}) = 0 do
              r_l \leftarrow r_{l-2}
              r_{l+1} \leftarrow r_{l-1}
              p_{l+2}(x) \leftarrow p_l/(x^2 - 2a_lx + a_l^2 + b_l^2)
              l \leftarrow l + 2
           end while
        end if
     end while
     find the roots of the cubic or quartic p_l using the closed forms in Section 1.2 or 1.3.
     polish r_0, \ldots, r_{n-1} using Newton's method on p(x)
  end if
```

Deflation may stop when the degree of the polynomial reduces to four or three, and closed-form roots in Sections 1.2 and 1.3 can be computed.

EXAMPLE 2. Find the roots of $p(x) = x^3 - x - 1$ using Müller's method. For each root the iteration start with initial guesses $x_{-2} = 1, x_{-1} = 1.5$, and $x_0 = 2.0$. We terminate the iteration at step *i* when $|\Delta x_i - \Delta x_{i-1}| \le 5 \cdot 10^{-5}$.

The method estimates the first root to be $r_1 = 1.324718$ with an accuracy about $3.4 \cdot 10^{-7}$.

i	x_i	$p(x_i)$
-2	1.0	-1
-1	1.5	0.875
0	2.0	5
1	1.33333	0.037037
2	1.32447	-0.00105
3	1.324718	$1.44 \cdot 10^{-6}$
4	1.324718	$7.15 \cdot 10^{-13}$

Next, we work with the deflated polynomial $q(x) = p(x)/(x - r_1)$ and find the second root to be $r_2 = -0.66236 + 0.56228i$ with an accuracy of $2.2 \cdot 10^{-5}$.

The third root must be a conjugate of the second root. So we have $r_3 = -0.66236 - 0.56228i$.

Let us do a more complete example.

EXAMPLE 3. Find the roots of the polynomial

$$p(x) = x^4 + 2x^2 - x - 1.$$

Earlier by checking the sign changes in the coefficient sequence we knew that p(x) has one positive root, one negative root, and one pair of complex conjugate roots.

Now let us look at the bound heuristics:

$$\rho = \min \left\{ n \frac{|a_0|}{|a_1|}, \sqrt[n]{\frac{|a_0|}{|a_n|}} \right\}$$
$$= \min\{4, 1\}$$
$$= 1.$$

Thus there is at least one zero inside the complex circle of radius one about the origin. Furthermore, all zeros of p(x) lie inside the circle of radius

$$r = 1 + \max_{0 \le k \le n-1} \left| \frac{a_k}{a_n} \right|$$

= 1 + \max\{1, 1, 2, 0\}
= 3.

Our search for zero need only focus on the complex disk of radius 3. For each root we start Müller's method with the initial guesses

$$x_0 = -\frac{1}{2}, \qquad x_1 = 0, \qquad x_2 = \frac{1}{2},$$

and terminate the search once $\Delta x_i \leq 5 \cdot 10^{-5}$.

roots	# iterations	accuracy
		-
0.8251098	5	$2.4 \cdot 10^{-7}$
-0.4818156	4	$1.4 \cdot 10^{-6}$
-0.171647 + 1.576686i	2	$5.1 \cdot 10^{-6}$
-0.171647 - 1.576686i		

Note that the two complex roots lie between the circle of radius 1 and the circle of radius 3.

Deflations were used in seeking the second and the third roots. We should next polish the four root estimates using the original polynomial p(x), which can be done automatically within Müller's method.

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