A Practical Root-finding Algorithm based on the Cubic Hermite Interpolation

Tatsuo Torii* and Tsuyako Miyakoda*

1. Introduction

An iterative method for finding a root of analytic function $f(z)$, real valued on real axis, is described.

We combine Newton method and the cubic interpolatory iteration to improve the former condition of the convergence, as stated below.

Let z_0 be an approximation of the root ζ of $f(z)$ and $g(z)$ be cubic Hermite interpolating polynomial of $f(z)$ on two points z_0 and its complex conjugate $\bar{z}_0$. If z_0 is sufficiently close to ζ such that z_0 satisfies the convergence theorem of Newton iteration owing to Ostrowski[1)], then we have Newton iteration. Otherwise we solve cubic polynomial equation $g(z) = 0$ and take a root z_1 of $g(z)$ nearest to z_0 as the next approximation of ζ .

Replacing z_1 by z_0 , we continue the way as before until the absolute value of residual $f(z_0)$ is smaller than the error bound of the value of the function at z_0 .

As an example, we apply this algorithm to the polynomial with real coefficients. Our algorithm will be rather practical than usual one such as Newton-Bairstow method.

2. Base of algorithm

Suppose given function $f(z)$ satisfies $f(z) = \overline{f(\bar{z})}$ on its domain. On an arbitrary point $z_0 \neq \bar{z}_0$ we construct a cubic Hermite interpolating polynomial:

$$g(z) = \frac{(z-\bar{z}_0)^2}{(z_0-\bar{z}_0)^2}\left\{ f(z_0) + (z-z_0)\left(f'(z_0) - \frac{2f(z_0)}{z_0-\bar{z}_0} \right)\right\}$$

$$+ \frac{(z-z_0)^2}{(\bar{z}_0-z_0)^2}\left\{ f(\bar{z}_0) + (z-\bar{z}_0)\left(f'(\bar{z}_0) - \frac{2f(\bar{z}_0)}{\bar{z}_0-z_0} \right)\right\}$$

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* Faculty of Engineering, Osaka University

of which remainder is given by

$$r(z) = (z-z_0)^2(z-\bar{z}_0)^2 \frac{\theta f^{(4)}(\xi)}{4!}$$

where θ is a complex number such that $|\theta| \leq 1$ and ξ is some point belonging to a convex hull of three points $z, z_0, \bar{z}_0$.

For brevity, rewrite variable z to s such that

$$z = x_0 + s\ , \qquad z_0 = x_0 + iy_0\ , \qquad y_0 > 0\ .$$

Then we have

$$g(z) = g(x_0+s) = (s^2+y_0^2)(\gamma_0 s + \gamma_1) + \gamma_2 s + \gamma_3$$

where real coefficients γ_0 , γ_1, γ_2 and γ_3 have expression:

$$\gamma_0 = \frac{1}{(2iy_0)^2}\left\{ f'(z_0) + \overline{f'(z_0)} - \frac{f(z_0) - \overline{f(z_0)}}{iy_0} \right\}$$

$$\gamma_1 = \frac{1}{4iy_0}\left\{ f'(z_0) - \overline{f'(z_0)} \right\}$$

$$\gamma_2 = \frac{1}{2iy_0}\left\{ f(z_0) - \overline{f(z_0)} \right\}$$

$$\gamma_3 = \frac{1}{2}\left\{ f(z_0) + \overline{f(z_0)} \right\} .$$

In case z_0 is real number, these coefficients are defined by the limit value approaching y_0 to 0.

That is

$$g(x_0+s) = f(x_0) + f'(x_0)s + \frac{f''(x_0)}{2!}s^2 + \frac{f'''(x_0)}{3!}s^3$$

We consider first interpolatory iteration using this cubic polynomial.

If $g(z)$ is not identically constant, it has at least one root. By solving $g(z) = 0$, let z_1 denote its root closest to z_0. If the initial value z_0 is sufficiently close to ζ a root of $f(z)$, z_1 is evidently more accurate than z_0 from the expression of remainder $r(z)$. By continuing this way , we get a sequence $\{z_n\}$ which converges to ζ . We will call this method cubic Hermite interpolatory iteration. In order to consider the speed of convergence, we denote

$$f(z) = f(\zeta + h) = \sum_{k=m}^{\infty} a_k h^k\ , \qquad a_m \neq 0\ , \qquad m \geq 1$$

$$g(z)=g(\zeta+h)=c_0+c_1h+c_2h^2+c_3h^3.$$

In case ζ is a complex root, by the definition of $g(z)$, we get, with somewhat complicated calculation, all the coefficients:

$$c_0=\frac{1}{(h_0-k_0)^3}\Big\{(m-1)k_0^3a_mh_0^m+(mk_0a_{m+1}+3a_m)k_0^2h_0^{m+1}$$
$$-2imh_0^2k_0^2\,\mathrm{Im}(a_mh_0^{m-1})+O(h_0^{m+2})\Big\}$$

$$c_1=\frac{-1}{(h_0-k_0)^3}\Big\{mk_0^3a_mh_0^{m-1}+O(h_0^m)\Big\}$$

$$c_2=\frac{1}{(h_0-k_0)^3}\Big\{mk_0^2(a_mh_0^{m-1}+2\,\mathrm{Re}(a_mh_0^{m-1})+O(h_0^m)\Big\}$$

$$c_3=\frac{-1}{(h_0-k_0)^3}\Big\{-2mk_0\,\mathrm{Re}(a_mh_0^{m-1})+O(h_0^m)\Big\}$$

for sufficiently small $|h_0|$.

Let h_1 be a root of $g(\zeta+h)$ nearest to h_0. Then we have

$$h_1=\begin{cases}\Big\{\dfrac{a_2}{a_1}+\dfrac{i}{2\,\mathrm{Im}\,\zeta}\Big(2+\dfrac{\overline{a}_1}{a_1}\Big)\Big\}h_0^2+O(h_0^3)\,, & m=1\\[2ex] \dfrac{m-1}{m}h_0+O(h_0^2)\,, & m>1\,.\end{cases}$$

In case ζ is a real root, by denoting $h_0=\rho e^{i\theta}$, we have

$$c_0=\sum_{k=m}^{\infty}a_k\rho^k\,\frac{(k-3)\sin(k-1)\theta-(k-1)\sin(k-3)\theta}{4\sin^3\theta}$$

$$c_1=\sum_{k=m}^{\infty}a_k\rho^{k-1}\,\frac{k(\sin(k-2)\theta+\sin(k-4)\theta)-2(k-3)\sin k\theta}{4\sin^3\theta}$$

$$c_2=\sum_{k=m}^{\infty}a_k\rho^{k-2}\,\frac{(k-3)(\sin(k+1)\theta+\sin(k-1)\theta)-2k\sin(k-3)\theta}{4\sin^3\theta}$$

$$c_3=\sum_{k=m}^{\infty}a_k\rho^{k-3}\,\frac{-(k-2)\sin k\theta+k\sin(k-2)\theta}{4\sin^3\theta}$$

Here, it is noteworthy that each a_k is a real number.

As the case ζ is a complex root, h_1 is written by

$$\frac{a_4}{a_1}|h_0|^4+O(h_0^5)\,,\qquad m=1$$

$$\sqrt{\frac{a_4}{a_2}}\,|h_0|^2+O(h_0^{\frac{5}{2}})\,,\qquad m=2$$

$$\sqrt[3]{\frac{a_4}{a_3}}|h_0|^{4/3} + O(h_0^{5/3}) \quad , m=3$$

$$O(h_0) \quad , m \geq 4$$

where the argument of quardatic root or cubic root of a real number is so determined that h_1 is closest to h_0 .

Thus, it concludes that the speed of convergence of this method is fourth and second order for a simple real root and a complex root, respectively.

Next, we consider the combination of Newton method and cubic Hermite interpolatory iteration to reduce the computing time and to improve the condition of the former convergence. As far as Newton method converges, we will use this algorithm. In other case we have cubic Hermite interpolatory iteration.

To select mechanically one of them in the iteration process, we note the convergence theorem of Newton method.

Theorem (Ostrowski)[1]. Let $f(z)$ be a complex function of complex variable z in a neighborhood of z_0 , $f(z_0)f'(z_0) \neq 0$, $h_0 = -f(z_0)/f'(z_0)$, $z_1 = z_0 + h_0$. Consider the circle $K_0 : |z-z_0| \leq |h_0|$, and assume $f(z)$ analytic in K_0 , $\max_{K_0}|f''(z)| = M$ and $2|h_0|M \leq |f'(z_0)|$. Form, starting with z_0 , the sequence z_n by the recurrence formula

$$z_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)} , \quad (n=0,1,\cdots \quad) .$$

Then all z_n lies in K_0 and we have

$$z_n \longrightarrow \zeta \quad (n \to \infty)$$

where ζ is the only zero in K_0 .

Since it is difficult to check mechanically these conditions for an arbitrary analytic function $f(z)$ except low degree polynomial, we test whether these conditions are satisfied or not in each new step for the cubic polynomial $g(z)$. Moreover, if the circle K_0 of which center is not on real axis intersects that line, we can not discriminate whether z_1 is real root of $g(z)$ or complex root by the finite Newton iterates.

We use, therefore, a criterion for the selection between two algorithms as follows.

Let

$$z_n = x_n + i y_n \quad (y_n \geq 0).$$

$$f(z_n) f'(z_n) \neq 0$$

$$2|h_n| M_n \leq |f'(z_n)|$$

$$\mathrm{Im}(z_n + h_n) > |h_n| \ , \quad \mathrm{Im}\, z_n > 0$$

where

$$h_n = -f(z_n)/f'(z_n)$$

$$M_n = 2|\gamma_1| + 6|\gamma_0|(y_n + 2|h_n|)$$

If all conditions above are satisfied, we have Newton iterates one or two times such that

$$z_{n+1} = \begin{cases} z_n + h_n & \mathrm{Im}\, z_n \neq 0 \\ z_n + h_n - \dfrac{(\gamma_0 h_n + \gamma_1) h_n^2}{3\gamma_0 h_n^2 + 2\gamma_1 h_n + \gamma_2} \ , & \mathrm{Im}\, z_n = 0 \end{cases}$$

Otherwise, cubic Hermite interpolatory iteration has to be used.

3. Application to the polynomial with real coefficients.

Suppose that a given function $f(z)$ is a n-th order polynomial with real coefficients:

$$f(z) = a_0 z^n + a_1 z^{n-1} + \cdots \quad + a_n \ , \quad a_0 \neq 0$$

for which we can easily construct a Hermite interpolating polynomial $g(z)$ at an arbitrary point z_0 and its complex conjugate $\bar{z}_0$.

Denote

$$z^2 + pz + q = (z - z_0)(z - \bar{z}_0) \ , \quad z_0 = x_0 + i y_0 \ , \quad y_0 \geq 0$$

From recurrence formulas

$$b_0 = a_0$$

$$b_1 = a_1 - p b_0$$

$$b_{k+1} = a_{k+1} - p b_k - q b_{k-1} \ , \quad k = 1, 2, \cdots, n-1$$

$$b_n^* = b_n - x_0 b_{n-1}$$

$$c_0 = b_0$$

$$c_1 = b_1 - p c_0$$

$$c_{k+1} = b_{k+1} - p c_k - q c_{k-1} \ , \quad k = 1, 2, \cdots, n-3$$

$$c_{n-3}^* = c_{n-3}$$

$$c_{n-2}^* = c_{n-2} - x_0 c_{n-3}$$

we get

$$g(z) = g(x_0+\delta) = (\delta^2 + y_0^2)(C^*_{n-3}\delta + C^*_{n-2}) + b^*_{n-1}\delta + b^*_n$$
$$f(z_0) = b^*_n + i y_0$$
$$f'(z_0) = b^*_{n-1} - 2y_0^2 C^*_{n-3} + 2i y_0 C^*_{n-2}$$

Hence, we can use the algorithm in the foregoing paragraph.

Next we consider the stopping criterion. In floating-point arithmetic with t binary digits, we have

$$fl(xRy) = (xRy)(1+\varepsilon) \quad , \qquad |\varepsilon| \le 2^{-t}$$

or
$$= (xRy)/(1+\varepsilon)$$

where R is one operation of $+-\times\div$.

Then the error bound $\varepsilon_1(z)$ of computed value $f(z)$ is determined by

$$\varepsilon_1(z) = 9 \times 2^{-t} \sum_{k=0}^{n} |b_k| |z|^{n-k}$$

This is slightly simplified but rough to Adams's formula[2]. So we determine the stopping rule:

$$|b^*_n + i y b^*_{n-1}| < \varepsilon_1(z)$$

For many examples this stopping rule has been efficiently operated. It is desirable that a suitable condition number is defined for each computed root to know the loss of significant digits of the approximate root.

Using the error bound $\varepsilon_1(z)$ and inequalities

$$\sum |b_k||z|^{n-k} \ge |zf'(z)| \quad , \quad \mathrm{Im}\, z = 0$$
$$\ge \frac{1}{2} |zf'(z)| \quad , \quad \mathrm{Im}\, z \ne 0$$

we can define a condition number for the root ζ such that

$$\mathrm{cond}(\zeta) = \begin{cases} \sum |b_k||z|^{n-k} / |\zeta f'(\zeta)| & , \ \mathrm{Im}\,\zeta = 0 \\ 2\sum |b_k||z|^{n-k} / |\zeta f'(\zeta)| & , \ \mathrm{Im}\,\zeta \ne 0 \end{cases} \quad , \ \zeta|f'(\zeta)| \ne 0.$$

Evidently, $\mathrm{cond}(\zeta) \ge 1$.

Test results are shown in our original Japanese paper.

Refferences

[1] Ostrowski, A.M.: Solution of Equations Systems of Equations, Academic Press, Inc., 2nd edition, 1966, pp. 59-66.

[2] Adams, D.A.: A Stopping Criterion for Polynomial Root Finding, Comm. ACM Vol. 10, 1967, pp. 655-658.