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Quadratically Convergent Multiple Roots Finding Method Without Derivatives

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Abstract—In this paper, an iteration method without derivatives for multiple roots is proposed. This method proved to be quadratically convergent. Its efficiency and accuracy are illustrated by numerical experiments. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords-Nonlinear algebraic equation, Multiple roots, Numerical method, Iteration method, Ill-conditioned problem.

1. INTRODUCTION

It is well known that multiple roots are ill-conditioned and quadratically convergent multiple roots finding methods are almost all dependent on derivatives (see [1-3], etc.), and they have only restricted applications. Hence, the purpose of this note is to present a quadratically convergent iteration method without derivatives. Its computational efficiency and accuracy exceed other methods which use derivatives, such as Newton's method, and yet for functions whose derivatives are too lengthy to evaluate, Newton's method may well be an inefficient algorithm relative to methods which avoid the use of derivatives (a review can be seen in [4]). This motivates formula (2) in the next section of this paper, which replaces the given function f(x) by a new function F(x) that has simple zeros.

2. A QUADRATICALLY CONVERGENT MULTIPLE ROOTS FINDING METHOD

We consider iteration methods for computing approximate solutions of the nonlinear algebraic equation

$$f(x) = 0, \tag{1}$$

where we restrict our attention to real functions single-valued and of a real variable.

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For convenience in the following discussion, we define a function

$$F(x) = \frac{\operatorname{sign}(f(x))f(x)|f(x)|^{1/m}}{\operatorname{sign}(f(x+\operatorname{sign}(f(x))|f(x)|^{1/m}) - f(x))f(x)|f(x)|^{1/m} + f(x+\operatorname{sign}(f(x))|f(x)|^{1/m}) - f(x)},$$
(2)

where m is a positive integer.

THEOREM 1. Let p be a root of multiplicity m of equation (1) and f'(x) is continuous in the neighborhood of p. Then p is only a simple root of the equation

$$F(x) = 0. \tag{3}$$

PROOF. We have

$$\begin{aligned} f\left(x + \operatorname{sign}(f(x))|f(x)|^{1/m}\right) - f(x) \\ &= \operatorname{sign}(f(x))|f(x)|^{1/m} \cdot f'\left(x + s \cdot \operatorname{sign}(f(x))|f(x)|^{1/m}\right), \qquad 0 < s < 1 \end{aligned}$$

by the mean value theorem. Then it follows that

$$F(x) = \frac{f(x)}{\operatorname{sign} \left(f(x + \operatorname{sign}(f(x))|f(x)|^{1/m} \right) - f(x) \operatorname{sign}(f(x))f(x) + f'(x + s \cdot \operatorname{sign}(f(x))|f(x)|^{1/m})}, 0 < s < 1.$$

From

$$\lim_{x \to p} \left(\operatorname{sign}(f(x + \operatorname{sign}(f(x))|f(x)|^{1/m}) \operatorname{sign}(f(x))f(x) + f'\left(x + s \cdot \operatorname{sign}(f(x))|f(x)|^{1/m}\right) = f'(p), \right)$$

we conclude that p is only a simple root of equation (3).

Clearly, for equation (3), the well-known bisection method can be employed directly to produce the approximate solution of the multiple roots, including evenly multiple roots of equation (1), although the convergence rate of bisection method is slow. Of course, we may use Newtonlike methods. However, in order to avoid the use of derivatives, we can employ the modified Steffensen's method (see [5,6])

$$\begin{aligned} x_{n+1} &= x_n - h_n \frac{F^2(x_n)}{t \cdot F^2(x_n) + F(x_n + F(x_n)) - F(x_n)} \\ &= x_n - h_n \frac{F(x_n)}{t \cdot F(x_n) + (F(x_n + F(x_n)) - F(x_n))/(F(x_n))}, \qquad n = 0, 1, 2, \dots, \end{aligned}$$
(4)

for computing the approximate solution of equation (3), where $h_n > 0$ is the iteration step size and $|t| < +\infty$.

THEOREM 2. Suppose that F(p) = 0 and U is a sufficiently close neighborhood of p and $t \cdot F(x) + F'(x) \neq 0$ in U. Then the iteration formula (4) is at least quadratically convergent for $h_n = 1$. PROOF. The iteration function relating to method (4) with $h_n = 1$ is as follows:

$$Q(x) = x - \frac{F(x)}{t \cdot F(x) + (F(x + F(x)) - F(x))/(F(x))}$$

From

$$\lim_{x\to p}\frac{F(x+F(x))-F(x)}{F(x)}=F'(p),$$

F(p) = 0, $F'(p) \neq 0$ by Theorem 1, and $t \cdot F(x) + F'(x) \neq 0$ in U, we can deduce that Q(p) = p and Q'(p) = 0. This means that iteration formula (4) is convergent of order two.

It should be noticed that, from the formulae above, the iteration formula (4) can be regarded as a deformation of the extended Newton-like method

$$x_{n+1} = x_n - h_n \frac{F(x_n)}{t \cdot F(x_n) + F'(x_n)},$$
(5)

where $|t| < +\infty$. And letting t = 0, $h_n = 1$ in (5), we get Newton's method. For iteration formula (5) with $h_n = 1$, we have the following results.

THEOREM 3. It is assumed that $F(x) \in C^1[a,b]$ and $t \cdot F(x) + F'(x) \neq 0$, $x \in [a,b]$. Then equation (3) has at most one root in [a,b].

PROOF. It follows immediately from the auxiliary function $G(x) = \exp(tx) \cdot F(x)$, and $G'(x) = \exp(tx) \cdot (t \cdot F(x) + F'(x))$ that if there are two different roots of equation (3) in [a, b], then there exists at least one value $\theta \in (a, b)$ such that $G'(\theta) = 0$ by Rolle's Theorem, contradicting the condition $G'(x) \neq 0$, $x \in [a, b]$.

THEOREM 4. If $F(x) \in C^1[a, b]$, $F(a) \cdot F(b) < 0$, and $t \cdot F(x) + F'(x) \neq 0$, then equation (3) has a unique root in (a, b).

PROOF. Let $G(x) = \exp(tx) \cdot F(x)$, then we have $G(a) \cdot G(b) < 0$. Thus, G(x) = 0 has a unique root in (a, b) under the given conditions. So does equation (3).

THEOREM 5. The iteration formula (5) with $h_n = 1$ is quadratically convergent for any t, $|t| < +\infty$.

PROOF. The iteration function relating to formula (5) with $h_n = 1$ is

$$\tilde{Q}(x) = x - \frac{F(x)}{t \cdot F(x) + F'(x)}.$$
 (6)

And it is easy to see that $\tilde{Q}(p) = p$ and $\tilde{Q}'(p) = 0$, indicating that formula (5) with $h_n = 1$ is quadratically convergent.

3. SOME REMARKS

REMARK 1. Let $\varepsilon_n = x_n - p$, n = 0, 1, 2, ... be the errors in applying (4), where p is the root of F(x) = 0. Subtracting p from both sides of (4), we obtain

$$= (x_n - p) - h_n \frac{x_{n+1} - p}{f(p + (x_n - p))} = (x_n - p) - h_n \frac{F(p + (x_n - p))}{f \cdot F(p + (x_n - p)) + (F(p + (x_n - p) + F(p + (x_n - p))) - F(p + (x_n - p)))/(F(p + (x_n - p)))},$$

$$n = 0, 1, 2, \dots,$$

i.e.,

$$arepsilon_{n+1} = (1-h_n) \cdot arepsilon_n + h_n \cdot \left[rac{\left(F'(p)+1\right)F''(p)}{2F'(p)} + t
ight] \cdot arepsilon_n^2 + O\left(arepsilon_n^3
ight), \qquad n = 0, 1, 2, \dots$$

Consequently, when appropriate h_n and t are chosen, some high-order methods can be gotten. It is obvious that when $h_n = 1$, formula (4) is quadratically convergent. Especially, when t = 0 and $h_n = 1$, formula (4) gives Steffensen's method

$$x_{n+1} = x_n - \frac{F(x_n)}{(F(x_n + F(x_n)) - F(x_n))(F(x_n))}.$$
(7)

And when t = 1, $h_n = 1$, formula (4) becomes

$$x_{n+1} = x_n - \frac{F(x_n)}{F(x_n) + (F(x_n + F(x_n)) - F(x_n))(F(x_n))}.$$
(8)

The errors in applying (7) and (8) behave as

$$\varepsilon_{n+1} = \left[\frac{(F'(p)+1)F''(p)}{2F'(p)}\right] \cdot \varepsilon_n^2 + O\left(\varepsilon_n^3\right)$$

and

$$\varepsilon_{n+1} = \left[\frac{(F'(p)+1)F''(p)}{2F'(p)} + 1\right] \cdot \varepsilon_n^2 + O\left(\varepsilon_n^3\right),$$

respectively. So if ((F'(p)+1)F''(p))(2F'(p)) < -1/2, (8) converges faster than (7). This is true of Example 1 and 2 below. Let us offer some numerical tests as follows. Every example tries to find the root p of the given equation F(x) = 0 in [a, b].

EXAMPLE 1.

$$F(x) = x \cdot \exp(-x) - 0.1 = 0, \qquad [a, b] = [0, 1]$$

EXAMPLE 2.

$$F(x) = \ln(x) = 0,$$
 $[a, b] = [-0.5, 5].$

EXAMPLE 3.

$$F(x) = \operatorname{arctg}(x) = 0, \qquad [a, b] = [-1, 3].$$

EXAMPLE 4.

$$F(x) = x + 1 - \exp(\sin(x)) = 0, \qquad [a, b] = [1, 4],$$

The numerical results are illustrated in Table 1.

Example	<i>x</i> ₀	n	x_n (by formula (8))	$F(x_n)$	x_n (by Steffensen's)
1	1	7	$1.118325610352252 \times 10^{-1}$	7.1083×10^{-18}	failed
2	5	8	1.000000000000000	0	divergent
3	3	9	0.000000000000000	0	divergent
4	4	10	1.696812386809752	3.2678×10^{-16}	not convergent to p in $[a,b]$

Table 1.

REMARK 2. For finding multiple roots, the class of methods (4) with $h_n = 1$, including Steffensen's method (7), all require four evaluations of f(x), thus the efficiency index of the class of methods (4) with $h_n = 1$ is $E = \sqrt[4]{2}$.

REMARK 3. A termination criterion can be chosen such that both $|f(x_n)| < \varepsilon_1$ and $|x_n - x_{n-1}| < \varepsilon_2$ are held, where ε_1 and ε_2 indicate the assigned working precision. Theoretically, if a termination criterion is chosen such that $|f(x_n)| < \varepsilon$, then the class of methods generally cannot give better than $\varepsilon^{1/m}$, because p is a root of equation (1) of multiplicity m. However, even if p is only a simple root of equation (3) in [a, b], it is better not to choose the termination criterion such that $|F(x_n)| < \varepsilon$, for the evaluation of $F(x_n)$ involves the determination of $f(x_n)$, and as the root is approached, $f(x_n)$ and $f(x_n + \operatorname{sign}(f(x_n))|f(x_n)|^{1/m})$ will be equal to the precision of the arithmetic used, leading to the nondetermination of $F(x_n)$. Some other termination criteria could also be adopted of course, for instance, $|f(x_n + \operatorname{sign}(f(x_n))|f(x_n)||f(x_n)|^{1/m})| < \varepsilon_1$ and $|(x_n - x_{n-1})/x_n| < \varepsilon_2$, where $x_n \neq 0$.

REMARK 4. The starting value x_0 should be chosen in [a, b], where $F(a) \cdot F(b) < 0$. With regard to t, it should be chosen such that $t \cdot F(x) + (F(x + F(x)) - F(x))/(F(x)) \neq 0$ keeps in [a, b]except p. For example, we can let $t = \operatorname{sign}(F(x + F(x)) - F(x))$ such that $\operatorname{sign}(t \cdot F(x)) = \operatorname{sign}((F(x + F(x)) - F(x))/(F(x)))$.

REMARK 5. It is easy to see that formula (4) can also be used for finding simple roots of equation (1). And (4) is suitable for complex roots, too.

4. NUMERICAL EXPERIMENTS FOR MULTIPLE ZEROS

We yield the following results by using iteration formula (8) in which F(x) is determined by (2) with m = 2 and adopting the termination criterion $|f(x)| < 10^{-18}$ and $|x_n - x_{n-1}| < 10^{-8}$. PROBLEM 1.

$$f(x) = \sin^4(x) = 0,$$
 $[a, b] = [-0.7, 0.7].$

PROBLEM 2.

$$f(x) = (x - 1)^4 = 0,$$
 $[a, b] = [0.5, 1.5].$

PROBLEM 3.

$$f(x) = 1 - \cos(x - 1) = 0,$$
 $[a, b] = [0, 2].$

PROBLEM 4.

$$f(x) = \operatorname{arctg}(x) - x = 0,$$
 $[a, b] = [-0.5, 0.5],$

PROBLEM 5.

$$f(x) = \ln(1+x) - x + \frac{x^2}{2} = 0,$$
 $[a, b] = [-0.5, 1]$

Table 2.

The numerical rusults are illustrated in Table 2.

Problem	x_0	n	x_n (by formula (8))	$ f(x_n) $	$ x_n - x_{n-1} $
1	0.7	7	0.16×10^{-15}	6.5×10^{-64}	8.36×10^{-14}
2	1.5	6	0.99999999789	5.6×10^{-36}	6.27×10^{-10}
3	2.0	6	1.0000000002	0	1.17×10^{-8}
4	0.5	8	0.318×10^{-7}	1.07×10^{-23}	7.06×10^{-9}
5	1.0	6	0.118×10^{-6}	4.30×10^{-20}	2.03×10^{-10}

All the numerical experiments in this paper are performed with double precision.

5. CONCLUSION

A new method with quadratic convergence for finding multiple zeros is proposed in this paper. A new formula is offered, which replaces the given function f(x) by a new function F(x) that has simple zeros. Some numerical experiments are presented to demonstrate the efficiency and accuracy of the new method.

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