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A SECANT METHOD FOR MULTIPLE ROOTS

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Abstract.

A superlinear procedure for finding a multiple root is presented. In it the secant method is applied to the given function divided by a divided difference whose increment shrinks toward zero as the root is approached. Two function evaluations per step are required, but no derivatives need be calculated.

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1. Introduction.

We seek a method of secant type for finding a real, multiple root α of the nonlinear equation $f(x)=0$. But direct application of the secant method to f,

$$(1) \qquad x_{n+2} = x_{n+1} - (x_n - x_{n+1}) \frac{f_{n+1}}{f_n - f_{n+1}}, \quad f_i \equiv f(x_i),$$

yields a procedure whose convergence for a root of multiplicity $m>1$ apparently is linear at best (see Espelid [3], Stewart [5], and Woodhouse [7]). That is, for given initial values x_0 and x_1, the order of convergence p is 1 in

$$(2) \qquad \lim_{n\to\infty} \frac{\varepsilon_{n+1}}{\varepsilon_n^p} = K_m,$$

for errors $\varepsilon_i = x_i - \alpha$. Stewart [5] has computed K_m for various $m>1$ as the positive root of $K^m + K^{m-1} - 1 = 0$.

Since it is well known that the function $F = f/f'$ has a simple root at α (see Traub [1], p. 235, for example), we can avoid the difficulty of (slow) linear convergence by applying (1) to F instead of to f. Using F, however, requires that a derivative as well as a function value be calculated each step; moreover f' is frequently more complicated than f.

The function F may also be used in Newton's method,

$$(3) \qquad x_1 = x_0 - \frac{F_0}{F'_0} = x_0 - \frac{f_0}{f'_0} \frac{1}{1 - \dfrac{f_0 f''_0}{f'^2_0}},$$

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where here and henceforth we suppress n in the subscripts. Since F has a simple root at α, the process converges quadratically ($p=2$), whereas f itself in Newton's method yields linear convergence with $K_m=(m-1)/m$ (see Rall [2]). The price of gaining quadratic convergence is having to calculate not only f and f' but also f''.

Inspired by a procedure due to Steffensen, Esser [6] has recently proposed that the derivatives of f in (3) be replaced by divided differences. The increment $(-f)$ for these differences is not constant, however, but shrinks as the root is approached. Such a scheme is a natural way of defining differences with the desired derivative properties. Esser's method indeed is quadratic, calls for three function evaluations per step, and provides the multiplicity m as well as the root α. Its efficiency index (see Traub [1], p. 263) is $2^{\frac{1}{3}}=1.260$.

2. A method for multiple roots.

In the same spirit we propose for multiple roots that the secant method be used not with the function $F=f/f'$ but rather with

$$G = \frac{f(x)}{\dfrac{f(x-f(x))-f(x)}{(x-f(x))-x}} = \frac{-f^2(x)}{f(x-f(x))-f(x)} . \tag{4}$$

Here again f' has been replaced by a divided difference of f, with increment $(-f)$. It will be instructive to compare G with F, to see why both yield superlinear convergence when used as secant method functions.

First of all we want to find the value of F and its first three derivatives at α. Note that if the function f has a root of multiplicity m at α, then it may be written as

$$f(x) = (x-\alpha)^m g(x), \; g(\alpha) \neq 0 . \tag{5}$$

Furthermore since the secant algorithm (1) gives x_2 as a linear function of x_0 and x_1, it follows that a translation of f by $(x-\alpha)$ enables us without loss of generality to take $\alpha=0$. Consequently $F(\alpha)$ may be expressed in terms of g as

$$F(0) = \left. \frac{xg(x)}{mg(x)+xg'(x)} \right|_{x=0} = 0 , \tag{6}$$

i.e., α is a root of F. Differentiating F we see that

$$F'(0) = \left. \frac{mg^2+x^2(g'^2-gg'')}{(mg+xg')^2} \right|_{x=0} = \frac{1}{m} \neq 0 , \tag{7}$$

so that in fact α is a simple root of F. Further differentiation shows that

$$F''(0) = -\frac{2}{m^2}\frac{g'(0)}{g(0)} \tag{8}$$

and that

$$F'''(0) = \frac{6(m+1)}{m^3}\left(\frac{g'(0)}{g(0)}\right)^2 - \frac{6}{m^2}\frac{g''(0)}{g(0)}. \tag{9}$$

It is known (for example, see Anderson and Björck [4], p. 258) that the asymptotic error equation for the secant method with a function F having a simple root at α is

$$\varepsilon_2 \cong \left\{\frac{1}{2}\frac{F''(\alpha)}{F'(\alpha)}\right\}\varepsilon_0\varepsilon_1 + \left\{\frac{1}{6}\frac{F'''(\alpha)}{F'(\alpha)} - \left(\frac{1}{2}\frac{F''(\alpha)}{F'(\alpha)}\right)^2\right\}\varepsilon_0\varepsilon_1(\varepsilon_0+\varepsilon_1), \tag{10}$$

where the coefficients may be written in terms of g and its derivatives at α by means of (7), (8), and (9). This error equation shows that for any multiplicity m the secant method (1) using F is superlinear. The asymptotic convergence rate, in fact, is 1.618.

But what about the function G? We can expand $f(x-f(x))$ in a Taylor series about x to get, for small F,

$$\begin{aligned} G(x) &= \frac{-f^2(x)}{\{f(x)-f(x)f'(x)+\frac{1}{2}f^2(x)f''(x)-\frac{1}{6}f^3(x)f'''(x)+\ldots\}-f(x)} \\ &= F\{1+\tfrac{1}{2}Ff''-\tfrac{1}{6}Fff'''+\ldots+\tfrac{1}{4}F^2f''^2+\ldots\}. \end{aligned} \tag{11}$$

Evaluating at $\alpha=0$ the results of some very tedious differentiations, we conclude that G and its derivatives at any α can be written as

$$\left\{\begin{aligned} G(\alpha) &= 0 \\ G'(\alpha) &= F'(\alpha) = \frac{1}{m} \\ G''(\alpha) &= F''(\alpha)+F'^2(\alpha)f''(\alpha) = -\frac{2}{m^2}\frac{g'(\alpha)}{g(\alpha)}+\frac{1}{m^2}f''(\alpha) \\ G'''(\alpha) &= F'''(\alpha)+3F'^2(\alpha)f'''(\alpha)+3F''(\alpha)F'(\alpha)f''(\alpha) \\ &\quad +\tfrac{3}{2}F'^3(\alpha)f''^2(\alpha)-F'^2(\alpha)f'(\alpha)f'''(\alpha) \\ &= \left\{\frac{6(m+1)}{m^3}\left(\frac{g'(\alpha)}{g(\alpha)}\right)^2-\frac{6}{m^2}\frac{g''(\alpha)}{g(\alpha)}\right\}+\left\{\frac{3}{m^2}\right\}f'''(\alpha) \\ &\quad -\left\{\frac{6}{m^3}\frac{g'(\alpha)}{g(\alpha)}\right\}f''(\alpha)+\left\{\frac{3}{2m^3}\right\}f''^2(\alpha)-\left\{\frac{1}{m^2}\right\}f'(\alpha)f'''(\alpha). \end{aligned}\right. \tag{12}$$

Furthermore the derivatives of f in (12) are given in terms of g and its derivatives at the root α, and for various values of multiplicity m, as entries in the following table:

	$m=1$	$m=2$	$m=3$	$m\geqq 4$
$f'(\alpha)$	$g(\alpha)$	0	0	0
$f''(\alpha)$	$2g'(\alpha)$	$2g(\alpha)$	0	0
$f'''(\alpha)$	$3g''(\alpha)$	$6g'(\alpha)$	$6g(\alpha)$	0 .

Thus G has a simple root at α, and otherwise exhibits behavior quite similar to that of F.

When G is used in the secant method,

$$x_2 = x_1-(x_0-x_1)\frac{G_1}{G_0-G_1}, \tag{13}$$

it produces superlinear convergence. The asymptotic error equation for this, the proposed method, is

$$\varepsilon_2 \cong \left\{\frac{1}{2}\frac{G''(\alpha)}{G'(\alpha)}\right\}\varepsilon_0\varepsilon_1+\left\{\frac{1}{6}\frac{G'''(\alpha)}{G'(\alpha)}-\left(\frac{1}{2}\frac{G''(\alpha)}{G'(\alpha)}\right)^2\right\}\varepsilon_0\varepsilon_1(\varepsilon_0+\varepsilon_1). \tag{14}$$

It is well known that for this procedure the order of convergence is $p=(1+5^{\frac{1}{2}})/2=1.618$. Since the two function evaluations $f(x_1)$ and $f(x_1-f(x_1))$ are required each step, it follows that the efficiency index is $(1.618)^{\frac{1}{2}}=1.272$.

Woźniakowski [8] has shown that secant iteration such as that proposed is stable provided only that G be computed by a well-behaved algorithm.* For example, a polynomial f used in forming G should be evaluated by Horner's rule rather than term by term. Furthermore one must remember that in order to calculate a multiple root accurately it is necessary to use multiprecision arithmetic.

3. Finding the multiplicity m.

From (11) and (6) we can see that for small ε_1

$$G_1 \doteq F_1 = \frac{\varepsilon_1 g(x_1)}{mg(x_1)+\varepsilon_1 g'(x_1)} \doteq \frac{\varepsilon_1}{m}. \tag{15}$$

Similarly we know that $G_2 \doteq \varepsilon_2/m$. Furthermore $\varepsilon_2-\varepsilon_1=x_2-x_1$. Consequently when nearing the root α we can estimate its multiplicity by computing

$$m \doteq \frac{x_2-x_1}{G_2-G_1}. \tag{16}$$

Thus m is approximately the reciprocal of the divided difference of G for successive iterates x_1 and x_2. It may be computed and displayed at each step along with the current iterate.

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4. Examples.

Results from three examples computed (in quadruple precision) on an IBM 370 are shown in Tables 1–3. In each case the predicted error ε_2 as calculated from (14) is seen to be a good approximation to the actual error $x-\alpha$, and the estimated multiplicity $\underline{m}$ from (16) approaches its actual value. No careful convergence criteria were either discussed in the analysis or used in the examples. The secant method was also applied to f directly for the examples; some 47, 69, and 66 steps, respectively, were required to obtain final accuracy comparable to that of the proposed method.

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Table 1.

f	g	m	α	$g(\alpha)$	$g'(\alpha)$	$g''(\alpha)$	$G'(\alpha)$	$G''(\alpha)$	$G'''(\alpha)$
$(x-1)^2 \tan(\pi x/4)$	$\tan(\pi x/4)$	2	1	1	$\pi/2$	$\pi^2/4$	1/2	$-\pi/4$	$3\pi^2/6+3\pi/2+3/4$

$$\varepsilon_{n+2} \cong (-\pi/4+1/2)\varepsilon_n\varepsilon_{n+1}+3\pi/4\varepsilon_n\varepsilon_{n+1}(\varepsilon_n+\varepsilon_{n+1})$$

n	x	f	G	$x-\alpha$	ε	m
0	.6	.0815241	−.359569	−.4		
1	.7	.0551521	−.205290	−.3		
2	.833064	.0213742	−.0934212	−.166936	−.232168	1.1894645
3	.9441851	.00285348	−.0285632	−.0558149	−.0693915	1.7132998
4	.99312248	.0000467920	−.00344590	−.00687752	−.00754945	1.9483516
5	.999836316	.267857(−7)	−.818460(−4)	−.000163684	−.000166258	1.9957541
6	.999999660145	.115501(−12)	−.169928(−6)	−.339855(−6)	−.339961(−6)	1.9999062
7	.999999999984	.252743(−21)	−.794895(−11)	−.158979(−10)	−.158979(−10)	1.9999998

Table 2.

f	g	m	α	$g(\alpha)$	$g'(\alpha)$	$g''(\alpha)$	$G'(\alpha)$	$G''(\alpha)$	$G'''(\alpha)$
$x(x-2)^3$	x	3	2	2	1	0	1/3	−1/9	38/9

$$\varepsilon_{n+2} \cong -1/6\varepsilon_n\varepsilon_{n+1} + 25/12\varepsilon_n\varepsilon_{n+1}(\varepsilon_n+\varepsilon_{n+1})$$

n	x	f	G	$x-\alpha$	ε	m
0	1.0	−1.0	−1.0	−1.0		
1	1.1	−.8019	−.803700	−.9		
2	1.509423	−.178210	−.250516	−.490577	−3.71250	.74012233
3	1.694836	−.0481646	−.124869	−.305164	−1.35268	1.4756629
4	1.879101	−.00332062	−.0422846	−.120899	−.273133	2.2312244
5	1.9734474	−.0000369443	−.00890302	−.0265526	−.0388973	2.8263022
6	1.99861000	−.536751(−8)	−.000463443	−.00139000	−.00152117	2.9815029
7	1.99999175536	−.112084(−14)	−.00000274822	−.00000824464	−.00000829992	2.9992887
8	1.99999999806	−.146785(−25)	−.647783(−9)	−.194335(−8)	−.194339(−8)	2.9999959

Table 3.

f	g	m	α	$g(\alpha)$	$g'(\alpha)$	$g''(\alpha)$	$G'(\alpha)$	$G''(\alpha)$	$G'''(\alpha)$
$(x-2)^4/((x-1)^2+1)$	$((x-1)^2+1)^{-1}$	4	2	1/2	−1/2	1/2	1/4	1/8	3/32

$$\varepsilon_{n+2} \cong 1/4\varepsilon_n\varepsilon_{n+1}$$

n	x	f	G	$x-\alpha$	ε	m
0	3.0	.2	.386861	1.0		
1	2.9	.142321	.328118	.9		
2	2.341439	.00485487	.0946965	.341439	.225	2.3929309
3	2.114837	.0000775386	.0295811	.114837	.0768237	3.4800082
4	2.0118941	.988848(−8)	.00298239	.0118941	.00980241	3.8702061
5	2.000351611	.763957(−14)	.0000879106	.000351611	.000341469	3.9877511
6	2.00000104590	.598310(−24)	.261474(−6)	.104590(−5)	.104552(−5)	3.9996473

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