MATH 335: Numerical Analysis

Problem Set 6, Solutions

★5 **This exercise is for practice only. It will not be graded. Just do it and then use the appropriate MATLAB/OCTAVE program to check yourself.**

CP 3.4.2 Here we seek zeros of the function

$$f(V) \;=\; RT(V-b)^{-1} - a(V^2+2bV-b^2)^{-1} - P\,,$$

whose derivative is

$$f'(V) = 2a(V+b)(V^2+2bV-b^2)^{-2} - RT(V-b)^{-2}\,.$$

(This f is a function of V alone since all other symbols have values supplied.) Here are the OCTAVE commands and selected output:

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octave:1> function y = f(V)
> y = 1.618*350./(V - .3) - 365./(V.^2+.6*V-.3^2) - 778;
> end

octave:2> function y = fprime(V)
> y = 2*365*(V + .3)./(V.^2+.6*V-.3^2)^2 - 1.618*350./(V-.3)^2;
> end

octave:4> secant(@f, 1, 1.5, .000001, 25)
_______________________________________________________________
iter      xn           f(xn)       f(xn+1)-f(xn)     |xn+1-xn|
_______________________________________________________________
 0      1.000000   -210.721854
 0      1.500000   -425.364379   -214.642525      0.500000
 1      0.509133   1160.933146   1586.297525      0.990867

 9      0.800338     -0.278969      5.296654      0.003544
10      0.800152      0.002247      0.281215      0.000187
11      0.800153     -0.000001     -0.002248      0.000001
12      0.800153     -0.000000      0.000001      0.000000

octave:5> newton(@f, @fprime, 1.25, .000001, 25)
_____________________________________________________________
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iter	x	f(x)	df(x)	|xn+1-xn|
0	1.250000	-346.124208	-398.407746	
1	0.381231	4908.589358	-79659.996035	0.868769
6	0.795268	7.441485	-1539.606460	0.042666
7	0.800102	0.077677	-1507.632945	0.004833
8	0.800153	0.000009	-1507.297526	0.000052
9	0.800153	0.000000	-1507.297488	0.000000

Both methods converge to the approximate root 0.800153, with secant doing it in 12 steps and Newton in 9. Thus, if it is the case that 2 secant steps present the same amount of computation time as 1 Newton step, then secant got to the root "faster."

⋆6 We have, for $p = (1+\sqrt{5})/2$,

$$|e_{n+2}| \;=\; A|e_{n+1}|^p \;=\; A\left(A|e_n|^p\right)^p \;=\; A^{1+p}|e_n|^{p^2}\ ,$$

where $q = p^2 = (1+\sqrt{5})^2/4 = (3+\sqrt{5})/2 \doteq 2.618$. Thus, if two secant steps are like one Newton one, then the secant method is faster, having "order of convergence" at least $(3+\sqrt{5})/2$.

⋆7 (a) Our Taylor expansion says

$$g(x) \;=\; g(\alpha) + g'(\alpha)(x-\alpha) + \frac{1}{2}g''(\xi)(x-\alpha)^2 \;=\; \alpha + \frac{1}{2}g''(\xi)(x-\alpha)^2\ .$$

Thus,

$$x_{n+1} \;:=\; g(x_n) \;=\; \alpha + \frac{1}{2}g''(\xi_n)(x_n-\alpha)^2\ ,$$

where ξ_n is between x_n and α; or, subtracting α to the other side and taking absolute values,

$$|x_{n+1}-\alpha| \;=\; \frac{1}{2}|g''(\xi_n)||x_n-\alpha|^2\ .$$

To write the Taylor expansion of g we assumed that g'' is continuous in an interval $I = [\alpha-\delta, \alpha+\delta]$ surrounding α, so by the Extreme Value Theorem there is an upper bound $|g''(x)| \le M$ for all $x \in I$. So, as long as x_n is inside I we have $|x_{n+1}-\alpha| \le (M/2)|x_n-\alpha|^2$, showing *at least quadratic* convergence.

(b) We have

$$g'(x) \;=\; 1 - \frac{2f(x)f'(x)[f(x+f(x))-f(x)] - [f(x)]^2\{f'(x+f(x))[1+f'(x)] - f'(x)\}}{[f(x+f(x))-f(x)]^2}$$

$$= \quad 1 - \frac{2f(x)f'(x)}{f(x+f(x)) - f(x)} + \frac{[f(x)]^2\{f'(x+f(x))[1+f'(x)] - f'(x)\}}{[f(x+f(x)) - f(x)]^2}$$

Now, as $x \to \alpha$, continuity of f gives that $f(x) \to f(\alpha) = 0$. Thus,

$$\lim_{x\to\alpha} \frac{f(x)f'(x)}{f(x+f(x)) - f(x)} \;=\; \left(\lim_{x\to\alpha} f'(x)\right)\left(\lim_{x\to\alpha} \frac{f(x+f(x)) - f(x)}{f(x)}\right)^{-1} \;=\; \frac{f'(\alpha)}{f'(\alpha)} \;=\; 1\,.$$

Similarly,

$$\begin{aligned}
&\lim_{x\to\alpha} \frac{[f(x)]^2\{f'(x+f(x))[1+f'(x)] - f'(x)\}}{[f(x+f(x)) - f(x)]^2} \\
&= \left(\lim_{x\to\alpha} \frac{f(x+f(x)) - f(x)}{f(x)}\right)^{-2} \left\{\lim_{x\to\alpha} f'(x+f(x))[1+f'(x)] - \lim_{x\to\alpha} f'(x)\right\} \\
&= [f'(\alpha)]^{-2}\,\{f'(\alpha)[1+f'(\alpha)] - f'(\alpha)\} \;=\; 1\,.
\end{aligned}$$

Thus,

$$\begin{aligned}
g'(\alpha) &= \lim_{x\to\alpha} g'(x) \\
&= 1 - 2\lim_{x\to\alpha} \frac{f(x)f'(x)}{f(x+f(x)) - f(x)} + \lim_{x\to\alpha} \frac{[f(x)]^2\{f'(x+f(x))[1+f'(x)] - f'(x)\}}{[f(x+f(x)) - f(x)]^2} \\
&= 1 - 2(1) + 1 \;=\; 0\,.
\end{aligned}$$

By part (a), the fixed-point iteration is at least quadratically convergent.

(c) When $g'(\alpha) \neq 0$, the $(x-\alpha)$ term does not disappear. We can expand $g(x)$ with 1st-order remainder term

$$g(x) \;=\; g(\alpha) + g'(\xi)(x-\alpha) \;=\; \alpha + g'(\xi)(x-\alpha)\,,$$

and so, evaluating both ends of this equation at x_n (and using the fact that $x_{n+1} = g(x_n)$), we get

$$|x_{n+1} - \alpha| \;=\; |g'(\xi_n)||x_n - \alpha| \;\leq\; M|x_n - \alpha|\,,$$

where M is an upper bound on values of $|g'(x)|$ for x in some interval I surrounding α. Thus, we do have *at least 1st-order* convergence.

(d) This time expanding $g(x)$ in a Taylor series about α so that we have 3rd-order remainder term, we get

$$\begin{aligned}
g(x) &= g(\alpha) + g'(\alpha)(x-\alpha) + \frac{1}{2}g''(\alpha)(x-\alpha)^2 + \frac{1}{6}g'''(\xi)(x-\alpha)^2 \\
&= \alpha + \frac{1}{6}g'''(\xi)(x-\alpha)^3\,,
\end{aligned}$$

leading to

$$|x_{n+1} - \alpha| \;=\; \frac{1}{6}|g'''(\xi_n)||x_n - \alpha|^3 \;\le\; \frac{M}{6}|x_n - \alpha|^3 \,,$$

where M is an upper bound on values of $|g'''(x)|$ for x in some interval I surrounding α. Thus, we have *at 3rd-order* convergence.

<u>3.6.5</u> First, note that this iteration is $c_{n+1} = g(c_n)$ where

$$g(x) \;=\; x - \tan x \;=\; x - \frac{\sin x}{d/dx(\sin x)}$$

so it is really Newton's method applied to finding a root of $f(x) = \sin x$. In light of the previous problem, we look at

$$g'(x) = 1 - \sec^2 x \,.$$

At each root $\alpha_n = n\pi$ of $\sin x$,

$$\begin{aligned} g'(\alpha_n) &= 1 - \sec^2(n\pi) \;=\; 0 \\ g''(\alpha_n) &= -2\sec^2(n\pi)\tan(n\pi) \;=\; 0 \\ g'''(\alpha_n) &= -4\sec^2(n\pi)\tan^2(n\pi) - 2\sec^4(n\pi) \;=\; -2 \,. \end{aligned}$$

Thus, we have *at least 3rd-order* convergence.

<u>3.6.6</u> Recall from class (or from Equation (3.16), p. 88) that the error $e_n := x_n - \alpha$ at the nth step satisfies

$$e_{n+1} \;=\; -e_n^2 \frac{f''(\xi_n)}{2f'(x_n)} \,.$$

Thus,

$$|e_{n+1}| \;=\; |e_n|^2 \left|\frac{f''(\xi_n)}{2f'(x_n)}\right| \;\le\; |e_n|^2 \frac{4}{2\cdot 2} \;=\; |e_n|^2 \,.$$

We then have the following error bounds:

n	1	2	3
bound on e_n	1/9	1/81	1/6561