

MATH 335: Numerical Analysis

Problem Set 6, Final version

Due Date: Mon., Feb. 23, 2009

Read Sections 3.4, 3.6 and 3.7 in Kharab & Guenther.

★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. Let $f(x) = x^3 - x - 1$. Calculate the first two iterates (approximating a zero of f) by hand using

- (a) the false position method, with $a_0 = 1.2$ and $b_0 = 1.4$. (By “next two iterates” here, I mean the next two bracketing intervals $[a_1, b_1]$ and $[a_2, b_2]$.)
- (b) Newton’s method, with $x_0 = 1.4$.
- (c) the secant method, with $x_0 = 1.2$ and $x_1 = 1.3$.

CP 3.4.2 The Peng-Robinson equation of state is given by

$$P = \frac{RT}{V - b} - \frac{a}{V(V + b) + b(V - b)},$$

where

P = Pressure,

V = Molar Volume, volume of one mole of gas or liquid,

T = Temperature (degrees K),

R = ideal gas constant.

Find V at $P = 778$ kPa and $T = 350$ K with $a = 365$ m⁶kPa/(kg mole)², $b = 0.3$ m³/kg mole, and $R = 1.618$. Use the secant method with $V_0 = 1.0$ and $V_1 = 1.5$ as initial estimates.

Determine this same V using Newton’s method with initial estimate $x_0 = 1.25$. Do the two methods converge to the same solution? Does Newton’s method require fewer than half the steps required by the secant method?

★6 The secant and Newton’s methods generate a sequence (x_n) which often converges to a root α of some function f of interest. Let us define the error at the n th step to be $e_n := \alpha - x_n$. In class we showed that, under ideal circumstances, these errors for Newton’s method satisfy $|e_{n+1}| \leq C|e_n|^2$ (i.e., Newton’s method converges at least

quadratically). Though we did not carry out the details, we asserted that the errors for the secant method satisfy $|e_{n+1}| \approx A|e_n|^p$ where $p = (1 + \sqrt{5})/2 \doteq 1.62$ (superlinear convergence). From this standpoint, Newton's method appears to be faster than the secant method. Nevertheless, we pointed out that the secant method requires only one new function evaluation per iteration whereas Newton requires two. Given that function evaluations often represent a significant portion of the computation time at each step, it may be more fair to compare two steps of the secant method with one step of Newton's. Use the relationship

$$|e_{n+1}| = A|e_n|^p, \quad p = \frac{1 + \sqrt{5}}{2}$$

to determine a relationship

$$|e_{n+2}| = B|e_n|^q$$

(most importantly, determine the value of q) to see how, under this two-secant-steps-to-one-Newton-step point of view, the two methods compare.

- ★7 (a) Assume that α is a fixed-point of a function g . Write out a Taylor expansion with 2nd-order remainder of $g(x)$, centering this expansion on α . Use it to show that, when $g'(\alpha) = 0$, the fixed-point iteration method

$$x_0 \text{ given,} \quad x_{n+1} = g(x_n)$$

is at least quadratically convergent.

- (b) **This part is optional, but read regardless.** Under suitable conditions on f , we showed that $g(x) := x - f(x)/f'(x)$ satisfied $g'(\alpha) = 0$ when $f(\alpha) = 0$. Your work in (a), then, provides an alternative method (to what we did in class) of showing Newton's method is quadratically convergent. Take yet another alteration of Newton: given x_0 , set

$$x_{n+1} = g(x_n), \quad \text{where} \quad g(x) := x - \frac{[f(x)]^2}{f(x + f(x)) - f(x)}.$$

Show that this scheme is also (at least) quadratically convergent (yet, obviously, avoids having to compute derivative values).

- (c) What if $g'(\alpha) \neq 0$? What breaks down in your demonstration of quadratic convergence in part (a)? Can you still show *at least linear* convergence? Compare with Example 3.13 in the text (pp. 90-92; in particular, Table 3.7).
- (d) What can be said about the order of convergence if, in addition to $g'(\alpha) = 0$, we have $g''(\alpha) = 0$?

3.6.5 Prove that the iteration

$$c_0 = 3, \quad c_{n+1} = c_n - \tan c_n, \quad n = 1, 2, \dots$$

converges. Find the order of convergence.

3.6.6 If f is such that $|f''(x)| \leq 4$ for all x and $|f'(x)| \geq 2$ for all x , and if the initial error in Newton's method is less than $1/3$, what is an upper bound on the error at each of the first 3 steps?