Computational Physics
Homework 1

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1 Problem a

Write a program to carry out the rootfinding algorithms and keep it flexible

1.1 Description of program

define functions for each method. keep it general so the function is input at the start. I've kept the option to turn 'verbose' off in which case the algorithm just returns the best estimate.

For bracketing methods a variable 'switch' was introduced which was used to distiguish between functions that went minus to plus and those that went plus to minus. In this way there is no need (at least in the bisection method) to keep a value of f(x) stored anywhere.

2 Problem b

run on some known functions

2.1 functions used

- $f(x) = x^2 - 2$
- $f(x) = \tanh(x)$
- $f(x) = \sin(x)$
- $f(x) = \cot(x)$

2.2 questions

- the errors decrease according to the theory until they hit the maximum precision allowed by the data type used.
- roundoff error doesn't seem to effect the algorithm except that it limits the accuracy of the final answer to be that of the data type
- increasing the initial condition to be far from x_* can cause Newton and secant to go crazy (e.g. $f(x) = \tan(x)$) but for some functions it doesn't make much difference (e.g. $f(x) = x^2 - 2$)).

3 Problem c

run on functions with multiple roots

3.1 functions used

- $f(x) = sin^2(x)$
- $f(x) = sin^3(x)$

3.2 questions

the errors converge much slower than expected for Newton and secant methods. Regula falsi and bisection are unaffected for the most part except that, as the function has the same sign on either side of the root in the case of double roots, it is not possible to bracket the root in the same way.

4 Problem d

automatically stop iterating when a certain accuracy is reached. then test on some functions

4.1 description of program

for methods that maintain bracketing I stopped when the bracket was narrower than the required accuracy. If just one estimate was made per iteration I compared this to the previous estimate and stopped when they differed by less than the required accuracy.

4.2 functions used

- $f(x) = e^x - 1$
- $f(x) = \frac{1}{x}$
- $f(x) = x^1 1$
- $f(x) = xe^{-\frac{1}{x^2}}$

4.3 questions

for $e^x - 1$ all methods worked and honed into the correct solution. for $\frac{1}{x}$ Newton and secant methods diverged horribly and couldn't find the answer. For $x^1 1$ Newton and Secant converged very very slowly to the point where they ran up to the maximum allowed iterations (which I set at 200). $xe^{-\frac{1}{x^2}}$ was even stranger because even the bisection method failed. This is because as x neared the root the computer was unable to distinguish $f(x)$ from zero and so was not able to correctly determine the sign.