Programming Assignment 4 Foundations of Computational Mathematics 1 Fall 2024

The solutions are due on Canvas by 11:59 PM on Monday December 9, 2024

General Task

Your task is to implement and demonstrate the capabilities of the methods discussed in the class: Regula Falsi, Secant method, (modified) Newton's method by answer questions motivated by Study Questions Set 6 using targetted empirical observations. You will also use the quadratically convergent Steffensen's method described next.

Steffensen's Method: Newtons method achieves quadratic convergence to a simple root of $f(x)$ by requiring the availability and evaluation each step of the derivative $f'(x)$. There is an alternate technique used to build methods that converge quadraticlly to a simple root but do not evaluate $f'(x)$. This is done using a nested evaluation of $f(x)$.

Steffensen's method for finding the roots of a nonlinear scalar function, $f(x)$, is defined by:

$$\theta(x_k) = \frac{f(x_k + f(x_k)) - f(x_k)}{f(x_k)}$$

$$g(x_k) = x_k - \frac{f(x_k)}{\theta(x_k)}$$

$$x_{k+1} = g(x_k)$$

where $x_k \in \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$. This method replaces $f'(x_k)$ with the difference approximation given by $\theta(x_k)$. Note that it can also be written as

$$x_{k+1} = x_k - \frac{f(x_k)^2}{f(x_k + f(x_k)) - f(x_k)}.$$

As with all of the rootfinding methods, care must be taken as $f(x_k)$ gets small in magnitude, i.e., as x_k converges to a root.

Experiments and Observations

You are not required to perform and condense a large number of experiments and their results. Simply run a few tests for each question and then select a small number to display and make your answer clear. This is similar to what is done in many of the homework and study questions answers and in the class notes/lectures. Also, remember the discussions in the lectures on convergence rate being an asymptotic statement and the description of how a higher order method displays its superior convergence rate in the sequence of x_k and $f(x_k)$.

Higher Order Roots

Consider Problem 6.2 in Study Question Set 2 and its solution. Change your Newton's method code to include the scalar m (which should be a floating point varialble even though here it will always be positive integer value corresponding to the multiplicity of the root sought) to the update of x_k. Clearly, taking $m = 1.0$ will correspond to the standard Newton's method.

Consider problems of the form $f(x) = (x - \rho)^d$, i.e., a single root at ρ of multiplicity d.

1. Use standard Newton's method, i.e., $m = 1$, and empirically demonstrate the convergence rate trends as you take $d = 2, 3, \ldots$. You should demonstrate the behavior with two to three different x_0 for each d and record your observations on the behavior.

2. Use modified Newton's method with $m = d$, and empirically demonstrate the convergence rate trends as you take $d = 2, 3, \ldots$. You should demonstrate the behavior with two to three different x_0 for each d and record your observations on the behavior.

3. How fast does Steffensen's method converge for $d = 2, 3, \ldots$? Does it appear quadratic?

4. Describe and comment on the behavior of Regula Falsi and Secant for $d = 2, 3, \ldots$. How does your choice of the two initial points required for each affect the convergence behavior?

5. What happens for these methods when $d = 1$?

6. Suppose $d \geq 2$ and $m \neq d$, i.e., suppose you have set m to something other than the degree of the root ρ. What is the behavior of modified Newton's method for $m > d$ and $m < d$? Does it still converge? If so, what rate does it appear to have? Does it diverge for any of your choices of m, d and x_0?

Distinct Roots and Trends as They Coalesce

Consider Problem 6.7 in Study Question Set 2 and its solution.

Three Distinct Roots and Newton compared to the Other Methods

Consider the generic cubic polynomial used in the problem with three distinct roots 0, $\rho > 0$ and $-\rho$ with the following form and properties:

$$f(x) = x(x-\rho)(x+\rho) = x^3 - \rho^2 x, \quad \rho > 0$$

$$f'(x) = 3x^2 - \rho^2 = 3(x^2 - \alpha^2) = 3(x-\alpha)(x+\alpha), \quad \alpha = \rho/\sqrt{3} > 0$$

Study Question 6.7 analyzes the behavior of Newton's method on the intervals

$$x > \rho$$

$$\alpha < x < \rho$$

$$-\xi < x < \xi$$

where ξ is the "cycling point" of Newton's method for this $f(x)$.

1. Demonstrate all of the behaviors give in the solution.
2. When examining the cycling behavior specifically address the observed behavior considering that ξ is almost certainly not representable exactly as a floating point number and therefore you are actually using an x_0 that is a floating point number slightly different the actual $\xi \in \mathbb{R}$. Consider the behvior as you take $x_0 = \xi \pm \epsilon$ for $\epsilon > 0$ with increasing values. Does the iteration actually cycle when $x_0 = \xi$ is use, i.e., x_0 is the floating point version of ξ given when you evaluate it in floating point?
3. For what values of x_0 does Newton's iteration move far away from x_0 yet still converges to one of the roots?
4. Is it possible to make Newton's method fail by producing numbers that are undefined or too large for the floating point system?
5. Compare the behavior of Regula Falsi, Secant and Steffensen' methods to Newton's method. What choices of the initial two points for Regular Falsi and Secant cause trouble for the methods? Does Steffensen's method demonstrate quadratic convergence like Newton's method? If so does it do so using the same x_0 values as Newton's method?

Scaling

Now suppose you replace the function $f(x)$ with $\tilde{f}(x) = \sigma f(x)$ where $\sigma > 0$.

1. How does this affect the behavior of Newton's method as σ grows larger?
2. How does this affect the behavior of the other methods?

Root Coalescing

Consider the function

$$\hat{f}(x) = x(x - \rho_1)(x - \rho_2) \quad \rho_1 > 0, \quad \rho_2 > 0$$

that has roots $0 < \rho_1 < \rho_2$.

These questions investigate the gradual degradation of the convergence rate from quadratic to linear to slower linear, i.e., linear with a larger contraction constant (see the slides on this as a function of the degree of the root).

1. What happens to the behavior of Newton's method as you take ρ_1 closer and closer to 0?

2. What happens to the behavior of Newton's method as you take ρ_1 **and** ρ_2 closer and closer to 0?

3. How does this afffect the behavior of the Secant Method?