Computational Science:
Computational Methods in Engineering

Introduction to Root Finding Methods

Outline

- Introduction
- Multiple Roots
- Conclusions

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Introduction

What is Root Finding?

What values of x makes $f(x) = 0$?

$$\text{Let } f(x) = ax^2 + bx + c = 0$$

This is easily solved algebraically

$$x_r = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

But what if…

$$f(x) = e^x - x = 0$$

This cannot be solved analytically.
A numerical method must be used.

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Root Finding Methods

- Bracketing Methods
  - Finding a single root that falls within a known range.
  - Very robust
  - Must know something ahead of time.
- Open Methods
  - Trial-and-error iterative methods
  - Do not need bounds, only an initial guess.
  - More efficient than bracketing methods
  - Can be unstable and not find a solution
- Roots of Polynomials
  - Algorithm specific to polynomials
  - Physics of your problem must be fit to a polynomial
  - Able to find all roots.

Requires initial bounds
$$x_{\mathrm{L}} \leq x_{\mathrm{r}} \leq x_{\mathrm{U}}$$

Requires an initial guess
$$x_{\mathrm{r}} \approx x_1$$

Requires multiple points
$$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$$

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Multiple Roots

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What are Multiple Roots?

Function with a single root: $x-2=0$

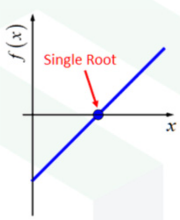
Function with a double root: $x^2-6x+9=(x-3)(x-3)=0$

Function with a triple root: $x^3-21x^2+147x-343=(x-7)(x-7)(x-7)=0$

Recognizing Number of Roots

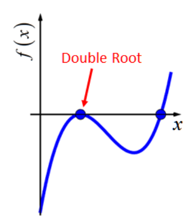
Single Root

- Sign changes on either side of root.
  $f(x_r-\delta)f(x_r+\delta)<0$
- Slope at root is not zero.
  $f'(x_r)\neq 0$



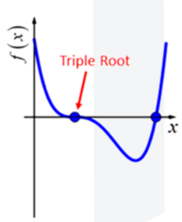
Double Root

- Sign is same on either side of root.
  $f(x_r-\delta)f(x_r+\delta)>0$
- Slope at root is zero.
  $f'(x_r)=0$
- Curvature is same on either side of root.
  $f''(x_r-\delta)f''(x_r+\delta)>0$



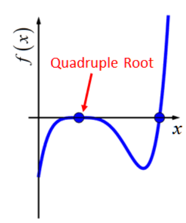
Triple Root

- Sign changes on either side of root.
  $f(x_r-\delta)f(x_r+\delta)<0$
- Slope at root is zero.
  $f'(x_r)=0$
- Curvature changes on either side of root.
  $f''(x_r-\delta)f''(x_r+\delta)<0$



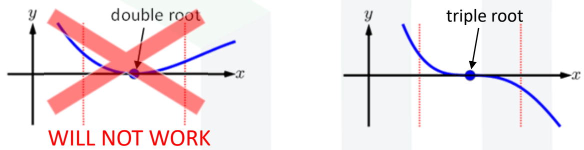
Quadruple Root

- Sign is same on either side of root.
  $f(x_r-\delta)f(x_r+\delta)>0$
- Slope at root is zero.
  $f'(x_r)=0$
- Curvature is same on either side of root.
  $f''(x_r-\delta)f''(x_r+\delta)>0$
- Curvature is broad and flat.



Problem with Multiple Roots: *Bracketing Methods*

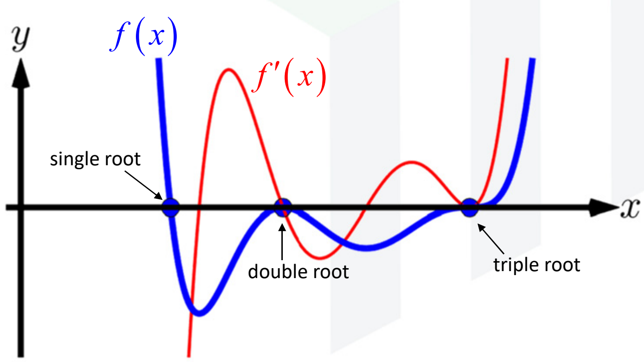
Bracketing methods require a sign change on either side of the root. This means they only work for an odd number of roots.



Problem with Multiple Roots: *Open Methods*

The update equation for both Newton-Raphson method and secant method involved $f(x)/f'(x)$.

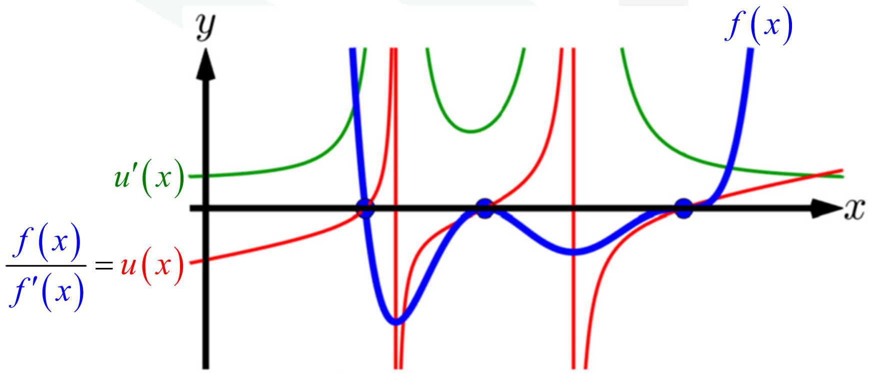
When there are multiple roots, both $f(x)$ and $f'(x)$ can go to zero at the root. This causes a divide by zero problem.



$$\frac{f(x)}{f'(x)} = \frac{0}{0} = \text{undefined}$$

The Fix

Define an auxiliary function $u(x)$ that will have the same roots as $f(x)$ but: (1) will always change sign on either side of any multiple root, and (2) who's derivative $u'(x)$ will not go to zero at the roots.



This is the same auxiliary function used for bracketing methods.

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Conclusions

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Generalizing Root Finding Algorithms

Root finding algorithms find values of x such that $f(x) = 0$.

What if it is desired to find values of x such that $f(x) = a$?

Generalization

$$f(x) = a$$

$$f(x) - a = 0$$

$$\text{Let } g(x) = f(x) - a$$

Now perform standard root finding on $g(x)$.

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Preliminary Root Location

The basic root finding algorithms all require that a root be roughly located. The root finding algorithm only refines the location of the root.

This means approximate locations of the roots must be somehow determined. This can be accomplished several ways.

1. Something is known about the physics of the problem being solved that provides information about where the roots should be.
2. If nothing else is known, plot the function to identify the rough location of the roots and feed each of those rough locations into a root-finding algorithm. Several plots may have to be generated while experimenting with axis scaling to find the roots.

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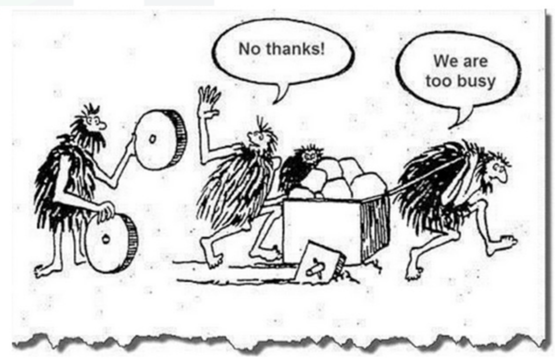
Need for Better Algorithms

In many circumstances, a single computation of $f(x)$ may take hours, days, weeks or much longer! In these cases it is highly desired to minimize the total number of computations of $f(x)$.

It is often worth the investment of a few hours to write an awesome code that runs in an hour than waiting days or weeks for the answer to come from a simple code you wrote in a few minutes.



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