ASTR 119: Session 8 Root finding Bisection & Newton-Raphson

Outline

- 1) Homework due 10/29 at 8:00am
- 2) Visualization of the Day
- 3) Root finding: Bisection Search
- 4) Root finding: Newton-Raphson
- 5) Save your work to GitHub



Homework, due Oct 29, 8:00am

1) Write a jupyter notebook to perform Bisection Search root finding. Numerically find the two roots of the function:

$$f(x) = 1.01x^2 - 3.04x + 2.07$$

Use a tolerance of 1.0e-6 for the allowed deviation of f(x) from 0.

- 2) Given your starting guesses for the bracketing values around the roots, how many iterations does your method take to converge?
- 3) Have your notebook make a plot of f(x) vs. x as a line, and indicated with differently colored points your initial bracketing values and the roots. In the plot, use limits of x=[0,3] and y=[-0.5, 2.1]. Add a horizontal line at y=0. Plot f(x) at a 1000 evenly spaced values of x=[0,3].
- 4) Create an issue for your repository and tag your TA. CLEAR ALL THE CELLS BEFORE YOU COMMIT THE NOTEBOOK.
- 5) Your TA will clone your code and email you commented version of the code and a grade. To get the full grade possible, all the notebooks will need to run to completion without errors and produce the requested plots.
- 6) Call the repository "astr-119-hw-4" and the notebook "hw-4.ipynb".

Algorithm for Bisection method

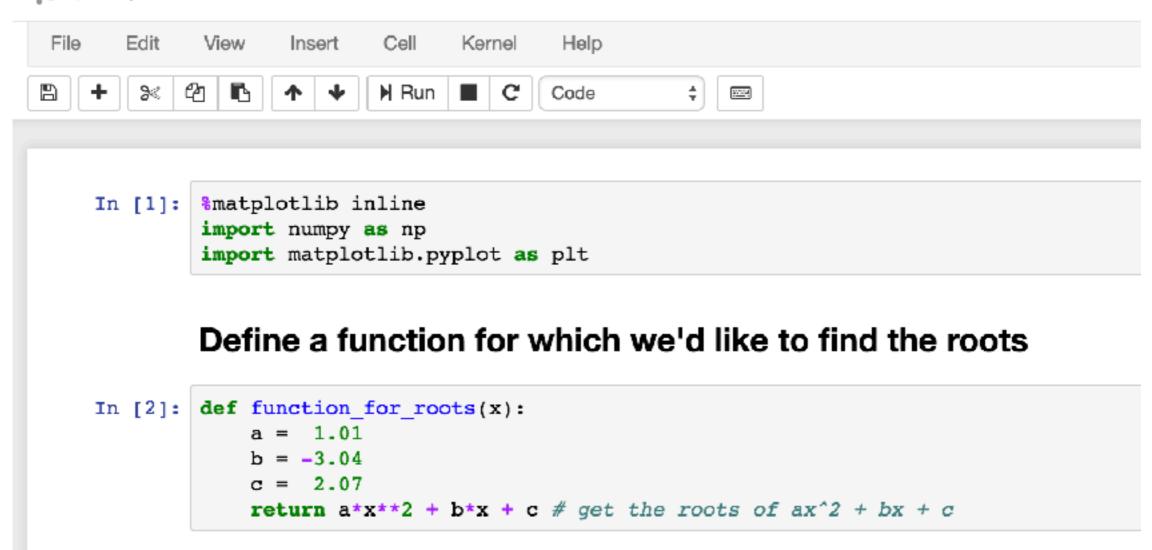
- 1. Declare variables.
- 2. Set maximum number of iterations to perform.
- 3. Set tolerance to a small value (eg. 1.0e-6). 4. Set the two initial bracket values.
 - (a) Check that the values bracket a root or singularity.
 - (b) Determine value of function fnct at the two bracket values.
 - (c) Make sure produce of functional values is less than 0.0. If not, then report this and stop.
 - (d) If the absolute value of one of the functional values is less than tolerance, then a root is found and write value to terminal and stop.
- 5. Set the counter of the number of iterations to zero. 6. Begin Bisection loop
 - (a) Find value midway between bracket values.
 - (b) Determine functional value at this midpoint.
 - (c) If the absolute value of function value at midpoint is less than tolerance, then exit Bisection loop.
 - (d) If produce of functional values at midpoint and at one of the endpoints is greater than zero, then replace this endpoint and its functional value with midpoint and its functional value.
 - (e) Otherwise, replace the other endpoint and its functional value with midpoint and its functional value.
 - (f) Increment the count of the number of iterations.
 - (g) If we have exceeded the maximum number of iterations, then exit Bisection loop.
- 7. End Bisection Loop
- 8. If root was not found in maximum number of iterations, write a warning message to the terminal.
- 9. Write to screen the value of root

Function funct: Given 1 argument (type float):

- 1. Declare any additional variables.
- 2. Calculate value of function at the given point.
- 3. Return value as a float.



Jupyter bisection_search_demo Last Checkpoint: a few seconds ago (autosaved)



We need a function to check whether our initial values are valid

```
In [9]: def check_initial_values(f, x_min, x_max, tol):
             #check our initial guesses
            y min = f(x min)
            y max = f(x max)
             #check that x min and x max contain a zero crossing
             if(y_min*y_max>=0.0):
                 print("No zero crossing found in the range = ",x min,x max)
                 s = "f(%f) = %f, f(%f) = %f" % (x min, y min, x max, y max)
                 print(s)
                 return 0
             # if x min is a root, then return flag == 1
             if(np.fabs(y min)<tol):</pre>
                 return 1
             # if x max is a root, then return flag == 2
             if(np.fabs(y max)<tol):</pre>
                 return 2
             #if we reach this point, the bracket is valid
             #and we will return 3
             return 3
```

Now we will define the main work function that actually performs the iterative search

```
def bisection root finding(f, x min start, x max start, tol):
    # this function uses bisection search to find a root
   x \min = x \min start
                            #minimum x in bracket
                            #maximum x in bracket
   x max = x max start
   x mid = 0.0
                             #mid point
   y min = f(x min) #function value at x min
   y max = f(x max) #function value at x max
   y mid = 0.0
                     #function value at mid point
    imax = 10000
                     #set a maximum number of iterations
                     #iteration counter
    i = 0
    #check the initial values
   flag = check_initial_values(f,x min,x max,tol)
    if(flag==0):
        print("Error in bisection root finding().")
       raise ValueError('Initial values invalid',x min,x max)
   elif(flag==1):
       # lucky guess
       return x min
   elif(flag==2):
       # another lucky guess
        return x max
   #if we reach here, then we need to conduct the search
```

```
#if we reach here, then we need to conduct the search
#set a flag
flag = 1
#enter a while loop
while(flag):
    x_mid = 0.5*(x_min+x_max) #mid point
   y mid = f(x mid) #function value at x mid
    #check if x mid is a root
    if(np.fabs(y_mid)<tol):</pre>
        flag = 0
    else:
        #x mid is not a root
        #if the product of the function at the midpoint
        #and at one of the end points is greater than
        #zero, replace this end point
        if(f(x_min)*f(x_mid)>0):
            #replace x min with x mid
            x \min = x \min d
        else:
            #replace x max with x mid
            x max = x mid
    #print out the iteration
    print(x_min,f(x_min),x_max,f(x_max))
```

```
#print out the iteration
    print(x min,f(x min),x max,f(x max))
    #count the iteration
    i += 1
    #if we have exceeded the max number
    #of iterations, exit
    if(i>=imax):
        print("Exceeded max number of iterations = ",i)
        s = "Min bracket f(%f) = %f" % (x_min,f(x_min))
        print(s)
        s = \text{"Max bracket } f(%f) = %f" % (x max, f(x max))
        print(s)
        s = "Mid bracket f(%f) = %f" % (x_mid,f(x_mid))
        print(s)
        raise StopIteration('Stopping iterations after ',i)
#we are done!
return x mid
```

Perform the search

```
In [57]: x min = 0.0
         x max = 1.5
         tolerance = 1.0e-6
         #print the initial guess
         print(x min, function for roots(x min))
         print(x max, function for roots(x max))
         x_root = bisection_root_finding(function_for_roots,x_min,x_max,tolerance)
         y_root = function_for_roots(x_root)
         s = "Root found with y(%f) = %f" % (x_root,y_root)
         print(s)
         0.0 2.07
         1.5 -0.21750000000000007
         0.75 0.358124999999996 1.5 -0.2175000000000007
         0.75 0.3581249999999996 1.125 <math>-0.07171875000000005
         0.9375 0.10769531249999975 1.125 -0.07171875000000005
         1.03125 0.009111328124999485 1.125 -0.07171875000000005
         1.03125 0.009111328124999485 1.078125 -0.033522949218749876
         1.03125 0.009111328124999485 1.0546875 -0.012760620117187482
         1.03125 \ 0.009111328124999485 \ 1.04296875 \ -0.0019633483886720704
         1.037109375 0.0035393142700193003 1.04296875 -0.0019633483886720704
         1.0400390625 0.0007793140411376243 1.04296875 -0.0019633483886720704
         1.0400390625 0.0007793140411376243 1.04150390625 -0.0005941843986509987
         1.040771484375 9.202301502186927e-05 1.04150390625 -0.0005941843986509987
         1.040771484375 9.202301502186927e-05 1.0411376953125 -0.0002512161433698701
         1.040771484375 9.202301502186927e-05 1.04095458984375 -7.963042706249368e-05
         1.040863037109375 6.1878282573424315e-06 1.04095458984375 -7.963042706249368e-05
         1.040863037109375 6.1878282573424315e-06 1.0409088134765625 -3.6723415833161965e-05
         1.040863037109375 6.1878282573424315e-06 1.0408859252929688 -1.5268322895334308e-05
         1.040863037109375 6.1878282573424315e-06 1.0408744812011719 -4.540379595852073e-06
         1.040863037109375 6.1878282573424315e-06 1.0408744812011719 -4.540379595852073e-06
         Root found with y(1.040869) = 0.000001
```

Newton-Raphson Root Finding

Consider the Taylor series approximation of f(x) about position x_i :

$$f(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{(x - x_i)^2}{2!}f''(x_i) + \dots$$

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$$f(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{(x - x_i)^2}{2!}f''(x_i) + \dots$$

We want to find where f(x)=0. We can make a guess at the value of the root x by using the Taylor expansion to linear order to find an approximation to the root, x_{i+1} :

$$\tilde{f}(x) = f(x_i) + (x - x_i)f'(x_i)$$

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$$\tilde{f}(x) = f(x_i) + (x - x_i)f'(x_i)$$

IF
$$\tilde{f}(x_{i+1}) = 0$$
 then $x_{i+1} = x_i - f(x_i)/f'(x_i)$

Consider the Taylor series approximation of f(x) about position x_i :

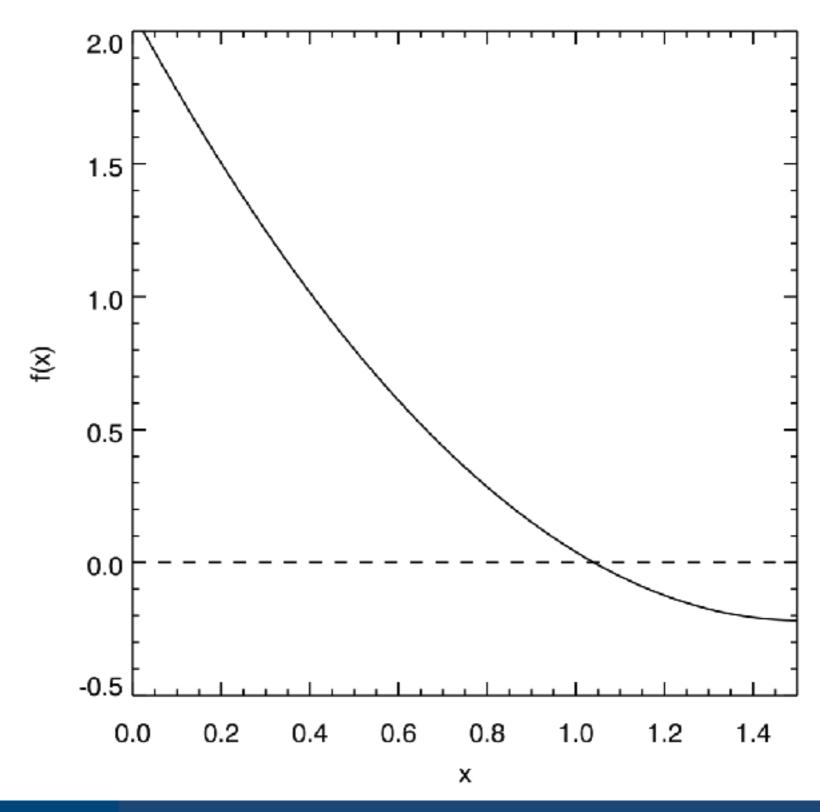
$$f(x) = f(x_i) + (x - x_i)f'(x_i) + \frac{(x - x_i)^2}{2!}f''(x_i) + \dots$$

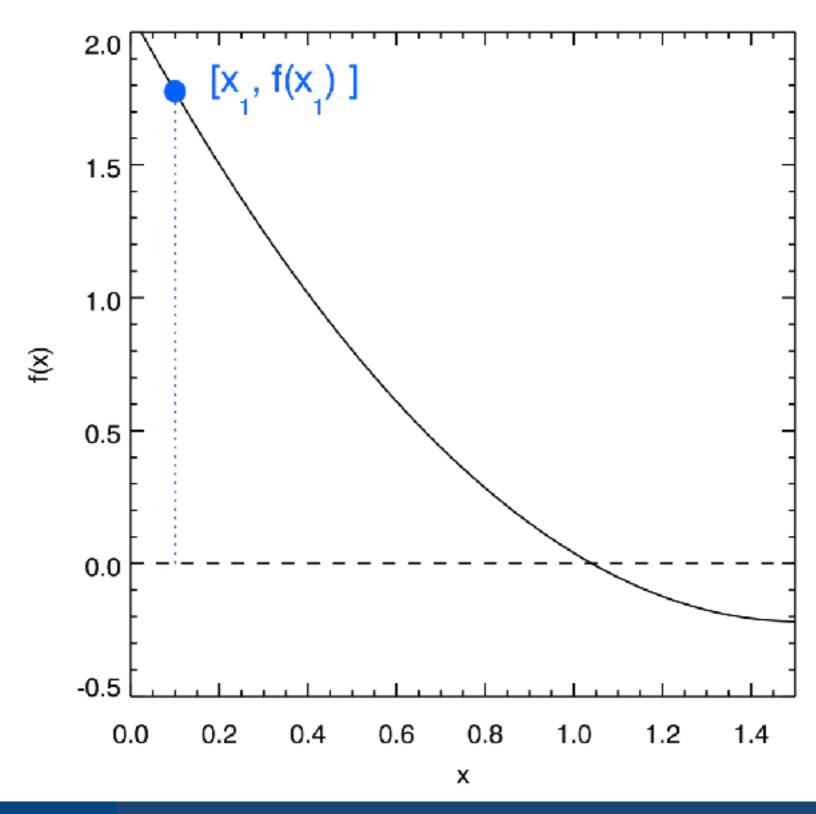
We want to find where f(x)=0. We can make a guess at the value of the root x by using the Taylor expansion to linear order to find an approximation to the root, x_{i+1} :

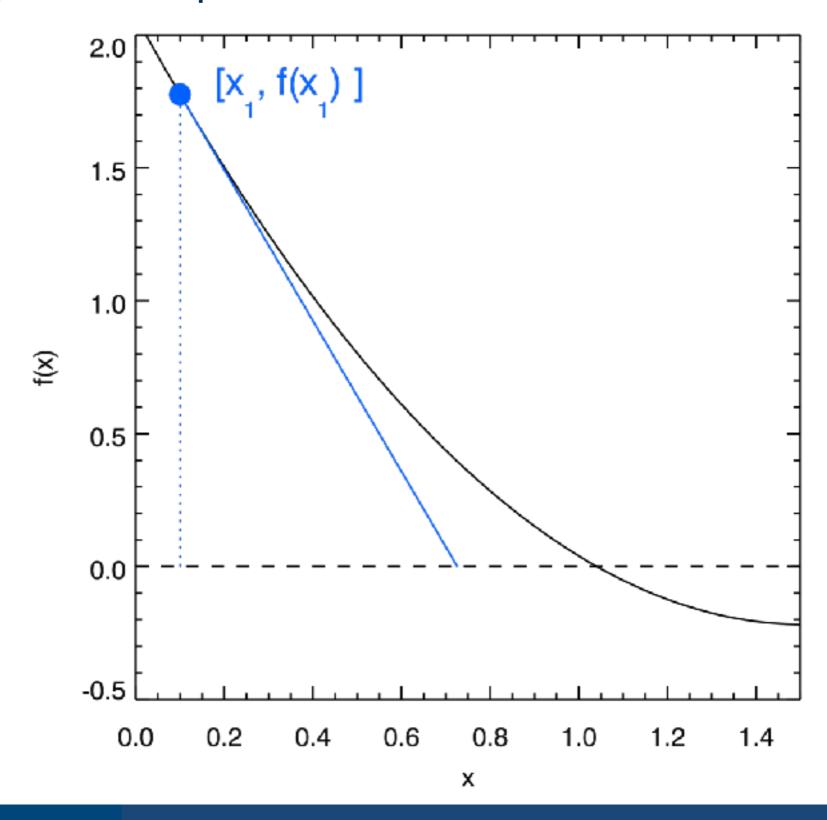
$$\tilde{f}(x) = f(x_i) + (x - x_i)f'(x_i)$$

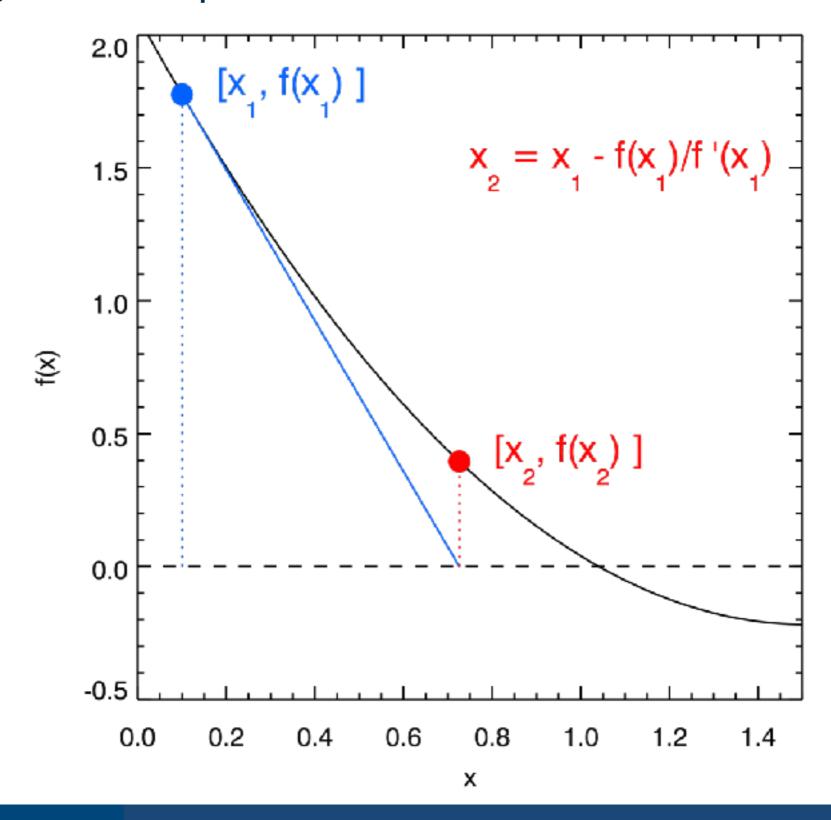
IF
$$\tilde{f}(x_{i+1}) = 0$$
 then $x_{i+1} = x_i - f(x_i)/f'(x_i)$

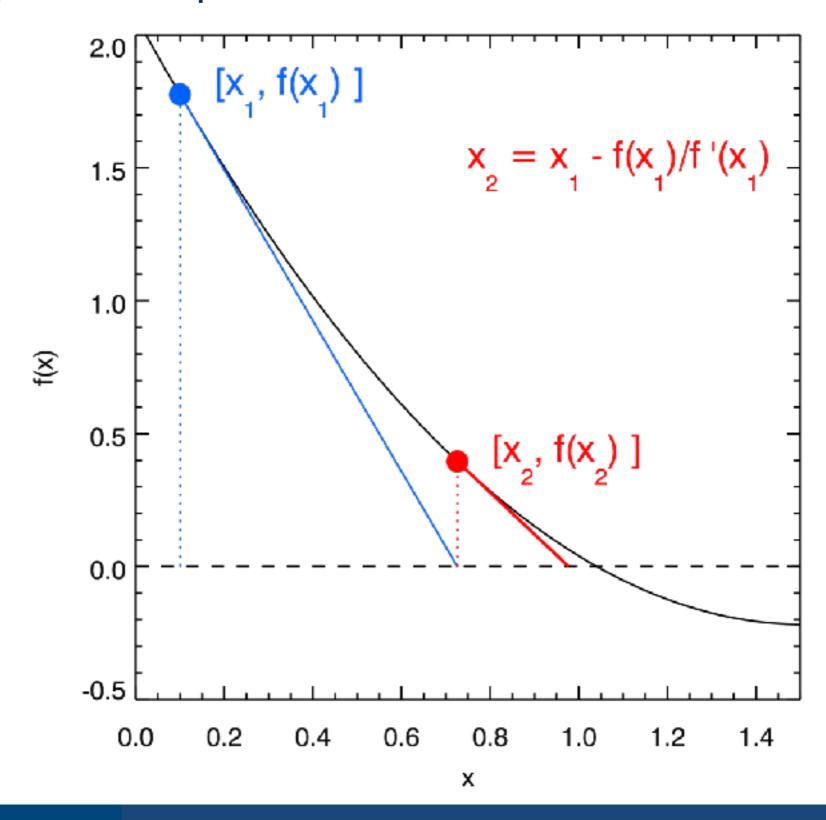
We can then replace x_i with x_{i+1} , and try again until $f(x_i) = 0$.

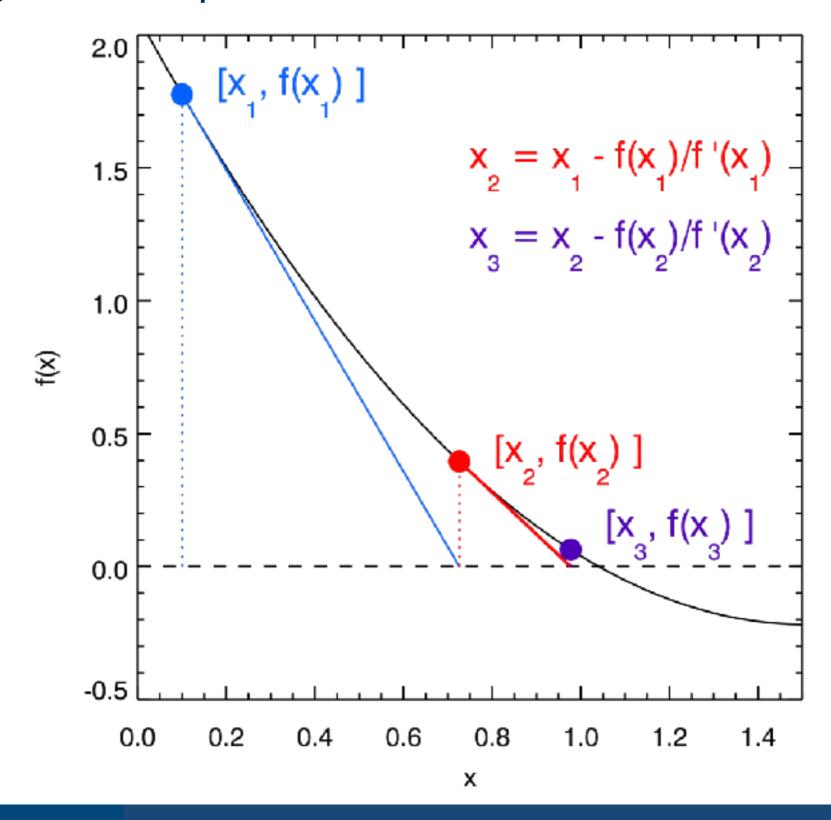












ALGORITHM FOR NEWTON-RAPHSON

Function fnct: Given 1 argument (type float):

- 1. Declare any additional variables.
- 2. Calculate value of function at the given point.
- 3. Return value as a float.

Function fnct_prime: Given 1 argument (type float):

- 1. Declare any additional variables.
- 2. Calculate the value of derivative of the function at the given point.
- 3. Return value as a float.



ALGORITHM FOR NEWTON-RAPHSON

- 1. Declare variables.
- 2. Set maximum number of iterations to perform.
- 3. Set tolerance to a small value (eg. 1.0e-6).
- 4. Set the initial guess. Set an iteration counter to zero.
- 5. Begin Newton-Raphson loop
 - (a) Find next guess via new_root = root fnct(root)/fnct_prime(root)
 - (b) If the absolute value of fnct(new_root) is less than tolerance, then a root is found and write value to terminal and stop.
 - (c) Increment the count of the number of iterations.
 - (d) If we have exceeded the maximum number of iterations, then stop Newton-Raphson loop.
- 6. If root was not found in maximum number of iterations, write a warning message to the terminal.
- 7. Write to terminal the value of root and number of iterations performed.

A Newton-Raphson Root Finding Implementation

```
* matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
```

Define the function for root finding

```
def function_for_root(x):
    a = 1.01
    b = -3.04
    c = 2.07
    return a*x**2 + b*x + c
```

Define the function's derivative

```
def derivative_for_root(x):
    a = 1.01
    b = -3.04
    return 2*a*x + b
```

Define the primary work function

```
def newton_raphson_root_finding(f, dfdx, x_start, tol):
    # this function uses newton-raphson search to find a root
    #set a flag
    flag = 1
    #set a maximum number of iterations
    imax = 10000
    #start a counter
    i = 0
    #define the new and old guesses
    x \text{ old} = x \text{ start}
    x new = 0.0
    y_new = 0.0
```

```
#start the loop
while(flag):
    #make a new quess
    x \text{ new} = x \text{ old} - f(x \text{ old})/dfdx(x \text{ old})
    #print out the iteration
    print(x new,x old,f(x old),dfdx(x old))
    #if the abs value of the new function value
    #is < tol, then stop
    y new = f(x new)
    if(np.fabs(y new)<tol):</pre>
         flag = 0 #stop the iteration
    else:
         #save the result
         x \text{ old} = x \text{ new}
         #increment the iteration
         i += 1
    if(i>=imax):
         printf("Max iterations reached.")
         raise StopIteration('Stopping iterations after ',i)
#we are done!
return x new
```

Perform the search

```
x_start = 0.5
tolerance = 1.0e-6

#print the initial guess
print(x_start,function_for_root(x_start))

x_root = newton_raphson_root_finding(function_for_root,derivative_for_root,x_start,tolerance)
y_root = function_for_root(x_root)

s = "Root found with y(%f) = %f" % (x_root,y_root)
print(s)
```

Perform the search

```
x  start = 0.5
tolerance = 1.0e-6
#print the initial guess
print(x start,function_for_root(x_start))
x root = newton raphson root finding(function for root, derivative for root, x start, tolerance)
y_root = function_for_root(x_root)
s = "Root found with y(%f) = %f" % (x root, y root)
print(s)
0.5 0.802499999999998
0.8953201970443347 0.5 0.802499999999999 -2.0300000000000002
1.023494648595172 0.8953201970443347 0.15784083877308386 -1.2314532019704438
1.040556119705499 1.023494648595172 0.016592976930660974 -0.9725408098377528
1.040869531981685 1.040556119705499 0.00029400473441354436 -0.9380766381948917
Root found with y(1.040870) = 0.000000
```

Save Your Work

Make a GitHub project "astr-119-session-8", and commit the programs my_first_jupyter_notebook.ipynb and test_matplotlib.ipynb you made today.

