

## Worksheet 2: Root finding

If you are using Julia or Python, we recommend using a jupyter notebook. In WeLearn, you need to submit this file. Please clearly indicate in the markup cells, the number of the question for which you are writing the program. Also, please remember to add documentation through comments in your program.

You may also use scripts and use REPL to evaluate them. In that case, please keep all your files for a particular worksheet in a folder and you may upload the compressed archive of that folder.

Please feel free to ask for help!

In all the root-finding methods, one does not look for an *exact* solution. If the function value is within certain small number  $\epsilon$  from the root, then we stop the search and declare the root is found. The value of  $\epsilon$  depends on the given problem's physical parameters and the required accuracy. Also, there must be a safe-guarding mechanism of having a maximum allowed iterations (to avoid infinite loops).

Given:

1. Maximum iteration count, `maxiter` = 50
  2.  $\epsilon$  or `eps` =  $1.0E-5$  (i.e.,  $10^{-5}$ )
  3. Use `numpy`: `import numpy as np`
1. (12 points) Use bisection, Secant and Newton-Raphson to solve the equation  $3x = \tan(x)$ . Plot the function in the range  $(0.0, 1.57)$ .
    - (a) Define a function to call the method, such as, `bisection(f,L,R,eps,maxiter)`, where `f` is the function whose root is within bracketing interval `L` and `R`.
    - (b) For bisection, the function should check if the bracketing interval is proper.
    - (c) The function should check if the given input points are roots.
    - (d) The function should return the required number of iterations and the root.
    - (e) For bisection, starting interval could be  $[1.2, 1.4]$ .
    - (f) For Secant the first two points could be  $[1.2, 1.25]$ .
    - (g) For Newton-Raphson, the starting point is 1.2.
  2. (8 points) Consider a particle moving in an asymmetric one-dimensional double-well potential  $V(x) = x^4 + \left(\frac{2x}{3}\right)^3 - x^2$  eV with a total energy  $-0.125$  eV. You need to find the turning points for the particle when it is in either potential well. Plot the function in the range  $(-1.25, 1.25)$ .
    - (a) (4 points) Use Bisection method.
    - (b) (4 points) Use Secant method.