Numerical methods
Bachelor in Physics

Practicum 1: Finding solutions of non-linear equations

Contact: jeroen.mulkers@uantwerpen.be U.305

1. In this exercise, we will determine the roots of the function

$$f(x) = 1 + x^2 - \tan(x),$$

by using the bisection method.

   (a) Download `bisect.m` from BB and read the code.

   (b) Plot $1+x^2$ and $\tan(x)$ in the same figure and pay attention to the intersections of both functions and the asymptotes of the tangent function.

   (c) Choose a suitable interval that contains the first positive root of $f(x)$, and determine the root with `bisect.m`.

   (d) How many iterations do you need to achieve an accuracy of 10^{-5}? Calculate this analytically (see lecture notes) and confirm numerically. On what does the necessary number of iterations depend?

   (e) Determine the negative root closest to zero.

2. The 'Regula Falsi' method: Similar to the bisection method, one starts by choosing an interval $[a, b]$ which contains a change of sign. Instead of taking the middle point as the next approximation of the root, in the 'Regula Falsi' method, one takes the intersection of the line through points $(a, f(a))$ and $b, f(b))$, and the x-axis.

   (a) Modify `bisect.m` and implement the 'Regula Falsi' method. Remove the error approximation $(b - a)/2$ since it is no longer correct.

   (b) Use the new script `regfals.m` to determine the roots of the previous exercise.

3. Implement the bisection method in a recursive way (e.i. write a function which calls itself and which does not contain a loop).

4. Use the method of Newton (see newton.m on BB) to determine the roots of exercise 1 and compare the rate of convergence between the Newton method and the bisection method.

5. One can use the method of Newton if the derivative of the function is known. The 'secant' method is a variant of the Newton method which does not require the derivative of the function. This method starts with 2 approximations of the root α, let's say x_1 and x_2. The intersection of the line through points $(x_1, f(x_1))$ and $(x_2, f(x_2))$, and the x-axis yields a new approximation x_3, and so on. Convince yourselves that the algorithm is given by

$$x_{n+1} = x_n - f(x_n) \cdot \left[\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \right], \text{ for } n = 2, 3, 4, \ldots.$$

   Implement this method by modifying newton.m. Name the new file secant.m. The method of Newton uses two function evaluations in each iteration. Make sure that in secant.m, only function evaluation is needed in each iteration.

   Use the new method secant.m to determine the roots of exercise 1. Compare again the convergence rate with the other methods.

6. Use the MATLAB command fzero to determine the roots of 1. Call the command fzero with the optional options argument which you can define as

   ```
   >> options= optimset('TolX',1.e-10,'Display','iter')
   ```

   Do not type ; to look at the set options.

7. Use Newton's method to determine the multiplicity of the root at $x = 0$ of the function $f(x) = x \sin(x^2) \tan(x)$.

8. Modify Newton's method for the determination of roots with a multiplicity > 1 (see lecture notes). Use the ordinary method of Newton in the first iteration steps to determine the multiplicity. Call the algorithm modnewton.m. Apply the new method to determine the roots of exercise 7. Compare the rate of convergence between Newton's method and the modified Newton's method.

9. The Schrdinger equation for a finite 1D potential well,

$$V = \begin{cases} V_0 & \text{for } |x| > a, \\ 0 & \text{for } |x| < a, \quad (V_0 > 0). \end{cases}$$

can not be solved exactly. However, the energy values $E = \hbar^2 k^2/2m$ can be found by solving the following transcendental equations numerically

$$\begin{aligned} ka \tan ka &= \kappa a \qquad &\text{(even solutions)} \\ ka \cot ka &= -\kappa a \qquad &\text{(odd solution),} \end{aligned}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

Visualize the problem by plotting the l.h.s. and the r.h.s. of both equations for different potential well depths. The intersections of these curves correspond with the different energy levels. Make a figure of the lowest energy levels as a function of the potential well depth. Check if the energy levels converge to the energy levels of the infinite potential well:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2m(2a)^2}.$$

Tip: it is good practice to limit the number of parameters by using reduced units. In this exercise, you can assume that $\hbar^2/2m = 1$. Furthermore, the transcendental equations can be simplified if you express the energy by $z = a\sqrt{E}$, and the depth of the potential well by $z_0 = a\sqrt{V_0}$. Under these conventions, the energy levels of the infinite potential well are given by $z_n = n\pi/2$.