<u>Exercise 1</u>: Roots and optimal values

The report must be delivered within 15 days after the corresponding practical lessons.

1. **Square root of a number:** it is possible to use a root finding algorithm to estimate the value of a square root of a number using a function like x^2-C=0.
    a. Implement the bissecion method to compute $\sqrt{4}$. Use as an initial interval [a,b] the intervals {[0.7,2.6]; [0.4,1.7]; [-3,0.6]}. Use as convergence criteria $\epsilon=10^{-5}$.
    b. Plot the estimated value *x* as a function of the number of iterations for each one of the initial intervals (draw all three curves in the same plot). Discuss the shape of the resulting curves and the values they converge.
    c. Implement the Newton method and the secant method for root finding. Apply them to the same function.
    d. Plot the logarithm of the error value of each method (value compared to the convergence criteria) as a function of the number of iterations. Discuss the results obtained.

2. **Oscillatory current in circuits:** an oscillatory current in a given circuit may be described by $I=9e^{-t}\sin(2\pi t)$, with I in mA.
    a. Using Newton method, find the values of time for which I=1.5mA, with a precision of 10^{-6} (Hint: use Mathematica derivate capabilities), using as initial values x0 = {0.6, 0.7, 0.75, 0.8, 0.9}. Discuss the obtained results for the various values of x0.
    b. Confirm the results obtained above with the Mathematica FindRoot function. Discuss the method used in Mathematica.

3. **Body attached to a spring:** a body attached to a spring is subject to a potential of $0.5*(x-2)^2$ [J].
    a. Implement the golden-section method for finding the maximum/mininum of a function and use it to find the position of equilibrium of this body. Use as initial intervals [a,b] the intervals {[-0.7,2.6], [0.4,1.7]}. Use a value of $\epsilon_r=0.001\%$ as a criteria for convergence. Discuss the resulting value for each initial interval.
    b. Implement the gradient descent method and apply it to solve the above problem. Use a maximum of 10 iterations, x0=0, a precision of $\epsilon=1\times10^{-5}$, and step size of $\lambda=\{0.1;0.5;1;2;2.1\}$
    c. Plot the resulting minima as a function of number of iterations for each step size λ (draw all curves in the same plot). Discuss the behaviour of each curve.

4. **Ionic bond distance:** The potential of interaction between the ion Na^+ and the ion Cl^- may be given by:

$$U(r)=Ae^{-Br}-\frac{C}{r}$$

where *A* = 80eV, *C* = 10eVÅ, *B* = 2Å^{-1}, and *r* is the distance between ions.

    a. Using the gradient descent method find their distance of equilibrium. Check the result with the Mathamatica FindMinimum function. Discuss the precision used by Mathematica.
    b. Consider now the potential in two dimensions, *U(x,y)*, with $r=\sqrt{x^2+y^2}$. Implement the gradient descent in two dimentions to find the minimum *(x,y)* of U(*x*,*y*) using as (x_0,y_0) = (5, -5) as a starting point (hint: compute the partial derivatives with Mathematica). Plot *'x'* and *'y'* as a function of number of iterations (both curves in the same plot). Place an inset plot with the trajectory (*y* as a function of *x*). Use FindMinimum to confirm the result. Compare this result with the one obtained previously (in one dimension).

Exercise 1 (optional): Roots and optimal values

This part is optional and doesn't need to go into report.

1. **Frictionless projectile:** a projectile is thrown at an heigth of $y_0 = 1$m, making and angle θ_0 with horizontal, with an initial speed of $v_0 = 30\, m/s$. The goal is to hit a target placed at an height of 1.8m and at some distance x. The trajectory may be described by:

$$y = \tan(\theta_0)\, x - \frac{g}{2 v_0^2 \cos^2(\theta_0)} x^2 + y_0$$

   a. Using the secant method find the values of θ_0 that hit a target at x=90m. Compute a table with every value of θ_0 found, the initial values used, the number of iterations and chosen prevision.
   b. Make a 3D plot using Mathematica with the above equation, as a function of θ_0 e x. Show graphically the function zeros (use function Plot3D[]).
   c. Elaborate a protocol, using any of the previous methods, to compute the zeros of the same function, but using both variables, θ_0 and *x*, as unknowns. Make a plot of *x* as function of θ_0.

2. **Body attached to a spring:** a body attached to a spring is subject to a potential of $0.5*(x-2)^2$ [J].
   a. Implement the gradient descent method in C++ and Python. Execute both for a maximum number of iterations of 1×10^{10}, a precision of $\epsilon = 1 \times 10^{-10}$, and step size of $\lambda = 1 \times 10^{-7}$. Compare the run-time taken by each implementation. Plot the run-time as a function of λ for both implementations.
   b. Implement a method similar to the golden-section, but using other ratios instead of the golden ratio. Compare the rate of convergence with a different ratio. How would you improve the algorithm presented in the classroom for efficiency?
   c. For the gradient descent, implement a protocal to optimise the step size λ at each step.

3. **Ionic bond distance:** The interaction potential between a ion Na^+ a ion ião Cl^- may be described by:

$$U(r) = A e^{-Br} - \frac{C}{r}$$

   where *A* = 80eV, *C* = 10eVÅ, *B* = 2Å^{-1}, and *r* is the distance between ions.

   a. Plot this function and identify the distance of equilibrium between the two ions (a minimum).
   b. Apply the gradient descent and newton methods to compute the identified distance of equilibrium. Plot the distance of equilibrium for both methods as a function of number of iterations (draw both curves in the same plot).
   c. Consider now the potential in two dimensions, *U(x,y)*, com $r = \sqrt{x^2 + y^2}$. Make a contour plot with Mathematica of the potential (use the ContourPlot[] function). Discuss the locations of the minimum in that plot.
   d. Implement the gradient descent method for U(x,y,z).