Evaluation Exercises
2022-2023

Students must do these exercises and delivery them using Moodle web page, **deadline: 10th March 2023**. Each exercise must have at least two files:

- The FORTRAN code (including the name of the student at the beginning of the code).
- A **pdf file** with the corresponding e**xplanations regarding the applied methods and comparison between them** (which one performs better, which one will you use....).

The final mark will take into account:

1. The program compiles without any error or warning.
2. It is well-structured and properly commented (add comments in the code).
3. It is effective, the result should be obtained using the least number of operations.
4. It is general for any function (use subroutines).

Part I: Integration of Functions

1 Write a program to solve the following integral

$$I = \int_1^3 sin(x^2) - cos(2x)dx$$

1. Using the **composite Simpson rule**. The program should:
   (a) Start with number of intervals (N) equal to 1.
   (b) Automatically double the number of subintervals.
   (c) At each iteration step the program must show the iteration step, subinterval number, integral value and the difference between a result and the preceding one.
   (d) Stop when convergence is reached (when the difference between a result and the preceding one is smaller than a threshold given by the user). Choose a threshold value of 10^{-8}.
   (e) Show the final iteration step, subinterval number, number of abscissa points employed and quadrature value.
2. Using the **Romberg's method** and a convergence criteria of $R(k,j)-R(k,j-1) < 10^{-8}$. The program should:
   (a) Show the entire triangular matrix up to $R_{10,10}$. (or just the triangular matrix until the converged $R_{k,j}$)
   (b) Print only the converged result and its position in the table.
3. Using the **Gauss-Legendre method** (*SubGauleg.f90* subroutine is provided by the teacher and it is accessible through Moodle). The program should:
   (a) Increase the number of quadrature points from 2 to 10, but stop calculation when the difference with respect to the previous iteration step is lower than 10^{-8}. Remember to change the limits and variables to the Gauss-Legendre optimum range.
   (b) At each step the program should show the number of quadrature points, integral value and the difference between a result and the preceding value.
   (c) Show the final quadrature value and total quadrature points employed.

Part II: Root-Finding and Function Optimization

2 Write a program that minimize/optimize the following two-dimensional function:

$$f(x, y) = sin(x + y) + (x - y)^2 - 1.5x + 3.5y + 3$$

1. Using **Steepest Descent method**, with a convergence threshold of 10^{-8} and a fix step size value of 0.3 to make the program simpler.
   (a) Hint: At the minimum, the gradient vector should be zero, but due to the method's limitation (and fix step size) the program will not converge. Set a maximum iteration number to finish the program (***maxiter*=40**).
   (b) Hint: Save coordinates in the *coord*(*maxiter*,2) matrix. Initial coordinates: $x = 1$, $y = 3$.
   (c) Hint: Calculate the gradient numerically (use subroutines) applying the **central finite difference approximation**, which must be a vector with two elements. **Normalize** the vector.
   (d) For each iteration step, the program must show the values of x, y, function, gradients, normalize gradients and convergence (error). Optionally, represent the x, y coordinates to observe the zig-zag pathway characteristic of the Steepest Descent method.
2. Using **Newton-Raphson method** and a convergence threshold of 10^{-8}.
   (a) Hint: Calculate the gradient and second derivative numerically (use subroutines) applying the **central finite difference approximation**. **Do not normalize** the gradient.
   (b) For each iteration step, the program must show the values of x, y, function, gradient, Hessian and convergence (error).
   (c) Show the final results: number of iterations needed, the coordinates of the minimum, gradient and Hessian.