Assignment 1

The potential energy function dictates the structure of a biomolecule. In particular, the most stable structure corresponds to the global minimum in the (free) energy function. So, finding the global minimum in a complex free energy surface is one of the most important steps in the structure prediction of the peptides or proteins. A number of numerical algorithms are available which either use the energy values, or their first derivative and second derivative information to locate the minimum. In order to find the global minimum this procedure should be performed for the entire range of different structural parameters (bond lengths, bond angles and dihedral angles). In order to get an understanding about this procedure here a model potential energy function is provided which has the following form:

$$U(r) = ((r-1)(r+2)(r-3))^2 - 8.0 + r \qquad \textbf{Equation -1}$$

Do the following tasks.

(i) Plot the potential energy function in the range -2.5 to 3.5 (use any tools such as xmgrace, grace, matlab,matplotlib) **[1 Mark]**

(ii) Write a program to find all the minima in this function using Steepest descent method and Newton's Raphson method **[3 Mark]**

(iii) Provide details about the global minimum after locating all the minima. **[0.5 Mark]**

(iv) Provide details about the timings taken by these two algorithms in finding the global minimum. **[0.5 Mark]**

TIPS : You can use any random number generator to get a random position for the search variable. Following pseudo code will give a random value in the given range of numbers range_min (-4) to range_max (4)

rval=rand()*(range_max-range_min)+range_min

The derivative at given r value for the function can be found using the following formula:

Derivative = (f(r+h)-f(r-h))/2h

Here, h is an increment in r. You can always set a threshold value (1.0d-6 or so) and if the change in r is less than this, the program can exit and print the value of r corresponding to minimum.

In the same way as described above, the second derivative of the function f(x) can also be obtained using the following formula.

$$f''(x) = \lim_{h\to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Equation -2

$U(x, y) = (2-x)^2 + 5(y-x^2)^2$

Do the following task.

Write a program to find global minima in this function using Steepest descent method and Newton's Raphson method. (Range x :[-5, 5], y:[-5, 5])
[2.5 Mark - Steepest descent, 2.5 Marks Newton's Raphson]

Hint:

new_points = old_points – $\text{hessian\_of\_U}_{(\text{old\_x, old\_y})}^{-1}$ * $\text{gradient\_of\_U}_{(\text{old\_x, old\_y})}$

* = matrix multiplication

new_points = $[\text{new\_x}, \text{new\_y}]^T$

old_points = $[\text{old\_x}, \text{old\_y}]^T$

$\text{gradient\_of\_U}_{(\text{old\_x, old\_y})} = [\, \partial U/\partial x, \partial U/\partial y]^T$

$\text{hessian\_of\_U}_{(\text{old\_x, old\_y})}^{-1}$ = Inverse of $\text{hessian\_of\_U}_{(\text{old\_x, old\_y})}$

$$\text{hessian\_of\_U}_{(x, y)} = \begin{pmatrix} \frac{\partial^2 U}{\partial x^2} & \frac{\partial^2 U}{\partial x \partial y} \\ \frac{\partial^2 U}{\partial y \partial x} & \frac{\partial^2 U}{\partial y^2} \end{pmatrix}$$

$\partial^2U/\partial x^2 = (U(x+h,y) - 2U(x,y) + U(x-h,y)) / h\text{^}2$

$\partial^2U/\partial y^2 = (U(x,y+h)- 2U(x,y) + U(x,y-h)) / h\text{^}2$

$\partial^2U/\partial xy = (U(x+h,y+h) - U(x+h,y-h) - U(x-h,y+h) + U(x-h,y-h)) / (4h\text{^}2)$

$\partial^2U/\partial xy = \partial^2U/\partial yx$

Inverse of 2x2 Matrix -

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$$A^{-1} = \frac{1}{\det A} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$