Algorithms In Computational Biology

Jai Singh, 2020070
Mohammad Sufyan Azam, 2020312

Assignment 1

INDRAPRASTHA INSTITUTE *of*
INFORMATION TECHNOLOGY **DELHI**

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1 Problem 1

1.1 Equation

$$\mathbf{U(r)} = ((r-1)(r+2)(r-3))^2 \text{ - } \mathbf{8.0} + \mathbf{r}$$

1.2 Task 1

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

Solution

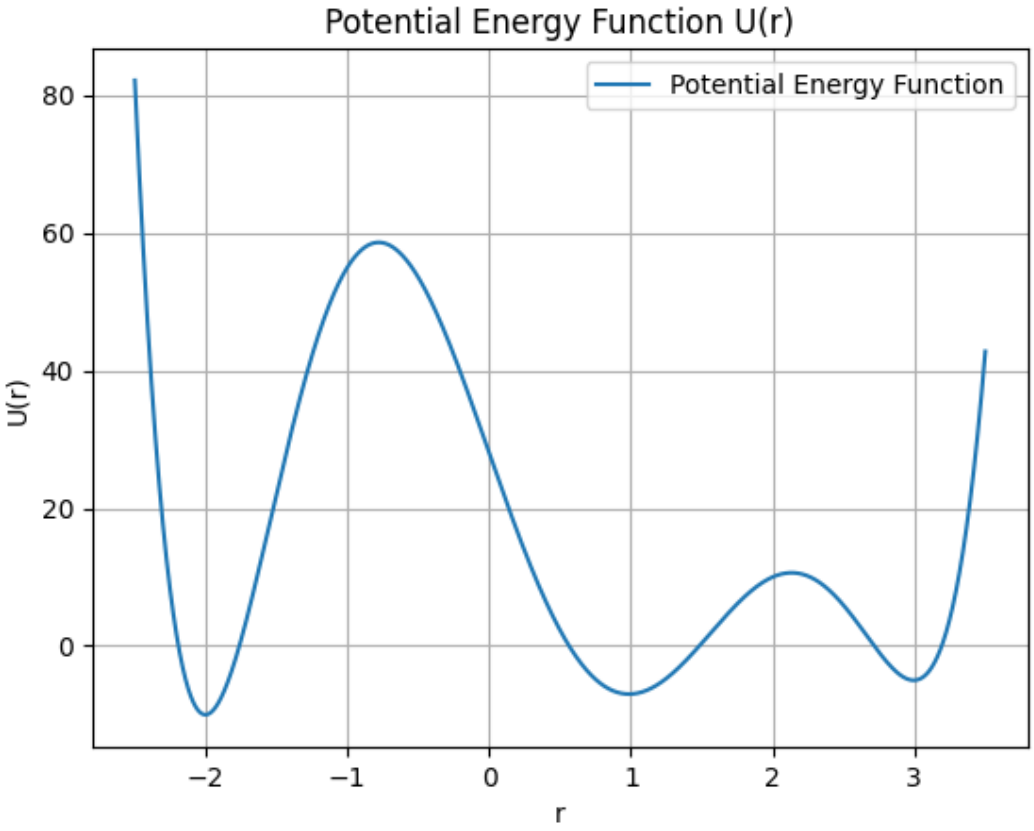

Figure 1: **Potential Function**

We have used Python (.ipynb format) with matplotlib and numpy libraries to generate the above graph.

1.3 Task 2

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

Solution

Newton Raphson Method

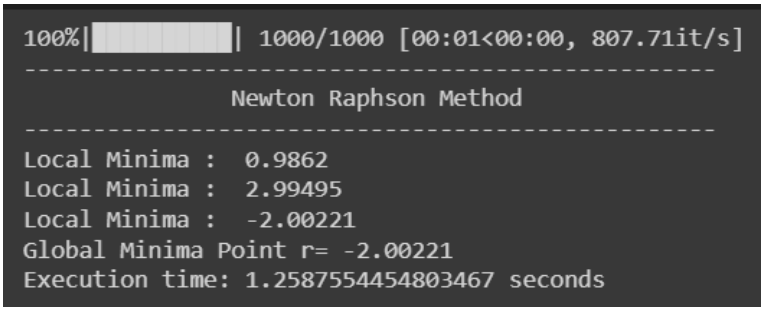

Figure 2: **Newton Raphson Method**

Steepest Descent Method

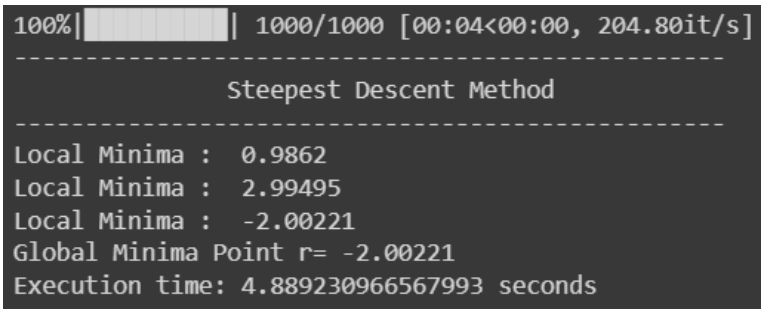

Figure 3: **Steepest Descent Method**

The Newton Raphson and the Steepest Descent method both provide a really accurate guess of all the local minima's present in the function. However, the execution time for steepest descent was lesser than Newton Raphson's method because steepest descent method typically requires fewer computations per iteration.

1.4 Task 3

Provide details about the global minimum after locating all the minima. [0.5 Mark]

Solution

The global minimum is at **r = -2.00221**.

The Value of Potential Energy **U(r) = -10.0011084847302**

```
The global minimum is at r = -2.00221
The Value of Potential Energy at Global Minima = -10.0011084847302
```

Figure 4: **Global Minima and its Corresponding Value**

1.5 Task 4

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

Solution

Newton Raphson Method

```
100%|██████████| 1000/1000 [00:01<00:00, 940.32it/s]
-----------------------------------------------
              Newton Raphson Method
-----------------------------------------------
Global Minima Point r= -2.00221
Execution time: 1.0737876892089844 seconds
```

Figure 5: **Newton Raphson Method(Execution Time)**

Steepest Descent Method

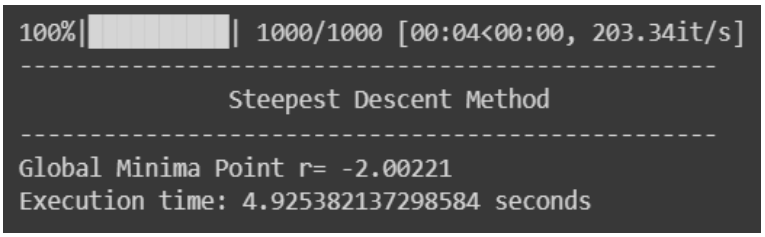

Figure 6: **Steepest Descent Method(Execution Time)**

The Newton-Raphson method often converges faster than the steepest descent method, especially for functions with well-behaved and convex properties. The Newton-Raphson method uses information from the second derivative (the Hessian matrix) of the function to directly approximate the local minimum. This allows it to take larger steps towards the minimum compared to the steepest descent method, which relies only on the first derivative (the gradient) and takes smaller steps.

2 Problem 2

2.1 Equation

$$\mathbf{U(x,\ y)} = (2 - x)^2 + 5(y - x^2)^2$$

2.2 Task 1 - Steepest Descent Method

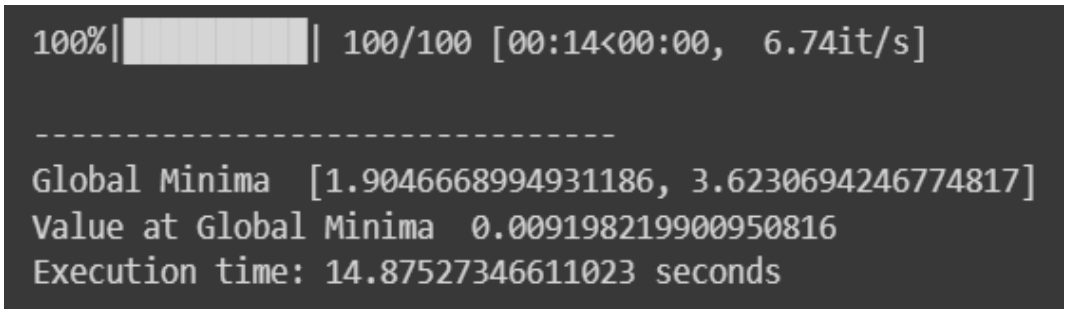

Figure 7: **Steepest Descent Method**

2.3 Task 2 - Newton Raphson's Method

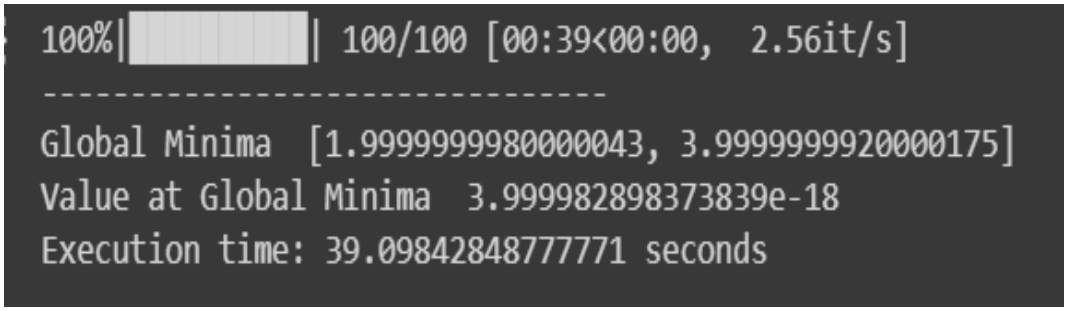

Figure 8: **Newton's Raphson Method**

We observe that steepest descent takes lesser time than Newton Raphson's method for finding the global minima, however, the Newton Raphson's method is more accurate. Steepest Descent takes around 14 sec while Newton Raphson's takes around 40 sec.