Student Name: Mina Gerges
ID: 70040441
Computational Physics_ PHYS624
HW1: Numerical Differentiation

UAEU كلية العلوم College of Science
جامعة الإمارات العربية المتحدة United Arab Emirates University

Numerical Differentiation

HW1

Write a program that compute the first and second derivative of the following function at 2 points in the specified intervals using (i) Forward difference (ii) Backward difference (iii) Central difference (iv) Richardson extrapolation and compare them with the analytic results

$f(x) = x^2 \cos x;\ x = [0,4]; h = [0.5, 0.25, 0.125]$

Answer:

Function to be differentiated → $f(x) = x^2 \cos x$

where (x) is measured in radians

$f'(x) = 2x\cos(x) - x^2 \sin(x)$ ← using Product Rule

$f''(x) = 2\cos x - 2x\sin x - 2x\sin x - x^2\cos x$

$f''(x) = 2\cos x - 4x\sin x - x^2\cos x$

The selected points are $x_1 = 1$, $x_2 = 2$

h is defined as a list of 3 values

$h = [0.5, 0.25, 0.125]$

* The analytic solution of 1st & 2nd derivative at the two points are as follows

at $x_1 = 1$ → $f'(1) = 0.2391336269$

$f''(1) = -2.825581633$

at $x_2 = 2$ → $f'(2) = -5.301777535$

$f''(2) = -6.442085741$5

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The Numerical Methods:- FD , BD , CD

Calculating The derivative at the three value of (h)

① **FD1** Forword difference for the first derivative

$h = 0.5 \quad f'(1) = \frac{f(1.5) - f(1)}{0.5}$

at $x=1$ $\quad h = 0.25 \quad f'(1) = \frac{f(1.25) - f(1)}{0.25}$

$h = 0.125 \quad f'(1) = \frac{f(1.125) - f(1)}{0.125}$

② **BD1** Backword difference for the first derivative

at $x=1$ for the 3 values of h

e.g → $h = 0.5 \quad f'(1) = \frac{f(1) - f(0.5)}{0.5}$

③ **CD1** Central difference

at $x=1$

$h = 0.5 \quad f'(1) = \frac{f(1.5) - f(0.5)}{1}$

for BD1 , CD1 same steps are repeated for

$h = 0.25$ & $h = 0.125$

④ Richardson Extrapolation

this step is calculated using the CD method

for $h_1 = 0.5$ & $h_2 = 0.25$ only

⑤ Same upper four steps are repeated to calculate FD2 , BD2 , CD2 For the second derivative using their specified formula as mentioned in Lectures

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The script runs as follows

1. define the function with x as a "double"
2. define a function for the first derivative.
3. define a function for the second derivative.
4. define functions for the numerical methods
   [FD1, BD1, CD1] → for the first derivative
   [FD2, BD2, CD2] → for the second derivative
5. define Richardson extrapolation using [h1, h2] as the first two values of list (h)
6. Repeating step 5 for Richardson extrapolation for the second derivative.

Computed values: [R1, R2], [R3, R4]

7. selecting x as $x_1 = 1$, $x_2 = 2$
8. Considering h as a step to be included in the function definition for each numerical method.
9. printing out the results

Technical tips in the script

Using "\t" as a tab character
Using "\n" to start new lines for the calculations.

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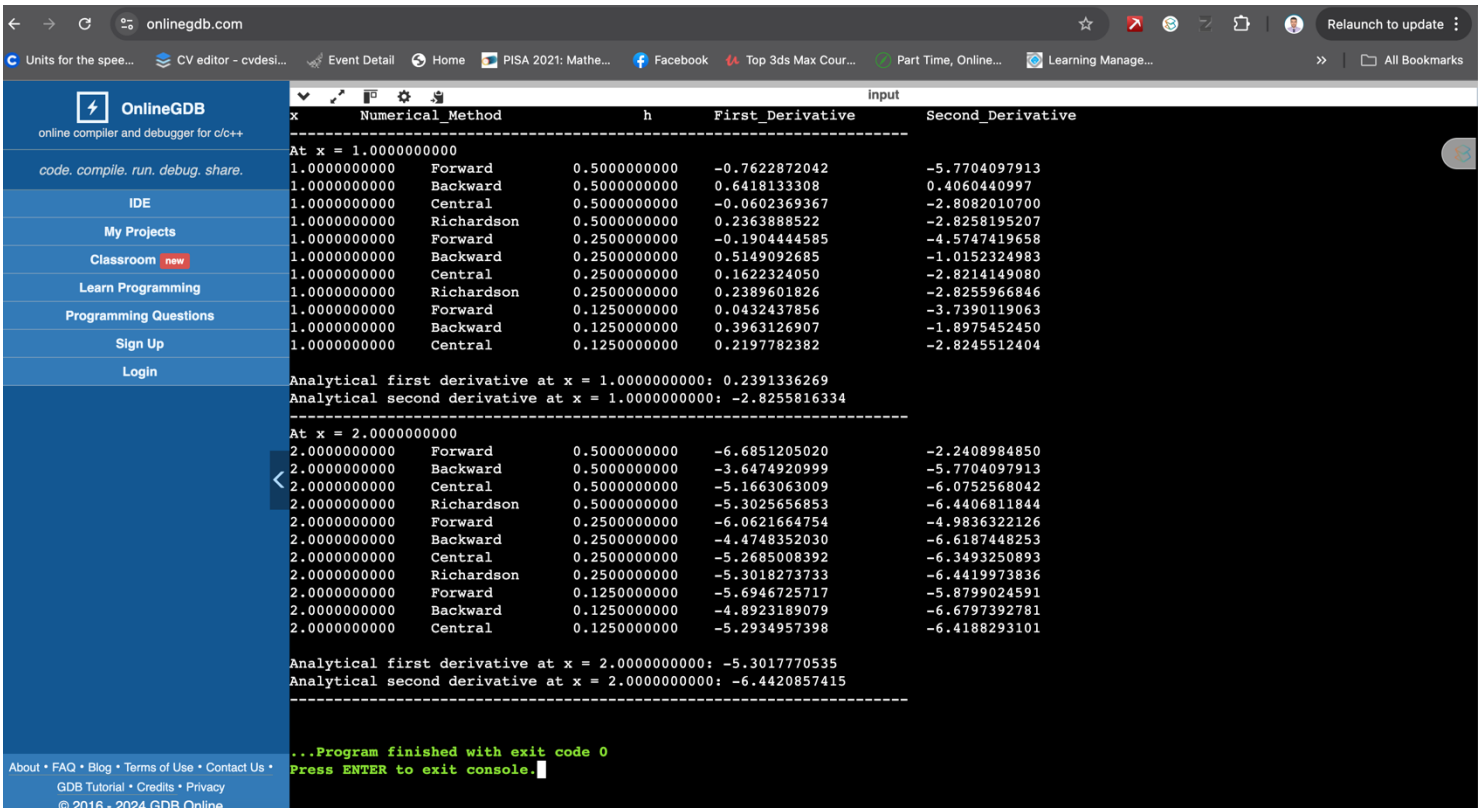
Code results:



The printed results

```
x     Numerical_Method          h      First_Derivative      Second_Derivative
------------------------------------------------------------------------
At x = 1.0000000000
1.0000000000   Forward      0.5000000000   -0.7622872042       -5.7704097913
1.0000000000   Backward     0.5000000000   0.6418133308        0.4060440997
1.0000000000   Central      0.5000000000   -0.0602369367       -2.8082010700
1.0000000000   Richardson   0.5000000000   0.2363888522        -2.8258195207
1.0000000000   Forward      0.2500000000   -0.1904444585       -4.5747419658
1.0000000000   Backward     0.2500000000   0.5149092685        -1.0152324983
1.0000000000   Central      0.2500000000   0.1622324050        -2.8214149080
1.0000000000   Richardson   0.2500000000   0.2389601826        -2.8255966846
1.0000000000   Forward      0.1250000000   0.0432437856        -3.7390119063
1.0000000000   Backward     0.1250000000   0.3963126907        -1.8975452450
1.0000000000   Central      0.1250000000   0.2197782382        -2.8245512404

Analytical first derivative at x = 1.0000000000: 0.2391336269
Analytical second derivative at x = 1.0000000000: -2.8255816334
------------------------------------------------------------------------
```

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At x = 2.0000000000

2.0000000000	Forward	0.5000000000	-6.6851205020	-2.2408984850
2.0000000000	Backward	0.5000000000	-3.6474920999	-5.7704097913
2.0000000000	Central	0.5000000000	-5.1663063009	-6.0752568042
2.0000000000	Richardson	0.5000000000	-5.3025656853	-6.4406811844
2.0000000000	Forward	0.2500000000	-6.0621664754	-4.9836322126
2.0000000000	Backward	0.2500000000	-4.4748352030	-6.6187448253
2.0000000000	Central	0.2500000000	-5.2685008392	-6.3493250893
2.0000000000	Richardson	0.2500000000	-5.3018273733	-6.4419973836
2.0000000000	Forward	0.1250000000	-5.6946725717	-5.8799024591
2.0000000000	Backward	0.1250000000	-4.8923189079	-6.6797392781
2.0000000000	Central	0.1250000000	-5.2934957398	-6.4188293101

Analytical first derivative at x = 2.0000000000: -5.3017770535
Analytical second derivative at x = 2.0000000000: -6.4420857415
