PH3120 – Computational Physics Laboratory 1
CPL102 – Numerical Differentiation and Integration
Section 1 & 2

1. First Derivatives

I. Answer the following questions based on first order numerical differentiation.

(a) Write down the Taylor series for an arbitrary function ($f(x)$) at $x = a$.

(b) Using the Taylor series expansion, derive the finite difference formulars for the first derivative. The three techniques that must be considered are

1. Forward difference
2. Backward difference
3. Central difference

(c) What is the truncation error in context of Taylor series approximation?

(d) Explain the truncation error in the above three methods. Which method has the lowest truncation error?

(e) Compare the forward, backward, and central difference methods for numerical differentiation. Discuss their advantages, disadvantages, and suitable applications for each method.

(f) Why is the choice of step size important in numerical differentiation methods? How does the step size affect the accuracy and stability of the derivative approximation obtained using the above three methods?

(g) Discuss the sources of error in the above methods. How does the error vary with respect to the step size and the smoothness of the function being differentiated?

II. Develop a python function with the following signature.

```python
def num_diff(f, x, h, method):
    """
    Compute the numerical derivative of a function using different difference methods.

    Parameters:
        f (function): The function for which to compute the derivative.
        x (float): The point at which to compute the derivative.
        h (float): The step size for the difference approximation.
        method (str): The differentiation method to use ('forward', 'backward', or 'central').

    Returns:
        float: The estimated derivative value.

    """
```

III. A function $f(x)$ is given as $f(x) = x^3 + 2x - 1$. Compute the derivative of $f(x)$ at $x = 2$ using the function you developed above and fill out the following table.

h	y' (forward)	y' (backward)	y' (Central)	Expected Solution	Error % (forward)	Error % (backward)	Error % (Central)
0.5							
0.2							
0.1							
0.05							
0.01							
0.001							

2. Second Order Derivatives

I. Answer the following questions based on higher order numerical differentiation.

(a) Derive an expression for 2nd order derivative based on the central difference method.

(b) What is the truncation error in the central difference formula for approximating the second derivative?

(c) Can you apply the above method to compute the second derivative, if the given step size is **non-uniform**? Explain your answer.

(d) Explain the accuracy of central difference method when it is used for a function which has discontinuities, sharp changes, and high-frequency components.

II. Develop a python function with the following signature.

```python
def central_diff(f, x, h, order=1):
    """
    Compute the central difference derivative of a function at a given point.

    Arguments:
    f -- function to differentiate
    x -- point at which to compute the derivative
    h -- step size
    order -- order of the derivative (1 for first derivative, 2 for second derivative) (default: 1)

    Returns:
    The approximate derivative of f at x.
    """
```

III. In simple harmonic motion, the position of the object can be described by the equation:

$$x(t) = A\,cos(\omega t + \varphi)$$

Where:

- $x(t)$ represents the position of the object at time t.
- A is the amplitude of the motion.
- ω is the angular frequency, given by ω = 2πf, where f is the frequency of the motion.
- φ is the phase constant that determines the initial position and velocity of the object.

Consider that an object undergoing simple harmonic motion with $\omega = 100$ rad s^{-1}, $A = 2$ cm, and $\phi = \frac{\pi}{6}$.

(a) Plot the position within the interval $-4s \leq t \leq 4s$ with 0.001s step size.
(b) Use the above central_diff() function to calculate the speed ($v(t)$) of the object as a function of time within $-4s \leq t \leq 4s$ interval and plot $v(t)$.
(c) Use the above central_diff() function to calculate the acceleration ($a(t)$) of the object as a function of time within $-4s \leq t \leq 4s$ interval and plot $a(t)$.

3. Integration: Trapezoidal Rule

I. Answer the following questions based on higher order numerical differentiation.

(a) Write down the trapezoidal rule for the following definite integral.

$$\int_a^b f(x)dx$$

(b) What are the advantages of using the trapezoidal rule for numerical integration?

(c) What is the order of accuracy of trapezoidal rule?

(d) What are the limitations of the trapezoidal rule?

(e) How can we use the trapezoidal rule for discontinuous functions?

(f) How can we use the above rule to integrate functions with high frequency or rapid changes?

II. Develop a python function with the following signature.

```python
def trapezoidal_integration(f, a, b, n):
    """
    Perform numerical integration using the trapezoidal rule.

    Arguments:
    f -- function to integrate
    a -- lower limit of integration
    b -- upper limit of integration
    n -- number of subintervals (higher n leads to higher accuracy)

    Returns:
    The approximate value of the definite integral of f(x) over the interval [a, b].
    """
```

III. The radial density of a disk is given by $\rho(x) = x\sqrt{x}$. Calculate the mass of a disk with radius 2 cm using the function developed in 3 (II). The mass is given by

$$m = \int_0^r 2\pi x\rho(x)dx$$

Find mass m using the function developed in 3 (III) and analytically.

n	m (Trapezoid)	m (Expected)	Error (%)
0.5			
0.1			
0.05			
0.01			
0.001			

IV. A particle is moving along a straight line with a velocity given by the function $v(t) = 2t - 1$ for $t < 2$s and $v(t) = 3$ for $t \geq 2$s.

(a) Plot $v(t)$ within the interval [0,4] seconds.

(b) Find the displacement (s) of the particle between $t = 0$s and $t = 4$s using the function developed in 3 (II) and analytically.

n	s (Trapezoid)	s (Expected)	Error (%)
0.5			
0.1			
0.05			
0.01			
0.001			

4. Integration: Simpson's Rule

I. Answer the following questions based on higher order numerical differentiation.

(a) Write down the Simpson's 1/3 rule for the following definite integral (Remember that you must consider the sum of the terms with even and odd indices separately).

$$\int_a^b f(x)dx$$

(b) What are the advantages of using the Simpson's 1/3 rule over trapezoidal rule for numerical integration?

(c) What is the order of accuracy of Simpson's 1/3 rule?

(d) What are the limitations of the Simpson's 1/3 rule?

(e) How can we use the Simpson's 1/3 rule for discontinuous functions?

(f) How can we use the above rule to integrate functions with high frequency or rapid changes?

II. Develop a python function with the following signature.

```
def simpsons_rule(f, a, b, n):
    """
    Simpson's rule for numerical integration.

    Args:
        f (function): The function to be integrated.
        a (float): The lower limit of integration.
        b (float): The upper limit of integration.
        n (int): The number of subintervals. n must be an odd integer.

    Returns:
        float: The approximate value of the definite integral of f(x) over the interval [a, b].
    """
```

III. Solve the question in 3 (III) using Simpson's 1/3 rule. Compare your results against that in 3 (III).

IV. Solve the question in Solve 3 (IV) using Simpson's 1/3 rule. Compare your results against that in 3 (IV).