# Computational Physics Exercise 1

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## Contents



## 1 Derivative Formula

Let $h$ be constant and let $f(x-2h), f(x-h), f(x+h), f(x+2h)$ contain the Taylor expansion up to order 4 with the error term in $O(h^5)$. We first construct the following;

$$f(x+h) + f(x-h) = 2f(x) + h^2 f^{''}(x) + \frac{h^4}{12} f^{''''}(x) + O(h^6) \tag{1}$$

Obtaining an error bound in $O(h^6)$ since derivatives of uneven order cancel out. Similarily we get;

$$f(x+2h) + f(x-2h) = 2f(x) + 4h^2 f^{''}(x) + \frac{16h^4}{12} f^{''''}(x) + O(h^6) \tag{2}$$

Multplying equation (1) by 16 and subtracting equation (2) we get the desired result;

$$-f(x+2h)+16f(x+h)+16f(x-h)-f(x-2h) = 30f(x)+12h^2 f^{''}(x)+O(h^6)$$
$$\Rightarrow f^{''}(x) = \frac{1}{h^2}[-\frac{1}{12}f(x+2h)+\frac{4}{3}f(x+h)-\frac{5}{2}f(x)+\frac{4}{3}f(x-h)-\frac{1}{12}f(x-2h)]+O(h^4) \tag{3}$$

Which is a **central 5-point formula** for the second derivative of **4-th order accuracy**.

# 2 2. Simpson Rule

## 2.1 Simpson integration in Python

The following function evaluates the integral of a given function $f(x)$ on a finite interval $x \in [a, b]$ using a set of $n$ equidistant sample points.

```
import math

def simpson(f, a, b, n):
    """Approximate the Integral of f in the interval
    between a and b using n equidistant sample points using
    Simpsons rule. The number of sample points can be even or odd."""
    # Enforce oddity
    n = max (n, 2)
    h = (b-a)/(n-1)
    odd_n = n -1 + n%2 # Enforce oddity
    S = f(a) + f(a+(odd_n-1)*h)
    # Integrate over alternating coefficients
    for i in range(1, n-1, 2):
S += 4*f(a + i * h)
    for i in range(2, n-2, 2):
S += 2*f(a + i * h)
    S *= h/3
    # Case n even
    if (n%2 == 0):
S += (h/12)* (5*f(b) + 8*f(b-h) - f(b-2*h))
    return S

# Lets output a test value
simpson(math.sin, 0, math.pi/2, 8)
```