**Introduction to Laboratory 8**

Laboratory 8 concerns the implementation of the **forward difference** and **central difference approximations** to calculate the first and second derivatives of a function $f(x)$. For example, the **forward difference approximation** for $f'(x)$ can be obtained from the Taylor expansion:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \cdots$$

which can be rewritten as

$$f'(x) = \frac{1}{h}\left[f(x+h) - f(x) - \frac{h^2}{2}f''(x) + \cdots\right]$$

giving the **forward difference approximation**

$$f'(x) = \frac{1}{h}[f(x+h) - f(x)] + E(h)$$

$$f'(x) \approx \frac{1}{h}[f(x+h) - f(x)]$$

where $E(h)$ is the error arising from the finite value of $h$, and it is given by

$$E(h) = -\frac{h}{2}f''(x) + \cdots$$

This shows that for small value of $h$ the error behaves linearly with respect to $h$, i.e. the error is of order 1 for the **forward difference approximation (FDA)**.

Similarly, we can derive expressions for the **central difference approximation (CDA)** and for the second derivative $f''(x)$ (see Laboratory 8).

In Laboratory 8 you have to:

1) Calculate the first and second derivatives of the function $f(x) = xe^x$ at $x = 2$ for different values of $h$, using both the **forward difference** and **central difference approximations**.

2) Calculate the error for different values of $h$ by making the difference between the numerical estimate and the exact value, i.e. $|E(h)| = \left|f'_{FDA\ or\ CDA} - f'_{Exact}\right|$.

3) Estimate the order of the error using the **Linear Least Squares method**. For small values of $h$ the error can be approximated by $|E(h)| \approx h^n$, where $n$ corresponds to the order of the error. This equation can be rewritten as $\ln|E(h)| \approx n \ln h$, which takes the form of a linear function ($y = ax$) with $y \equiv \ln|E(h)|$, $x \equiv \ln h$ and $a \equiv n$. By using the data points $x_i = \ln h_i$ and $y_i = \ln|E(h_i)|$ calculated from different values of $h$, the order of the error $n$ can be obtained with the **Linear Least Squares method** (see Figure 1).

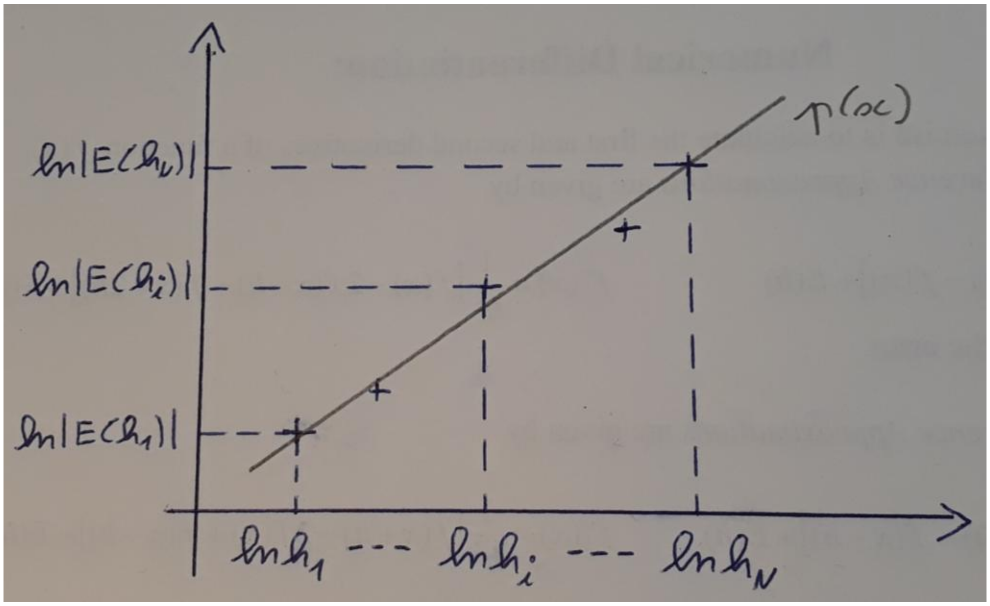

Figure 1: Plot of $\ln|E(h)|$ in function of $\ln h$. The slope $a$ of the linear function $p(x)$ interpolating the data points gives the order of the error.

In the **Linear Least Squares method** the interpolating polynomial is a linear function $p(x) = ax + b$. The coefficients $a$ and $b$ defining $p(x)$ are obtained by minimizing the quantity $S$ (summation of the squared differences):

$$S = \sum_{i=1}^{N} (p(x_i) - y_i)^2$$

where $N$ is the number of data points.

$S$ is a function of the two variables $a$ and $b$. Using the relations for a minimum, i.e. $\partial S/\partial a = 0$, $\partial S/\partial b = 0$, $\partial^2 S/\partial a^2 > 0$ and $\partial^2 S/\partial b^2 > 0$, we can find expressions for the coefficients $a$ and $b$ that minimize $S$. Thus, it is found that $S$ is minimum for

$$a = \frac{N \sum_{i=1}^{N} x_i y_i - \sum_{i=1}^{N} \sum_{j=1}^{N} x_i y_j}{N \sum_{i=1}^{N} x_i^2 - (\sum_{i=1}^{N} x_i)^2}$$

$$b = \frac{\sum_{i=1}^{N}\sum_{j=1}^{N} x_i^2\, y_j - \sum_{i=1}^{N}\sum_{j=1}^{N} x_i y_i x_j}{N\sum_{i=1}^{N} x_i^2 - \left(\sum_{i=1}^{N} x_i\right)^2}$$

In Laboratory 8, you should find values of the slope $n$ close to 1 and 2 for the **FDA** and **CDA**, respectively.