Computational Methods - Lesson 1 (Luxembourg, 16.09.2020)

Numerical differentiation and integration

Matteo Barborini*,[a], Valentin Vassilev Galindo*,[b], Prof. Alexandre Tkatchenko*

Theoretical Chemical Physics group

Faculté des Sciences, des Technologies et de Médecine - Département Physique et sciences des matériaux

*Campus Limpertsberg, Université du Luxembourg - 162 A, avenue de la Faïencerie, L-1511 Luxembourg

[a]matteo.barborini@uni.lu, [b]valentin.vassilev@uni.lu

1. Introduction

Before discussing numerical integration and differentiation, we have to recall the two main tools on which the various approaches are based. The first is **Taylor's Theorem** which states that if a function $f(x)$ is continuous and differentiable $n+1$ times in the interval $[a,b]$ and $x_0 \in [a,b]$, then for all $x \in [a,b]$ there exists a real number $\xi \in [\min(x_0,x), \max(x_0,x)]$ for which we can write

$$f(x) = P_n(x) + R_n(x) \tag{1}$$

where $P_n(x)$ is a **Taylor polynomial** of order n defined as:

$$P_n(x) = \sum_{k=0}^{n} \frac{1}{k!} \left.\frac{d^k f(x)}{dx^k}\right|_{x=x_0} (x-x_0)^k \tag{2}$$

and $R_n(x)$ is the **reminder term** (or truncation error) of the expansion (in Lagrange's formalism), defined as:

$$R_n(x) = \frac{1}{(n+1)!} \sup_{\xi \in [a,b]} \left.\frac{d^{n+1} f(x)}{dx^{n+1}}\right|_{x=\xi} (x-x_0)^{n+1}. \tag{3}$$

The second tool are the **Lagrange polynomials**, commonly used as interpolation tools to approximate a function in a finite interval (see Fig. 1). Let us suppose to have n data points $[(x_1,y_1),(x_2,y_2),\ldots,(x_n,y_n)]$ in the interval $[a,b]$ of the function $f(x)$ ($y_n = f(x_n)$), then we can construct the Lagrange polynomial of order n as

$$L_{n-1}(x) = \sum_{j=1}^{n} y_j Y_j(x) \tag{4}$$

where $Y_j(x)$ are polynomial functions (Lagrange coefficients) that are chosen to be equal to

$$Y_j(x) = C \prod_{i(\neq j)=1}^{n} (x - x_i). \tag{5}$$

To determine the constant factor C we can impose the interpolation condition that $L_{n-1}(x_i) = y_i$ so that $Y_j(x_i) = \delta_{ij}$, and we obtain that

$$Y_j(x_j) = C \prod_{i(\neq j)=1}^{n} (x_j - x_i) = 1 \quad \text{and} \quad C = \prod_{i(\neq j)=1}^{n} \frac{1}{(x_j - x_i)}. \tag{6}$$

Substituting this value of the constant in eq. 5 we get the final expression of the Lagrange coefficients

$$Y_j(x) = \prod_{i(\neq j)=1}^{n} \frac{x - x_i}{x_j - x_i}, \tag{7}$$

and consequently the Lagrange polynomial of order n will be defined as:

$$L_{n-1}(x) = \sum_{j=1}^{n} y_j \prod_{i(\neq j)=1}^{n} \frac{x - x_i}{x_j - x_i}. \tag{8}$$

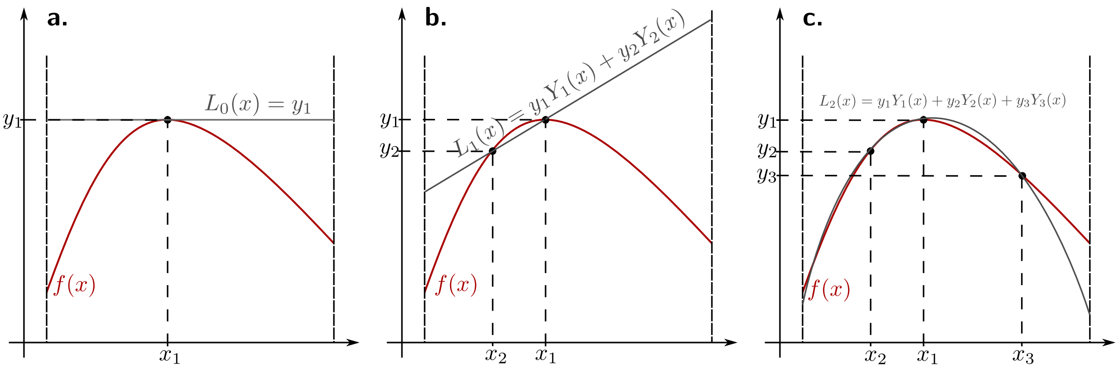

Figure 1: Approximation the $f(x)$ function in a given integral with and order 0 **a.**, and order 1 **b.** and an order 2 **c.** Lagrange polynomial.

It is also useful for the following discussions, to recall that the **reminder term** for the Lagrange expansion of a function $f(x)$ is written as[1]

$$R_n(x) = \frac{1}{n!} \sup_{\xi \in [a,b]} \left. \frac{d^n f(x)}{dx^n} \right|_{x=\xi} \prod_{i=1}^{n} (x - x_i) \tag{9}$$

where ξ is the value of x in the interval $[a, b]$ that maximises the value of the nth order derivative of $f(x)$.

2. Numerical differentiation

The definition of the first order derivative of a function $f(x)$ in a point x_0 is written through the limits

$$\left. \frac{df(x)}{dx} \right|_{x=x_0} = \lim_{h\to 0} \frac{f(x_0+h) - f(x_0)}{h} = \lim_{h\to 0} \frac{f(x_0) - f(x_0-h)}{h} = \lim_{h\to 0} \frac{f(x_0+h) - f(x_0-h)}{2h}, \tag{10}$$

and represents the angular coefficient of the tangent to the function $f(x)$ in x_0. If the displacement h is small enough, it is possible to approximate the derivative in x_0 through the three ratios

$$\left. \frac{df(x)}{dx} \right|_{x=x_0} \approx \begin{cases} \frac{f(x_0)-f(x_0-h)}{h} & \textit{backward difference} \\ \frac{f(x_0+h)-f(x_0-h)}{2h} & \textit{central difference} \\ \frac{f(x_0+h)-f(x_0)}{h} & \textit{forward difference} \end{cases} \tag{11}$$

that give slightly different results and converge differently as orders of h (An example of the forward difference in Python 3.0 can be found in the file `les01.1.py`).
To study the order of the error associated to the three differences, we can expand the function $f(x)$ in Taylor series around x_0

$$f(x) = f(x_0) + \left. \frac{df(x)}{dx} \right|_{x=x_0} (x - x_0) + \frac{1}{2} \left. \frac{d^2 f(x)}{dx^2} \right|_{x=x_0} (x - x_0)^2 + \frac{1}{6} \left. \frac{d^3 f(x)}{dx^3} \right|_{x=x_0} (x - x_0)^3 + \dots \tag{12}$$

so that the values of the function in $x_0 + h$ and $x_0 - h$ will written as

$$\begin{aligned} f(x_0+h) &= f(x_0) + \left. \tfrac{df(x)}{dx} \right|_{x=x_0} h + \tfrac{1}{2} \left. \tfrac{d^2 f(x)}{dx^2} \right|_{x=x_0} h^2 + \tfrac{1}{6} \left. \tfrac{d^3 f(x)}{dx^3} \right|_{x=x_0} h^3 + \dots \\ f(x_0-h) &= f(x_0) - \left. \tfrac{df(x)}{dx} \right|_{x=x_0} h + \tfrac{1}{2} \left. \tfrac{d^2 f(x)}{dx^2} \right|_{x=x_0} h^2 - \tfrac{1}{6} \left. \tfrac{d^3 f(x)}{dx^3} \right|_{x=x_0} h^3 + \dots \end{aligned} \tag{13}$$

By substituting these expansions in the finite differences in eq. 11 we can rewrite the derivatives in the three cases as

$$\left. \frac{df(x)}{dx} \right|_{x=x_0} = \begin{cases} \frac{f(x_0)-f(x_0-h)}{h} + \frac{h}{2} \left. \frac{d^2 f(x)}{dx^2} \right|_{x=x_0} - \frac{h^2}{6} \left. \frac{d^3 f(x)}{dx^3} \right|_{x=x_0} + \dots \\ \frac{f(x_0+h)-f(x_0-h)}{2h} - \frac{h^2}{6} \left. \frac{d^3 f(x)}{dx^3} \right|_{x=x_0} + \dots \\ \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2} \left. \frac{d^2 f(x)}{dx^2} \right|_{x=x_0} - \frac{h^2}{6} \left. \frac{d^3 f(x)}{dx^3} \right|_{x=x_0} + \dots \end{cases} \tag{14}$$

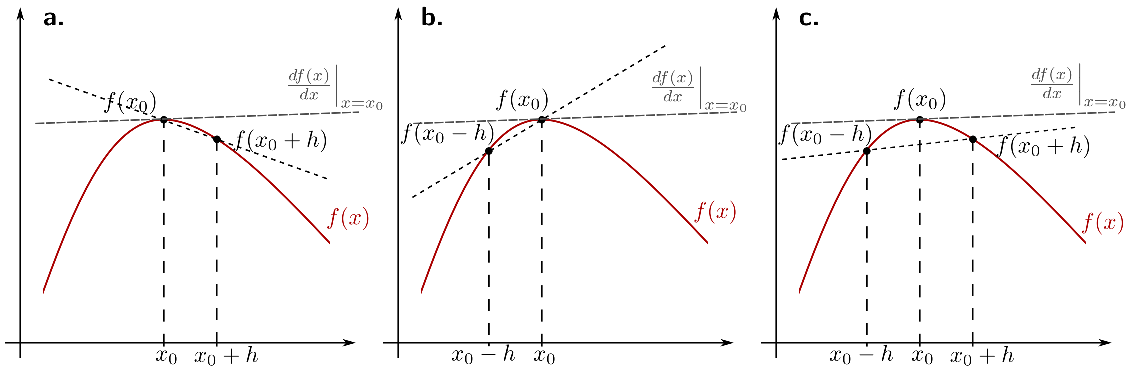

Figure 2: The grey line is the tangent to the function $f(x)$ in x_0 which is compared to the dotted black lines with angular coefficient obtained with the *forward difference* **a**, *backward difference* **b** and *central difference* **c** approximations.

so that approximating the derivatives with the first terms in the expansion

$$\frac{df(x)}{dx}\bigg|_{x=x_0} \approx \begin{cases} \frac{f(x_0)-f(x_0-h)}{h} + O(h) \\ \frac{f(x_0+h)-f(x_0-h)}{2h} + O(h^2) \\ \frac{f(x_0+h)-f(x_0)}{h} + O(h) \end{cases} \tag{15}$$

it is clear that the residual error for the first two methods is of order $O(h)$ while for the *central difference* approach it is of order $O(h^2)$. The fact that the *central difference* approach is more accurate can also be deduced from Fig. 2, where we compare the graphical representation of the derivative of $f(x)$ in x_0 with that obtained with numerical differentiation. In the example of Fig. 2 x_0 is near a saddle point of $f(x)$ so that the discrepancies between the three numerical methods become more evident. Clearly if the derivative is computed on a point x_0 where the function $f(x)$ has a more linear behaviour, then the differences between the three approaches vanish.

To better understand why the *central difference* approach is more accurate let us consider the Lagrange expansion of the function $f(x)$ on nth points in the interval $[a,b]$

$$f(x) = \sum_{j=1}^{n} f(x_j) Y_j(x) + \frac{1}{n!} \sup_{\xi\in[a,b]} \frac{d^n f(x)}{dx^n}\bigg|_{x=\xi} \prod_{j=1}^{n} (x - x_j)\,. \tag{16}$$

By computing the derivative with respect to x we obtain the expansion

$$\frac{df(x)}{dx} = \sum_{j=1}^{n} f(x_j)\frac{dY_j(x)}{dx} + \frac{1}{n!} \sup_{\xi\in[a,b]} \frac{d^n f(x)}{dx^n}\bigg|_{x=\xi} \sum_{k=1}^{n} \left[\prod_{j(\neq k)=1}^{n} (x - x_j)\right] \tag{17}$$

that computed on one of the nth points will be equal to:

$$\frac{df(x)}{dx}\bigg|_{x=x_i} = \sum_{j=1}^{n} f(x_j)\, \frac{dY_j(x)}{dx}\bigg|_{x=x_i} + \frac{1}{n!} \sup_{\xi\in[a,b]} \frac{d^n f(x)}{dx^n}\bigg|_{x=\xi} \prod_{j(\neq i)=1}^{n} (x_i - x_j)\,. \tag{18}$$

Now let us consider the case in which $n = 3$ for which the three derivatives of the Lagrange coefficients will be (with a bit of algebra)

$$\frac{dY_1(x)}{dx} = \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} \quad \frac{dY_2(x)}{dx} = \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} \quad \frac{dY_3(x)}{dx} = \frac{2x - x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)}.$$

In this case eq. 18 reduces to

$$\frac{df(x)}{dx}\bigg|_{x=x_i} = f(x_1)\frac{2x_i - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} + f(x_2)\frac{2x_i - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} + \\ + f(x_3)\frac{2x_i - x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)} + \frac{1}{3!} \sup_{\xi\in[a,b]} \frac{d^3 f(x)}{dx^3}\bigg|_{x=\xi} \prod_{j(\neq i)=1}^{3} (x_i - x_j)\,. \tag{19}$$

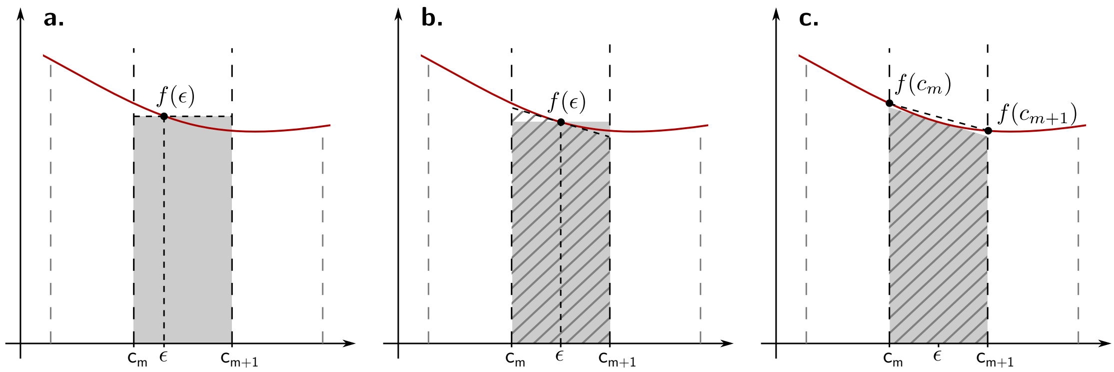

Figure 3: a. In the *rectangle rule* the area of the grey rectangle is used to estimate the integral of $f(x)$ in the interval $[c_m : c_{m+1}]$. The height of the rectangle is given by $f(\epsilon)$ were ϵ is an arbitrary value in $[c_m : c_{m+1}]$. **b.** In the *midpoint method* $\epsilon = (c_{m+1} + c_m)/2$ and the area of the grey rectangle is equal to the area of the trapezoid defined by an line passing through the midpoint (the line can be also the derivative of the function in the midpoint). **c.** In the *trapezoid rule* the area that approximates the integral is the trapezoid defined by the two points $(c_{m+1}, f(c_{m+1}))$ and $(c_m, f(c_m))$ at the edges of the interval. The trapezoid obtained from this rule is compared to that obtained from the *midpoint method*.

Now assuming, for simplicity, that the three points are equidistant, $x_1 = x_0$, $x_2 = x_0 + h$, $x_3 = x_0 + 2h$, the three derivatives of the function $f(x)$ on $x_1,\ x_2$ and x_3 will be written as

$$\begin{cases} \left.\frac{df(x)}{dx}\right|_{x=x_0} = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \\ \left.\frac{df(x)}{dx}\right|_{x=x_0+h} = \frac{1}{2h}\left[-f(x_0) + f(x_0+2h)\right] - \frac{h^2}{6}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \\ \left.\frac{df(x)}{dx}\right|_{x=x_0+2h} = \frac{1}{2h}\left[f(x_0) - 4f(x_0+h) + 3f(x_0+2h)\right] + \frac{h^2}{3}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \end{cases},$$

and finally, by transforming the variable in the second equation as $x_0 + h = x_0'$ and in the third equation as $x_0 + 2h = x_0''$, we obtain the formulas for the first order derivatives in three point approximations:

$$\begin{cases} \left.\frac{df(x)}{dx}\right|_{x=x_0} = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \\ \left.\frac{df(x)}{dx}\right|_{x=x_0'} = \frac{1}{2h}\left[-f(x_0'-h) + f(x_0'+h)\right] - \frac{h^2}{6}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \\ \left.\frac{df(x)}{dx}\right|_{x=x_0''} = \frac{1}{2h}\left[f(x_0''-2h) - 4f(x_0''-h) + 3f(x_0'')\right] + \frac{h^2}{3}\sup_{\xi\in[a,b]} \left.\frac{d^3f(x)}{dx^3}\right|_{x=\xi} \end{cases}$$

which correspond to the three-point *forward difference*, *central difference* and *backward difference*. From this result it is evident that the two-point central difference is a special case of the 3point numerical differentiation and this is the reason why the error is of order $O(h^2)$

3. Numerical integration

The solution of problems of scientific nature often requires the evaluation of integrals. The simplest type of integrals are those computed on finite intervals

$$I = \int_a^b f(x)dx. \tag{20}$$

If the antiderivative (or primitive function) $F(x)$ of $f(x)$ is known in the integration interval, clearly the problem can be solved analytically as $I = F(b) - F(a)$, yet this knowledge is not always straightforward, and in this case it is possible to apply methods for numerical integration. The idea at the basis of these methods lies in the discretization of the integral space in $\mathcal{M}$ subspaces taking advantage of the additive property of the integrals:

$$I = \int_a^b f(x)dx = \sum_{m=1}^{\mathcal{M}} \int_{c_m}^{c_{m+1}} f(x)dx = \sum_{m=1}^{\mathcal{M}} I_m \tag{21}$$

with $c_1 = a$ and $c_{\mathcal{M}+\infty} = b$ and $a \leq c_m \leq b \; \forall m \in [1, \mathcal{M}]$, so that the value I is reduced to a sum of the $\mathcal{M}$ integrals on their subspaces. Still, the exact solution of the integrals I_m intervals requires the knowledge of the antiderivative of the function $f(x)$ which is not known. Yet, since we can choose $\mathcal{M}$ as large as we want, it is possible to reduce the subspaces of I_m, until in those intervals the function $f(x)$ behaves in a sufficiently regular manner. At this point it is possible to approximate the function $f(x)$ with a simpler one (for example a polynomial) of which the primitive function is known. For polynomial interpolation, it is common to use the Lagrange polynomials $L_{n-1}(x)$ previously defined, so that

$$I_m \approx I_m^{(n)} = \int_{c_m}^{c_{m+1}} L_{n-1}(x) dx, \tag{22}$$

where n represents the order of the polynomial used for the interpolation of the $f(x)$ function. The absolute value of the truncation is equal to

$$\Delta_n = |f(x) - L_{n-1}(x)| \leq \frac{1}{n!} \sup_{\xi \in [a:b]} \left| \frac{d^n f(x)}{dx^n} \bigg|_{x=\xi} \right| \prod_{i=1}^{n} |x - x_i| \,, \tag{23}$$

and thus we can define the error in the integration over the mth interval as

$$\delta_m^{(n)} = |I_m - I_m^{(n)}| = \int_{c_m}^{c_{m+1}} \Delta_n dx \leq \frac{1}{n!} \sup_{\xi \in [c_m:c_{m+1}]} \left| \frac{d^n f(x)}{dx^n} \bigg|_{x=\xi} \right| \int_{c_m}^{c_{m+1}} \prod_{i=1}^{n} |x - x_i| \, dx. \tag{24}$$

Supposing again that the lengths of the integration intervals are all the same ($h = c_{m+1} - c_m \; \forall \, m$) and defining the change of variables

$$x = \frac{c_{m+1} + c_m}{2} + \frac{c_{m+1} - c_m}{2} t = \frac{h + 2c_m}{2} + \frac{h}{2} t = \frac{h}{2}(t+1) + c_m \tag{25}$$

we can rewrite the error as[1]

$$\delta_m^{(n)} \leq \frac{1}{n!} \left(\frac{h}{2} \right)^{n+1} \sup_{\epsilon \in [c_m:c_{m+1}]} \left| \frac{d^n f(x)}{dx^n} \bigg|_{x=\epsilon} \right| \int_{-1}^{1} \prod_{i=1}^{n} |t - t_i| \, dt, \tag{26}$$

where the integral does not depend on the specific interval on which it is calculated. Finally, defining

$$S_m^{(n)} [f(x)] = \sup_{\epsilon \in [c_m:c_{m+1}]} \left| \frac{d^n f(x)}{dx^n} \bigg|_{x=\epsilon} \right| \quad \text{and} \quad T_n = \frac{1}{n!} \int_{-1}^{1} \prod_{i=1}^{n} |t - t_i| \, dt, \tag{27}$$

we have that the error accumulated over the algorithmic integration of $f(x)$ over the interval $[a, b]$ will be written as the sum of all the errors

$$\delta^{(n)} = \sum_{m=0}^{\mathcal{M}-1} \delta_m^{(n)} \leq \left(\frac{h}{2} \right)^{n+1} T_n \sum_{m=0}^{\mathcal{M}-1} S_m^{(n)} [f(x)] \leq \mathcal{M} \left(\frac{h}{2} \right)^{n+1} T_n \mathcal{S}^{(n)} [f(x)] \tag{28}$$

where

$$\mathcal{S}^{(n)} [f(x)] = \max_{m \in [1:\mathcal{M}]} S_m^{(n)} [f(x)] = \sup_{\epsilon \in [a:b]} \left| \frac{d^n f(x)}{dx^n} \bigg|_{x=\epsilon} \right|. \tag{29}$$

Finally, considering that $\mathcal{M}h = b - a$ we can estimate the integration error as

$$\delta^{(n)} \leq \frac{b-a}{2^{n+1}} h^n T_n \mathcal{S}^{(n)} [f(x)] \tag{30}$$

which, as expected, decreases as the nth power of the length h, that is equivalent to saying that it decreases if we increase the number $\mathcal{M}$ of intervals in which we divide $[a : b]$.

[1]Differentiating the new variable we have that $dx = \frac{h}{2} dt$ and the new extremes of the integration can be obtained by setting $c_m = \frac{h}{2}(t_m + 1) + c_m$ so that $t_m = -1$ and by setting $c_{m+1} = \frac{h}{2}(t_{m+1} + 1) + c_m$ from which $t_{m+1} = 1$.

3.1. Rectangle rule. The simplest Legendre polynomial with which we can approximate the true function $f(x)$ is that of order zero, with $n = 1$, such that

$$I_m \approx I_m^{(1)} = \int_{c_m}^{c_{m+1}} L_0(x)dx = f(x_0)(c_{m+1} - c_m) \tag{31}$$

where $x_0 \in [c_m : c_{m+1}]$ is an arbitrary number in the integration interval. Equation 31 is the so called rectangular rule, that takes its name from the fact that the integral under the function $f(x)$ in the interval $[c_m : c_{m+1}]$ is approximated by a rectangle with the width $(c_{m+1} - c_m)$ and the height $f(x_0)$. Usually, this very rough approximation is used only if the function $f(x)$ is unknown except for some points obtained for example through experimental measurements. The error in the integration in this case will be equal to

$$\delta^{(1)} \le \frac{b-a}{4} h T_1 \mathcal{S}^{(1)}\left[f(x)\right] \tag{32}$$

where

$$\mathcal{S}^{(1)}\left[f(x)\right] = \sup_{\epsilon \in [a:b]} \left| \left. \frac{df(x)}{dx} \right|_{x=\epsilon} \right| \quad \text{and} \quad T_1 = \int_{-1}^{1} |t - t_1|\, dt. \tag{33}$$

3.2. Midpoint method. A particular case of the rectangle rule is the so called *midpoint method* for which in eq. 31 the function $f(x)$ is evaluated at the midpoint $x_0 = (c_{m+1} + c_m)/2$ of the interval $[c_m : c_{m+1}]$. Although, the quadrature formula remains the same as the *rectangle rule*, the error in this case is much smaller. As a matter of fact, the area of the rectangle is the same as the area below any line passing through the middle point in the given interval (An example of the Midpoint method in Python 3.0 can be found in the file `les01.2.py`). By considering that the Taylor expansion of the function $f(x)$ around the point x_0 defined above

$$\begin{aligned} f(x) \approx f\left(\frac{c_{m+1}+c_m}{2}\right) + \left.\frac{df(x)}{dx}\right|_{x=\frac{c_{m+1}+c_m}{2}} \left(x - \frac{c_{m+1}+c_m}{2}\right) + \\ + \frac{1}{2}\left.\frac{d^2 f(x)}{dx^2}\right|_{x=\frac{c_{m+1}+c_m}{2}} \left(x - \frac{c_{m+1}+c_m}{2}\right)^2 + \dots \end{aligned} \tag{34}$$

we have that the first two terms correspond to a line passing through the middle point, thus the error of the integral in the mth interval will be

$$\begin{aligned} \delta_m^{(1)} \le \frac{1}{2}\left| \left.\frac{d^2 f(x)}{dx^2}\right|_{x=\frac{c_{m+1}+c_m}{2}} \right| \left| \int_{c_m}^{c_{m+1}} \left| x - \frac{c_{m+1}+c_m}{2}\right|^2 dx = \right. \\ = \frac{1}{48}\left| \left.\frac{d^2 f(x)}{dx^2}\right|_{x=\frac{c_{m+1}+c_m}{2}} \right| (c_{m+1} - c_m)^3 \end{aligned} \tag{35}$$

and thus the total error will be (considering that $T_1 = 1$):

$$\delta^{(1)} \le \frac{1}{24} \mathcal{S}^{(2)}\left[f(x)\right] h^2 (b-a) \tag{36}$$

that is of the same order of $\delta^{(2)}$ and differs only for a prefactor. The reason for this is that the *midpoint method* corresponds to approximating the function with a Lagrange polynomial of the first degree passing through two coinciding points that correspond to the midpoint.

3.3. Trapezoidal rule. The trapezoidal rule is obtained by approximating the function $f(x)$ with a Lagrange polynomial of n=2 passing through the points at the edges of the interval $[c_m : c_{m+1}]$:

$$I_m \approx I_m^{(2)} = \int_{c_m}^{c_{m+1}} L_1(x)dx = \frac{f(c_{m+1}) + f(c_m)}{2}(c_{m+1} - c_m) \tag{37}$$

with an error equal to ($T_2 = \frac{2}{3}$)

$$\delta^{(2)} \le \frac{b-a}{12} h^2 \mathcal{S}^{(2)}\left[f(x)\right]. \tag{38}$$

3.4. Simpson's rule. A more accurate approximation of the integral can be obtained by approximating the function in the interval $[c_m, c_{m+1}]$ with a parabola passing through the integration limits and the midpoint of the interval. By constructing the Lagrange polynomial we obtain Simpson's formula

$$I_m \approx I_m^{(3)} = \int_{c_m}^{c_{m+1}} L_2(x)dx = \frac{f(c_{m+1}) + 4f((c_m + c_{m+1})/2) + f(c_m)}{6}(c_{m+1} - c_m) \tag{39}$$

for which it can be shown that the error

$$\delta^{(3)} \leq (b-a)h^4 \mathcal{S}^{(3)}\left[f(x)\right] T_3. \tag{40}$$

is of the fourth order in h.

References

(1) Howell, G. W. Derivative error bounds for Lagrange interpolation: An extension of Cauchy's bound for the error of Lagrange interpolation. *J. Approx. Theo.* **1991**, *67*, 164 – 173.