CHAPTER V
NUMERICAL DIFFERENTIATION AND INTEGRATION

Nabil R. Nassif and Dolly K. Fayad

April 2012

1 Introduction

As in the previous chapter, let D_n be a set of $n+1$ given points in the (x, y) plane:

$$D_n = \{(x_i, y_i) |\, 0 \leq i \leq n; a = x_0 < x_1 < ... < x_n = b;\, y_i = f(x_i)\}, \tag{1}$$

for some function $f(x)$. Our basic objectives in this chapter are to seek accurate "approximations", based on D_n for:

1. $f'(x_i)$ and $f"(x_i)$: $i = 0, 1, ..., n$ (Numerical Differentiation),
2. $I = \int_a^b f(x)\, dx$ (Numerical Integration).

In what follows and unless stated otherwise, we shall assume that the x-data in D_n are equi-spaced, with:

$$h = x_{i+1} - x_i.$$

The topics of Numerical differentiation and Integration shall be made, solely relying on the standard Taylor's formula and the Intermediate Value Theorem, thus completely independant of the theory of interpolation as classically used in most textbooks (see [**?**], [**?**], [**?**]). To start, our discussion shall be illustrated on the following set of data related to the Bessel's function:

Example 1 *Consider the following table of data associated with the function $f(x) = J_0(x)$, the 0-th order Bessel's function of the first kind.*

i	$\mathbf{x_i}$	$\mathbf{y_i}$
0	0.00	1.0000000
1	0.25	0.98443593
2	0.50	0.93846981
3	0.75	0.86424228
4	1.00	0.76519769
5	1.25	0.64590609
6	1.50	0.51182767
7	1.75	0.36903253
8	2.00	0.22389078

Table 1. Data for $J_0(x)$, $x = 0.0\, 0.25, ..., 2.00$

The data is associated with 8 equidistant intervals of size $h = 0.25$.

2 Mathematical Prerequisites

In this section, we give a review of some basic results in Calculus.

2.1 Taylor's formula

Let $h_0 > 0$ and $m \in \mathrm{I\!R}$. Assume the function $f(x) \in C^{k+1}[(m - h_0, m + h_0)]$ that is, its derivatives:

$$\{f^{(j)}(x) : j = 1, ..., k, k+1\}$$

are continuous in the interval $(m - h_0, m + h_0)$. Then for all $h < h_0 \in \mathrm{I\!R}$, there exists $t \in (0, 1)$, such that:

$$f(m+h) = f(m) + f'(m)h + f^{(2)}(m)\frac{h^2}{2} + ... \tag{2}$$
$$... + f^{(k)}(m)\frac{h^k}{k!} + f^{(k+1)}(c)\frac{h^{k+1}}{(k+1)!},$$

with $c = m + th$. Formula (2) will be refered to as "Taylor's development about m" up to the $k-$th order, the "remainder term" being $R_k = f^{(k+1)}(c)\frac{h^{k+1}}{(k+1)!}$. Using the big-$O(.)$ notation, we abbreviate the formula as follows:

$$f(m+h) = f(m) + f'(m)h + f^{(2)}(m)\frac{h^2}{2} + ... + f^{(k)}(m)\frac{h^k}{k!} + O(h^{k+1}) \tag{3}$$

or for more convenience give it a form that is independent of the order of the development, that is under the assumption that the derivatives of f are continuous up to any order ($f \in C^{\infty}[(m - h_0, m + h_0)]$):

$$f(m+h) = f(m) + f'(m)h + f^{(2)}(m)\frac{h^2}{2} + ... + f^{(k)}(m)\frac{h^k}{k!} + ... \tag{4}$$

Hence, we will consider as equivalent (2), (3) or (4).

2.2 Intermediate Value Theorem

Let g be a continuous function defined over some subset $D \subset \mathrm{I\!R}$. Then for every finite ordered subset of points $\{m_1, m_2, ..., m_k\}$ in D, there exists a number $c \in D$, such that:

$$\sum_{i=1}^{k} g(m_i) = kg(c). \tag{5}$$

2.3 Mean Value Theorems

1. **First Mean Value Theorem**
   This theorem results from the application of Taylor's formula where the error term is expressed in terms of the first order derivative, specifically:

   $$f(m+h) - f(m) = hf'(c),\ c \in (m, m+h),$$

   which is equivalent to:

   $$\int_m^{m+h} f'(x)dx = f'(c)h. \tag{6}$$

2. **Second Mean Value Theorem**
   This one generalizes the previous one, (6) becoming:

$$\int_m^{m+h} w(x)g(x)dx = g(c)\int_m^{m+h} w(x)dx, \tag{7}$$

   where $g(x)$ and $w(x)$ are continuous functions with $w(x) \geq 0$ (or $w(x) \leq 0$).

3 Numerical Differentiation

3.1 1^{st} order Derivatives and Divided Differences

Based on the set of points (1), Divided Differences appear to provide efficient "discrete" tools to approximate derivatives. This is illustrated by the following proposition which is essential in this chapter.

Theorem 1 *Assume that the function f is k-times continuously differentiable in D. Then for every subset of distinct points $\{x_i, x_{i+1}, ..., x_{i+k}\}$ in D, there exists $c \in (x_i, x_{i+k})$, such that*

$$[x_i, x_{i+1}, ..., x_{i+k}] = \frac{f^{(k)}(c)}{k!}. \tag{8}$$

This theorem suggests the following approximation formulae for 1^{st} order derivatives (k=1):

$$f'(x_i) \approx \begin{cases} .[x_i, x_{i+1}] = \frac{y_{i+1}-y_i}{h} = \frac{\Delta_h y_i}{h} & (9.1) \\ .[x_{i-1}, x_i] = \frac{y_i - y_{i-1}}{h} = \frac{\nabla_h y_i}{h} & (9.2) \\ .[x_{i-1}, x_{i+1}] = \frac{y_{i+1}-y_{i-1}}{2h} = \frac{\delta_h y_i}{2h} & (9.3) \end{cases} \tag{9}$$

These approximations to the 1^{st} derivative are successively: **the Forward Difference (9.1), the Backward Difference (9.2) and the Central (9.3) Approximations.**
Obviously, in the example above, the 1^{st} approximation formula for the derivative is particularly suitable at the top of the table above, while the 2^{nd} approximation can be used at the bottom. The 3^{rd} one approximates $f'(x_i)$ anywhere in between.

3.2 Error Analysis: Order of the methods

Let h be a positive number, such that $0 < h < 1$.

- Forward Difference approximation:
  Using Taylor's formula up to first order, we can write:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(c_1) \tag{10}$$

  where c_1 is in the interval $(x, x+h)$, which leads to:

$$f'(x) = \frac{1}{h}[f(x+h) - f(x)] - \frac{1}{2}hf^{(2)}(c_1)$$

or equivalently:

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

Hence the approximation:

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

is the 1^{st} order **Forward Difference** approximation (9.1) to $f'(x)$, with a truncation error whose most dominant term is of order h. We write then: $E = O(h)$.

- Backward Difference approximation:
  Likewise, replacing h by $(-h)$, equation (10) implies then:

(11) $$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(c_2)$$

where c_2 is in the interval $(x-h, x)$, leading to:

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

Hence the approximation:

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

is the 1^{st} order **Backward Difference** approximation (9.2) to $f'(x)$, and its truncation error term is of order h, that is $E = O(h)$.

Remark 1 *Note that for the Forward and Backward Difference approximations, it is enough that $f \in C^2(D)$. The truncation error in these approximation formulae remains $O(h)$ when calculations are performed with higher order regularity conditions on f, that is when $f \in C^k(D)$, with $k > 2$.*

- Central Difference approximation:
  It is advantageous to have the convergence of numerical processes occur with higher orders. At this stage, we aim to obtain an approximation to $f'(x)$ in which the error behaves like $O(h^2)$. One such result is achieved based on the Central Difference approximation with the aid of Taylor's series where f is assumed to have continuous derivatives up to order 3 at least, that is $f \in C^k(D)$, with $k \geq 3$. Thus:

(12) $$f(x+h) = f(x) + hf'(x) + \frac{1}{2!}h^2 f^{(2)}(x) + \frac{1}{3!}h^3 f^{(3)}(c_1)$$

where $x < c_1 < x + h$.

and similarly:

$$f(x-h) = f(x) - hf'(x) + \frac{1}{2!}h^2 f^{(2)}(x) - \frac{1}{3!}h^3 f^{(3)}(c_2) \tag{13}$$

where $x - h < c_2 < x$.

By subtraction and using the Intermediate Value Theorem, we obtain:

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2}{3!}h^3 f^3(c) \tag{14}$$

where $c_1 < c < c_2$.

This leads to a new approximation for $f'(x)$:

$$f'(x) = \frac{1}{2h}[f(x+h) - f(x-h)] + O(h^3) \tag{15}$$

where the approximation

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} = \frac{\delta_h f(x)}{2h}$$

is the 1^{st} order **Central Difference** approximation to $f'(x)$, with its truncation error $E = O(h^2)$.

Remark 2 *In the derivation of the Central Difference approximation formula, in case one considers Taylor's series expansion up to* <u>*first order only*</u>*, then equations (12) and (13) lead to:*

$$f'(x) = \frac{\delta_h f(x)}{2h} + \frac{h}{4}\epsilon_h$$

where $\epsilon_h = f"(c_1) - f"(c_2)$ *and* $x - h < c_1 < c_2 < x + h$.

- *If* $f \in C^2(D)$*:* $\lim_{h \to 0} \epsilon_h = 0$*, that is in a "naive" sense,* ϵ_h *behaves "nearly" like* $O(h)$*. Consequently, he truncation error* $E = O(h^+)$*, or also* $E \approx O(h^2)$

- *If* $f \in C^3(D)$*: by the Mean Value theorem* $f"(c_1) - f"(c_2) = hf'(c)$*, implying obviously that* $E = O(h^2)$.

Based on these results, when using the Central Difference approximation formula to the derivative, we shall consider $f \in C^3(D)$. ■

The basic approximation results to the 1^{st} derivatives are then summarized as follows:

Proposition 1 *Let* $0 < h < 1$*. Then*

$$f'(x) = \begin{cases} \frac{\Delta_h f(x)}{h} - f^{(2)}(c_1)\frac{h}{2} = \frac{\Delta_h f(x)}{h} + O(h);\ (f\ in\ C^2) & (16.1) \\ \frac{\nabla_h f(x)}{h} + f^{(2)}(c_2)\frac{h}{2} = \frac{\nabla_h f(x)}{h} + O(h);\ (f\ in\ C^2) & (16.2) \\ \frac{\delta_h f(x)}{h} - f^{(3)}(c)\frac{h^2}{6} = \frac{\delta_h f(x)}{2h} + O(h^2);\ (f\ in\ C^3) & (16.3) \end{cases} \tag{16}$$

where $c_1 \in (x, x+h)$, $c_2 in(x-h, x)$ and $c \in (x-h, x+h)$.

In case $x = x_i$, the formulae above are written in terms of 1^{st} order finite divided differences as follows:

$$f'(x_i) = \begin{cases} \frac{\Delta_h f(x_i)}{h} + O(h) = [x_i, x_i + h] + O(h) \\ \frac{\nabla_h f(x_i)}{h} + O(h) = [x_i - h, x_i] + O(h) \\ \frac{\delta_h f(x_i)}{2h} + O(h^2) = [x_i - h, x_i + h] + O(h^2) \end{cases}$$

Example 2 *In the data of Table 1, find approximations to* $J_0'(0) = 0$ *using the forward difference approximation formula.*

Applying formula (16.1), one has the following results.

h	$\frac{1}{h}\Delta_h f(0)$
0.25	-0.06225629
0.50	-0.12306039
0.75	-0.18101029
1.00	-0.23480231

Table 2. Approximations for $J_0'(0)$, with $h = 0.25, 0.50, 0.75, 1.00$

Example 3 *In the data of Table 1, find approximations to* $J_0'(0.25) = -0.12402598$ *using the forward difference, the backward difference and the central difference approximations formulae.*

h	$\frac{1}{h}\Delta_h f(0.25)$	$\frac{1}{2h}\delta_h f(0.25)$	$\frac{1}{h}\nabla_h f(0.25)$
0.25	-0.18386448	-0.12306038	-0.06225628

Table 3. Approximations for $J_0'(0.25) = -0.12402598$, using the formulae in (16) with $h = 0.25$

Example 4 *In the data of Table 1, find approximations to* $J_0'(1) = -0.44005059$ *using the central difference approximation formula.*

Applying formula (16.3), one has the following results.

h	$\frac{1}{2h}\delta_h f(1)$
0.25	-0.43667238
0.50	-0.42664214
1.00	-0.38805461

Table 4. Approximations for $J_0'(1) = -0.44005059$, using (16.3) with $h = 0.25, 0.50, 1.00$

In order to obtain higher order approximations to the derivatives, it is possible to use a powerful technique known as **Richardson Extrapolation**. We illustrate this process on the basis of the forward ($\equiv$ backward) difference and central difference approximations to $f'(x)$.

3.3 1^{st} order derivatives and Richardson extrapolation

3.3.a Forward and Backward Difference Richardson Extrapolation

Recall that for a function $f \in C^{\infty}$, the infinite Taylor' s series expansion formula of $f(x+h)$ is as follows:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f^{(2)}(x) + \frac{h^3}{3!}f^{(3)}(x) + ...$$

leading to:

$$f'(x) = \frac{\Delta_h f(x)}{h} + a_1 f^{(2)}(x)h + a_2 f^{(3)}(x)h^2 + a_3 f^{(4)}(x)h^3 + ... \qquad (17)$$

where the $\{a_i\}$'s are universal constants independent of h and f.

Define now

$$\phi_h(.) = \frac{1}{h}\Delta_h(.) \qquad (18)$$

- Considering successively h then $2h$ in (17), one has:

  (17.a) $f'(x) = \phi_h(f(x)) + a_1 f^{(2)}(x)h + a_2 f^{(3)}(x)h^2 + a_3 f^{(4)}(x)h^3 + ...$

  (17.b) $f'(x) = \phi_{2h}(f(x)) + a_1 f^{(2)}(x)2h + a_2 f^{(3)}(x)(2h)^2 + a_3 f^{(4)}(x)(2h)^3 + ...$

  The algebraic operation $2 \times (17.a) - (17.b)$ yields then:

  $$f'(x) = 2\phi_h(f(x)) - \phi_{2h}(f(x)) - 2a_2 f^{(3)}(x)h^2 + O(h^3).$$

  Introducing **the 1^{st} order Forward Richardson extrapolation** operator, let:

  $$\phi_h^1(f(x)) = 2\phi_h(f(x)) - \phi_{2h}(f(x)) \qquad (19)$$

  One obtains:

  $$f'(x) = \begin{cases} \phi_h^1(f(x)) + a_2' f^{(3)}(x)h^2 + a_3' f^{(4)}(x)h^3 + ... \\ \phi_h^1(f(x)) + O(h^2) \end{cases} \qquad (20)$$

  Therefore, by eliminating (or "killing") the most dominant term in the error series using simple algebra, $\phi_h^1(f(x))$ provides a forward approximation to $f'(x)$ with an error term of order $O(h^2)$.

- The process can be further continued, i.e. one can consider **second order Richardson extrapolations**. From equation (20), one has simultaneously:

  (20.a) $f'(x) = \phi_h^1(f(x)) + a_2' f^{(3)}(x)h^2 + a_3' f^{(4)}(x)h^3 + ...$

  (20.b) $f'(x) = \phi_{2h}^1(f(x)) + a_2' f^{(3)}(x)(2h)^2 + a_3' f^{(4)}(x)(2h)^3 + ...$

The algebraic operation $4 \times (20.a) - (20.b)$ eliminates again the dominant term in the error series and yields:

$$f'(x) = \frac{4\phi_h^1(f(x)) - \phi_{2h}^1(f(x))}{3} - \frac{4}{3}a_3' f^{(4)}(x)h^3 + O(h^4)$$

Introducing the 2^{nd} **order Richardson extrapolation operator**, let

(21) $$\phi_h^2(f(x)) = \frac{4\phi_h^1(f(x)) - \phi_{2h}^1(f(x))}{3}$$

One obtains:

(22) $$f'(x) = \begin{cases} \phi_h^2(f(x)) - \frac{4}{3}f^{(4)}(x)h^3 + ... \\ \phi_h^2(f(x)) + O(h^3) \end{cases}$$

This is yet another improvement in the precision to $O(h^3)$ i.e. $\phi_h^2(f(x))$ provides a third order approximation to $f'(x)$. The successive Richardson extrapolation formulae and error estimates are then as follows:

(23) $$f'(x) = \begin{cases} \phi_h(f(x)) + O(h) \\ \phi_h^1(f(x)) + O(h^2) \\ \phi_h^2(f(x)) + O(h^3) \\ \phi_h^3(f(x)) + O(h^4) \\ ...... \end{cases}$$

where:
$\phi_h(.) = \frac{\Delta_h(.)}{h}$; $\phi_h^1 = \frac{2^1\phi_h(.) - \phi_{2h}(.)}{2^1-1}$; $\phi_h^2(.) = \frac{2^2\phi_h^1(.) - \phi_{2h}^1(.)}{2^2-1}$ and $\phi_h^3(.) = \frac{2^3\phi_h^2(.) - \phi_{2h}^2(.)}{2^3-1}$
The k^{th}**-order Forward Richardson operator** is then:

$$\phi_h^k(.) = \frac{2^k\phi_h^{k-1}(.) - \phi_{2h}^{k-1}(.)}{2^k - 1}$$

with the error term of order $O(h^{k+1})$.
The same procedure can be repeated over and over again to kill higher and higher terms in the error series. This is Richardson extrapolation!

Remark 3 *In the process above, let* $\phi_h^k(.) = F(\phi_h^{k-1}(.), \phi_{2h}^{k-1}(.))$ *be the function approximating the derivative* $f'(.)$ *in terms of 2 valid previous evaluations, with an error* $E = O(h^{k+1})$*. Richardson extrapolation method allows to obtain an improved approximation formula* $\phi_h^k(.)$ *without decreasing the value of* h *(that would favour increasing round-off errors). Thus through that process, the new approximation is "extrapolated" to the exact value of the derivative.*

Example 5 *On the basis of Table 2, find improvements of the results using Richardson's extrapolation of the 1st and second order to* $f^{'}(x)$*.*

We apply (19) and , (21) yielding the following results:

h	$\phi_h = \frac{1}{h}\Delta_h(f(0))$	$\phi_h^1(f(0))$	$\phi_h^2(f(0))$
1.00	-0.23480231	.	.
0.50	-0.12306039	-0.01131847	.
0.25	-0.06225628	-0.00145217	0.001836597

Table 5. Approximations for $J_0'(0)$.

Note that we can also derive Richardson extrapolation formulae based on the Backward difference approximation to $f'(x)$ (9.2), i.e. starting with

$$f'(x) = \frac{\nabla_h(f(x))}{h} + b_1 f^{(2)}(x)h + b_2 f^{(3)}(x)h^2 + ...$$

where the $\{b_i\}$ are constants independent of h, we let then:

$$\chi_h(.) = \frac{\nabla_h(.)}{h} \tag{24}$$

It is easy to verify that the successive **Backward Difference Richardson operators** thus obtained, have the same constant coefficients as those of the corresponding Forward Difference formulae. More explicitly:

$$f'(x) = \begin{cases} \chi_h(f(x)) + O(h) \\ \chi_h^1(f(x)) + O(h^2) \\ \chi_h^2(f(x)) + O(h^3) \\ ...... \end{cases} \tag{25}$$

where: $\chi_h(.) = \frac{\nabla_h(.)}{h}$ and $\chi_h^k(.) = \frac{2^k\chi_h^{k-1}(.) - \chi_{2h}^{k-1}(.)}{2^k - 1}$ where the error term is $O(h^{k+1})$.

3.3.b Central Difference Richardson Extrapolations

In the preceding section, we verified that the Central Difference approximation to $f'(x)$ satisfies the following equation:

$$f'(x) = \frac{\delta_h(f(x))}{2h} + d_1 f^{(3)}(x)h^2 + d_2 f^{(5)}(x)h^4 + ... = \frac{\delta_h(f(x))}{2h} + O(h^2).$$

With such information, it is possible to rely again on the powerful technique of Richardson extrapolation to wring more accuracy out of the method in the approximation-formulae of $f'(x)$. Specifically, let

$$\psi_h(.) = \frac{\delta_h(.)}{2h}$$

Obviously, then:

(26) $$f'(x) = \psi_h(f(x)) + d_1 f^{(3)}(x)h^2 + d_2 f^{(5)}(x)h^4 + ... = \psi_h(f(x)) + O(h^2)$$

Taking successively h then $2h$ in the equation above, one has:

(26.a) $f'(x) = \psi_h(f(x)) + d_1 f^{(3)}(x)h^2 + d_2 f^{(5)}(x)h^4 + ...$

(26.b) $f'(x) = \psi_{2h}(f(x)) + d_1 f^{(3)}(x)(2h)^2 + d_2 f^{(5)}(x)(2h)^4 + ...$

The algebraic operation $4 \times (26.a) - (26.b)$ yields:

$$f'(x) = \frac{4\psi_h(f(x)) - \psi_{2h}(f(x))}{3} + O(h^4)$$

Let the 1^{st} **order Richardson extrapolation** operator be defined by

$$\psi_h^1(.) = \frac{2^2\psi_h(.) - \psi_{2h}(.)}{2^2 - 1}$$

One can write then:

(27) $$f'(x) = \psi_h^1(f(x)) + O(h^4)$$

Leading therefore to the following identities:

(27.a) $f'(x) = \psi_h^1(f(x)) + d_2' f^{(5)}(x)h^4 + d_3' f^{(7)}(x)h^6 + ...$

(27.b) $f'(x) = \psi_{2h}^1(f(x)) + d_2' f^{(5)}(x)(2h)^4 + d_3' f^{(7)}(x)(2h)^6 + ...$

The algebraic operation $16 \times (27.a) - (27.b)$ yields:

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

or equivalently:

$$f'(x) = \psi_h^2(f(x)) + O(h^6)$$

Again, the process can be repeated to obtain higher order accuracy in the approximations of $f'(x)$.

Therefore, the 1st **Central Difference Richardson extrapolation formulae** obtained are as follows:

$$f'(x) = \begin{cases} \psi_h(f(x)) + O(h^2) \\ \psi_h^1(f(x)) + O(h^4) \\ \psi_h^2(f(x)) + O(h^6) \\ \ldots\ldots \end{cases} \tag{28}$$

where $\psi_h(.) = \frac{\delta_h(.)}{2h}$, $\psi_h^1(.) = \frac{2^2\psi_h(.)-\psi_{2h}(.)}{2^2-1}$, $\psi_h^2(.) = \frac{2^4\psi_h^1(.)-\psi_{2h}^1(.)}{2^4-1}$....
The k^{th}-order operator is then defined as follows:

$$\psi_h^k(.) = \frac{2^{2k}\psi_h^{k-1}(.) - \psi_{2h}^{k-1}(.)}{2^{2k}-1}$$

where the error term is $O(h^{2k+2})$

3.4 2^{nd} Order Derivatives and Divided Differences.Error Analysis

A direct application of Theorem 1 with $k = 2$ suggests the following approximation formulae for the 2^{nd} derivative of f:

$$f''(x_i) \approx \begin{cases} 2[x_i, x_{i+1}, x_{i+2}] = \frac{y_{i+2}-2y_{i+1}+y_i}{h^2} = \frac{\Delta_h^2 y_i}{h^2}; & \text{Forward Difference} \\ 2[x_{i-2}, x_{i-1}, x_i] = \frac{y_i-2y_{i-1}+y_{i-2}}{h^2} = \frac{\nabla_h^2 y_i}{h^2}; & \text{Backward Difference} \\ 2[x_{i-1}, x_i, x_{i+1}] = \frac{y_{i+1}-2y_i+y_{i-1}}{h^2} = \frac{\delta_h^2 y_i}{h^2}; & \text{Central Difference} \end{cases}$$

We start by estimating the order of convergence of each approximation formula:

- Forward Difference approximation
  Consider the 2 Taylor's series expansions of f up to $2nd$ order given by:

  (i) $f(x+h) = f(x) + \frac{h}{1!}f'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f^{(3)}(c_1)$; $c_1 \in (x, x+h)$

  (ii) $f(x+2h) = f(x) + \frac{(2h)}{1!}f'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f^{(3)}(c_2)$; $c_2 \in (x, x+2h)$

  where f is assumed to be a C^3-function.
  The algebraic operation: $f(x+2h) - 2f(x+h)$ leads to the **Forward Difference Approximation** to $f''(x)$ verifying the following:

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h) = \frac{\Delta_h^2 f(x)}{h^2} + O(h) \tag{29}$$

- Backward Difference approximation
  Furthermore, replacing h by $-h$ in equations (i) and (ii) above, one also has:

  (iii) $f(x-h) = f(x) - \frac{h}{1!}f'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f^{(3)}(c_3)$; $c_3 \in (x-h, x)$

(iv) $f(x-2h) = f(x) - \frac{(2h)}{1!}f'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f^{(3)}(c_4)$; $c_4 \in (x-2h, x+)$

The algebraic operation: $f(x-2h) - 2f(x-h)$ leads to the **Backward Difference Approximation** to $f''(x)$ verifying the following:

$$f''(x) = \frac{f(x-2h) - 2f(x-h) + f(x)}{h^2} + O(h) = \frac{\nabla_h^2 f(x)}{h^2} + O(h) \tag{30}$$

- Central Difference approximation
  In this case we start by writing Taylor's series expansions up to the 3^{rd} order successively for $f(x+h$ and $f(x-h)$ and then sum up the two series. This leads to:

$$f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + \frac{h^4}{4!}(f^{(4)}(c_1) + f^{(4)}(c_2))$$

  Dividing by h^2 and using the Intermediate Value Theorem, one concludes that:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12}f^{(4)}(c) = \frac{\delta_h^2}{h^2}(f(x)) + O(h^2)$$

Based on the results above, the following proposition is satisfied:

Proposition 2 *Let* $0 < h \leq 1$. *Then*

$$f''(x) = \begin{cases} \frac{\Delta_h^2 f(x)}{h^2} + O(h), & (31.1) \\ \frac{\nabla_h^2 f(x)}{h^2} + O(h), & (31.2) \\ \frac{\delta_h^2 f(x)}{h^2} + O(h^2), & (31.3) \end{cases} \tag{31}$$

where f is assumed to have up to third order continuous derivatives for the first 2 approximations ($f \in C^3$), and up to fourth order continuous derivatives for the third approximation ($f \in C^4$).

In terms of finite differences, these results are expressed as follows:

$$f''(x_i) \approx \begin{cases} 2[x_i, x_{i+1}, x_{i+2}] = \frac{\Delta_h^2 y_i}{h^2} + O(h); & \text{Forward Difference} \\ 2[x_{i-2}, x_{i-1}, x_i] = \frac{\nabla_h^2 y_i}{h^2} + O(h); & \text{Backward Difference} \\ 2[x_{i-1}, x_i, x_{i+1}] = \frac{\delta_h^2 y_i}{h^2} + O(h^2); & \text{Central Difference} \end{cases}$$

Remark 4 *Based on Theorem 1, the following approximation formulae for the* 3^{rd} *derivative of* f *are obtained:*

$$f'''(x_i) \approx \begin{cases} 6[x_i, x_{i+1}, x_{i+2}, x_{i+3}] = \frac{\Delta_h^3 y_i}{h^3}; & ForwardDifference \\ 6[x_{i-3}, x_{i-2}, x_{i-1}, x_i] = \frac{\nabla_h^3 y_i}{h^3}; & BackwardDifference \\ 6[x_{i-2}, x_{i-1}, x_{i+1}, x_{i+2}] = \frac{\delta_h^3 y_i}{h^3}; & CentralDifference \end{cases}$$

3.5 2^{nd} order derivatives and Richardson Extrapolation

In order to improve the order of the approximations of the 2^{nd} derivative, we can use as precedingly the powerful tool of Richardson extrapolation applied successively to the Forward, Backward and Central Difference formulae.
In this section, we analyze only the **Richardson extrapolation Central Difference approximation** to $f''(x)$. In the equations above:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = \frac{\delta_h^2 f(x)}{h^2} \tag{32}$$

Define then:

$$\psi_h(.) = \frac{\delta_h^2(.)}{h^2}$$

Adding the infinite series for $f(x+h)$ and $f(x-h)$, one can write successively:

$$f''(x) = \psi_h(f(x)) + d_1 f^{(4)}(x)h^2 + d_2 f^{(6)}(x)h^4 + ... \tag{33}$$

$$f''(x) = \psi_{2h}(f(x)) + d_1 f^{(4)}(x)(2h)^2 + d_2 f^{(6)}(x)(2h)^4 + ... \tag{34}$$

In order to eliminate the most dominant term of the error in the above 2 series, the algebraic operation $4 \times (33) - (34)$ yields:

$$f''(x) = \frac{4\psi_h(f(x)) - \psi_{2h}(f(x))}{3} + O(h^4) \tag{35}$$

Defining the 1^{st} **order Richardson extrapolation operator** by

$$\psi_h^1(.) = \frac{2^2\psi_h(.) - \psi_{2h}(.)}{2^2 - 1},$$

one rewrites (35) as:

$$f''(x) = \psi_h^1(f(x)) + O(h^4)$$

which improves the order of approximation.

Obviously, one can derive the following estimates:

$$f''(x) = \begin{cases} \psi_h(f(x)) + O(h^2) \\ \psi_h^1(f(x)) + O(h^4) \\ \psi_h^2(f(x)) + O(h^6) \\ ...... \end{cases} \tag{36}$$

where $\psi_h(.) = \frac{\delta_h^2(.)}{2h}$, $\psi_h^1(.) = \frac{2^2\psi_h(.) - \psi_{2h}(.)}{2^2-1}$, $\psi_h^2(.) = \frac{2^4\psi_h^1(.) - \psi_{2h}^1(.)}{2^4-1}$.

4 Numerical Integration

We consider now the approximation of $I(a,b) \equiv \int_a^b f(x)dx$, based on the data D_n. As in the numerical differentiation process, we assume the x-data to be equidistant, with:

$$h = x_{i+1} - x_i, \forall i.$$

Depending on the parity of n (i.e on the number of subintervals), we start by decomposing the integral I into the sum of simple integrals over the subintervals $[x_i, x_{i+1}]$ as follows:

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + ... + \int_{x_{n-1}}^{x_n} f(x)dx = \sum_{k=0}^{n-1} \int_{x_k}^{x_{k+1}} f(x)dx, \forall n$$

and in particular:

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... + \int_{x_{2m-2}}^{x_{2m}} f(x)dx = \sum_{k=0}^{m-1} \int_{x_{2k}}^{x_{2k+2}} f(x)dx, \underline{\forall n = 2m}$$

Thus, we will be dealing with 2 types of formulae:

1. **Simple Numerical integration** formulae

$$I_k = \int_{x_k}^{x_{k+1}} f(x)dx \;\; \forall \; n \;\; \text{, or } \; I'_k = \int_{x_{2k}}^{x_{2k+2}} f(x)dx \;\; , \forall \; n = 2m$$

   Subsequently,

2. **Composite Numerical integration** formulae

$$I = \int_a^b f(x)dx = \sum_{k=0}^{n-1} I_k \;\; \forall \; n \; \text{, or } I = \int_a^b f(x)dx = \sum_{k=0}^{m-1} I'_k \;\; , \forall \; n = 2m$$

We start with the simplest approximation method, called the **Midpoint Rectangular Rule**.

4.1 The Midpoint Rectangular Rule

Such rule applies only in the case when the number of subintervals is even, that is when $\underline{n = 2m}$.

1. **The formulae**
   A simple geometric argument consists in considering the integral I'_k as being the area of the region between the x- axis, the curve $y = f(x)$ and the vertical lines $x = x_{2k}$ and $x = x_{2k+2}$. Such area is then approximated by the surface of the rectangle which vertical sides are $x = x_{2k}$ and $x = x_{2k+2}$, and horizontal sides $y = 0$ and $y = f(x_{2k+1})$. In such case, the function values at the midpoints are known. For example, in the case of the data in Table 1,

i	x_i	$f(x_i)$
0	0.00	1.0000000
1	0.25	0.98443593
2	0.50	0.93846981
3	0.75	0.86424228
4	1.00	0.76519769
5	1.25	0.64590609
6	1.50	0.51182767
7	1.75	0.36903253
8	2.00	0.22389078

the set of midpoints is $\{x_1, x_3, x_5, x_7\}$.This leads first to the **simple Midpoint (rectangular) rule**, given by:

(37) $$I'_k = \int_{x_{2k}}^{x_{2k+2}} f(x)dx \approx M_k = 2hf(x_{2k+1}), k = 0, 1, ..., m-1.$$

and subsequently to the **composite Midpoint rule** given by:

(38) $$I \equiv I(a, b) = \int_a^b f(x)dx \approx M(h) = \Sigma_{k=0}^{m-1} 2hf(x_{2k+1})$$

2. **Error analysis**
   The error analysis of this method is based on either one of Taylor's formulae where the expansion is made about the point $x = x_{2k+1}$, yielding:

(39) $$f(x) = f(x_{2k+1}) + f'(x_{2k+1})(x - x_{2k+1}) + f''(c_k(x))\frac{(x - x_{2k+1})^2}{2}$$

where $c_k(x) = x_{2k+1} + t(x - x_{2k+1})$, $0 < t < 1$.
Obviously, it is required that the function f is at least in $C^2[a, b]$.

Integration of equation (39) from x_{2k} to x_{2k+2} and the use of the second Mean-value theorem leads to:

(40) $$\int_{x_{2k}}^{x_{2k+2}} f(x)dx = 2hf(x_{2k+1}) + f''(c_k)\int_{x_{2k}}^{x_{2k+2}} \frac{(x - x_{2k+1})^2}{2}dx$$

where c_k is a point in (x_{2k}, x_{2k+2}). One easily verifies that the integrals of odd powers of $(x - x_{2k+1})$ in (39) cancel out, with only the integrals of even powers contributing to the final result, thus yielding:

(41) $$I'_k = M_k + f''(c_k)\frac{h^3}{3}$$

Summing up (41) over k yields:

$$I(a,b) = \sum_{k=0}^{m-1} I'_k = \sum_{k=0}^{m-1} M_k + \frac{h^3}{3}\sum_{k=0}^{m-1} f''(c_k) = M(h) + \frac{h^3}{3}\sum_{k=0}^{m-1} f''(c_k).$$

Using the intermediate value theorem, one has:

$$\sum_{k=0}^{m-1} f''(c_k) = mf''(d) = \frac{b-a}{2h} f\text{"}(d),\ d \in (a,b)$$

and therefore, noting that the length of the interval of integration is

$$nh = (2m)h = b - a$$

the following result is reached:

$$I = I(a,b) = M(h) + \frac{(b-a)}{6} f''(d)h^2 \tag{42}$$

Proposition 3 *Let f be a function in $C^2[a,b]$, interpolating the set of data D_n where $n = 2m$. Then*

$$I = \int_a^b f(x)dx = M(h) + O(h^2)$$

where

$$M(h) = 2h\sum_{k=0}^{m-1} f(x_{2k+1})$$

Furthermore, when $h = \frac{b-a}{2^l}$, $l = 0, 1, 2, ...$, it can be proved that:

$$I = I(a,b) = M(h) + \mu_1 h^2 + \mu_2 h^4 + .. + \mu_j h^{2j} + ..., \tag{43}$$

where the sequence $\{\mu_j\}$ is <u>independent from h</u>, and depends on the function f (and its derivatives) at a and b.

4.2 The Trapezoidal Rule

Unlike the composite Midpoint rule that is only applicable when the number of intervals is even, the composite **Trapezoid rule** can be used in all cases.

1. **The formulae**
   A simple geometric argument consists in approximating the surface between the x-axis, the curve $y = f(x)$ and the vertical lines $x = x_k$ and $x = x_{k+1}$ by the area of the rectangular trapezoid, which vertices are $(x_k, 0)$, $(x_{k+1}, 0)$, $(x_k, f(x_k))$ and $(x_{k+1}, f(x_{k+1}))$. This leads first to the **simple Trapezoidal rule**, given by:

$$I_k = \int_{x_k}^{x_{k+1}} f(x)dx \approx T_k = \frac{h}{2}(f(x_k) + f(x_{k+1})), \tag{44}$$

and subsequently to the **composite Trapezoid rule** given by:

$$I \equiv I(a,b) = \int_a^b f(x)dx \approx T(h) = \frac{h}{2}\,\Sigma_{k=0}^{n-1}(f(x_k) + f(x_{k+1})), \tag{45}$$

More precisely: $T(h) = \frac{h}{2}\,(y_0 + 2(y_1 + ... + y_{n-1}) + y_n)$

Remark 5 *Note that when $n = 2m$, then:*

$$I \approx T(2h) = \Sigma_{k=0}^{m-1} T'_k = \Sigma_{k=0}^{m-1} h(f(x_{2k} + f(x_{2k+2}))$$

On the other hand:

$$M(h) = \Sigma_{k=0}^{m-1} M_k = 2h\Sigma_{k=0}^{m-1} f(x_{2k+1})$$

Considering then $(T(2h) + M(h))/2$, one gets:

$$T(h) = \frac{1}{2}(T(2h) + M(h)) \tag{46}$$

To prove this result note that:

$$T(2h) + M(h) = h\sum_{k=0}^{m-1}(f(x_{2k}) + f(x_{2k+2})) + 2f(x_{2k+1}) =$$

$$= h\sum_{k=0}^{m-1}[f(x_{2k}) + f(x_{2k+1})] + [f(x_{2k+1}) + f(x_{2k+2})]$$

$$= h\sum_{k=0}^{n-1}(f(x_k) + f(x_{k+1})) = 2T(h).$$

This result is summarized in:

Proposition 4 *For $n = 2m$, $T(h) = \frac{1}{2}(T(2h) + M(h))$.*

2. **Error analysis**
   Note that:

$$T_k = \int_{x_k}^{x_{k+1}} p_{k,k+1}(x)dx \tag{47}$$

where $p_{k,k+1}(x) = y_k + [x_k, x_{k+1}](x - x_k)$, is the linear interpolation polynomial to $f(x)$ at x_k and x_{k+1}. Furthermore, it is well known (section 4.5) that:

$$f(x) = p_{k,k+1}(x) + \frac{1}{2}(x - x_k)(x - x_{k+1})f''(c(x)),$$

with $c(x) \in (x_k, x_{k+1})$ depending continuously on x. By integration of this identity over the interval (x_k, x_{k+1}) and use of the second Mean Value Theorem with (47), one gets:

$$I_k = T_k + \frac{f''(c_k)}{2} \int_{x_k}^{x_{k+1}} (x - x_k)(x - x_{k+1})\, dx$$

leading to:

$$I_k = T_k - \frac{h^3}{12} f''(c_k), \tag{48}$$

where $c_k \in (x_k, x_{k+1})$. Summing up (48) over k, one gets an expression for the composite Trapezoidal rule error term (likewise for the Midpoint rule in (42)):

$$I = I(a,b) = \sum_{k=0}^{n-1} I_k = T(h) - \frac{(b-a)}{12} f''(c) h^2 \tag{49}$$

where $c \in (a, b)$.

Proposition 5 *Let the data* $D_n = \{(x_k, f(x_k)) | k = 0, 1, ..., n\}$, *be a set representing a function* f *in* $C^2([a, b])$, *then:*

$$I = \int_a^b f(x)dx = T(h) + O(h^2),$$

with:

$$T(h) = \frac{h}{2} \Sigma_{k=0}^{n-1} (f(x_k) + f(x_{k+1})).$$

On the other hand, as in (43), can prove that when $h = \frac{b-a}{2^l}$, $l = 0, 1, 2, ...$:

$$I = I(a,b) = T(h) + \tau_1 h^2 + \tau_2 h^4 + .. + \tau_j h^{2j} + ..., \tag{50}$$

where the sequence $\{\tau_j\}$ depends on the function f (and its derivatives) at a and b and consequently **independent from** h.

4.3 Trapezoid Rule / Richardson's extrapolation: Romberg formulae

1. **The formulae**
   On the basis of (50), we can implement Richardson's extrapolation, by writing this equation simultaneously for h and $\frac{h}{2}$. Specifically, in that case we obtain:

   (a) $I = T(h) + \tau_1 h^2 + \tau_2 h^4 + ... + \tau_j h^{2j} + ...$

   (b) $I = T\left(\frac{h}{2}\right) + \tau_1 \left(\frac{h}{2}\right)^2 + \tau_2 \left(\frac{h}{2}\right)^4 + ... + \tau_j \left(\frac{h}{2}\right)^{2j} + ...$

In order to eliminate the dominant term of the error, by performing the algebraic operation $4(b) - (a)$, we obtain:

$$3I = 4T\left(\frac{h}{2}\right) - T(h) + O(h^4)$$

and therefore:

(51) $$I = \frac{4T\left(\frac{h}{2}\right) - T(h)}{3} + t_2h^4 + t_3h^6 + ...$$

where the sequence $\{t_i\}$ is independent of h.
Defining the first Romberg integration operator as:

(52) $$R^1(h/2) = \frac{4T\left(\frac{h}{2}\right) - T(h)}{3} \text{ or equivalently } R^1(h) = \frac{4T(h) - T(2h)}{3}$$

equation (51) provides then an approximation to the integral $I(a, b)$ of order $O(h^4)$ verifying:

(53) $$I = R^1(h) + O(h^4)$$

In a similar way, we can derive a second Romberg integration formula by writing again the equation above simultaneously in terms of h and $\frac{h}{2}$:

(a) $I = R^1(h) + t_2h^4 + t_3h^6 + ...$

(b) $I = R^1\left(\frac{h}{2}\right) + t_2\left(\frac{h}{2}\right)^4 + t_3\left(\frac{h}{2}\right)^6 + ...$

Performing the algebraic operation $16(b) - (a)$ yields:

$$15I = 16R^1\left(\frac{h}{2}\right) - R^1(h) + O(h^6)$$

And therefore:

(54) $$I = \frac{16R^1\left(\frac{h}{2}\right) - R^1(h)}{15} + t_3h^6 + t_4h^8 + ...$$

where the sequence $\{t_i\}$ is independent of h.
Defining the second Romberg integration operator as:

(55) $$R^2(h) = \frac{16R^1(h) - R^1(2h)}{15}$$

equation (5.52) is then equivalent to:

(56) $$I = R^2(h) + O(h^6)$$

As for differentiation, this process can be repeated.

The first Romberg extrapolation formulae obtained based on the Composite Trapezoid Rule are as follows:

Proposition 6 *Let f belong to $C^\infty[a,b]$*

$$I = I(a,b) = \int_a^b f(x)dx = \begin{cases} R^1(h) + O(h^4) \\ R^2(h) + O(h^6) \\ R^3(h) + O(h^8) \\ \dots \end{cases}$$

Where $R^1(h) = \frac{2^2T(h)-T(2h)}{2^2-1}$; $R^2(h) = \frac{2^4R^1(h)-R^1(2h)}{2^4-1}$; $R^3(h) = \frac{2^6R^2(h)-R^2(2h)}{2^6-1}$, *and in general:* $R^k(h) = \frac{2^{2k}R^{k-1}(h)-R^{k-1}(2h)}{2^{2k}-1}$,

2. **Simpson's Rule**
Simpson's Rule is applicable only if the number of subintervals is even (n=2m). It can be derived from a linear combination of the Midpoint Rule and the Trapezoid Rule. Specifically, the **simple integration Simpson's Rule** is defined as follows

(57) $$S_k = \frac{2}{3}M_k + \frac{1}{3}T_k$$

Consequently:

$$S_k = \frac{2}{3}[f(x_{2k+1})2h] + \frac{1}{3}[\frac{f(x_{2k}) + f(x_{2k+1})}{2}2h]$$

leading to:

(58) $$I'_k = \int_{x_{2k}}^{x_{2k+2}} f(x)dx \approx S_k = \frac{h}{3}(f(x_{2k}) + 4f(x_{2k+1}) + f(x_{2k+2}))$$

Summing up this last equation over k, one derives the **Composite Simpson's Rule**, namely:

(59) $$I = I(a,b) = \Sigma_{k=0}^{m-1} S_k = \Sigma_{k=0}^{m-1}(\frac{2}{3}M_k + \frac{1}{3}T_k) = \frac{2M(h) + T(2h)}{3}$$

Referring to Proposition (4), since $M(h) = 2T(h) - T(2h)$, then one concludes that:

$$S(h) = \frac{4T(h) - T(2h)}{3} = R^1(h)$$

meaning that Simpson's Composite Numerical Integration formula is equivalent to the first Romberg Trapezoidal Extrapolation formula.
Thus, the following error estimate is obviously deduced:

Proposition 7 *Let f be a function in $C^4[a,b]$, interpolating the set of data D_n. Then:*

$$I = I(a,b) = S(h) + O(h^4)$$

Remark 6 *The error estimate of the Composite Simpson's rule can also be derived by noting that*

$$S_k = \int_{x_{2k}}^{x_{2k+2}} p_{2k,2k+1,2k+2}(x)dx$$

where $p_{2k,2k+1,2k+2}(x)$ is the quadratic interpolating polynomial to $f(x)$ at $x_{2k}, x_{2k+1}, x_{2k+2}$. Specifically one proves that:

$$I_k = S_k - \frac{1}{90} f^{(4)}(c_k(x))h^5.$$

leading therefore to:

$$I = S(h) - (b-a)\frac{1}{180} f^{(4)}(c)h^4.$$

where $S(h) = (y_0 + 4\sum_{k=0}^{m-1} y_{2k+1} + 2(\sum_{k=1}^{m-1} y_{2k}) + y_{2m})\frac{h}{3}$

In a consistent manner with the Composite Midpoint and Trapezoidal Rules, one also has when $h = \frac{b-a}{2^l}, l = 0, 1, 2, ...$:

$$I = I(a,b) = S(h) + s_2 h^4 + s_6 h^6 + ... + s_j h^{2j} + ...$$

where all the coefficients $\{s_i\}$ are independent of h.

In the last part of this chapter, we explore a totally different approach of estimating definite integrals. We will show that we can use sequences of random numbers for these approximations, a problem that seemingly has nothing to do with randomness.

5 Monte Carlo Methods and Random Numbers

PROBLEMS

Numerical Differentiation

1. If $\phi(h) = L - c_1 h - c_2 h^2 - c_3 h^3 - ...$, then what combination of $\phi(h)$ and $\phi(h/2)$ should give an accurate estimate of L ?

2. If $\phi(h) = L - c_1 h^{1/2} - c_2 h^{2/2} - c_3 h^{3/2} - ...$, then what combination of $\phi(h)$ and $\phi(h/2)$ should give an accurate estimate of L ?

3. Consider the following table of data associated with some unknown function $y = f(x)$

i	$\mathbf{x_i}$	$\mathbf{y_i}$
0	0.00	1.000
1	0.25	2.122
2	0.50	3.233
3	0.75	4.455
4	1.00	5.566
5	1.25	-1.000
6	1.50	-1.255
7	1.75	-1.800
8	2.00	-2.000

   (a) Find an approximation to $f'(0.25)$ using successively the forward, backward and central difference approximations if $h = 0.25$.

   (b) Find approximations to $f'(1)$ using the central difference approximation with $h = 0.25$, $h = 0.50$ then $h = 1.00$. Improve the results obtained using central difference Richardson's extrapolation of the first and second order to approximate $f'(1)$, if $h = 0.25$.

   (c) Approximate $f'(0)$ and $f'(2)$ with $h = 0.25$.

   (d) Find approximations to $f''(1)$ using the forward, backward and central difference approximations, with $h = 0.25$. Improve the results obtained using forward difference Richardson's extrapolation of the first and second order to approximate $f''(1)$, if $h = 0.25$.

   (e) Find approximations to $f'''(1.25)$ using the forward, backward and central difference approximations, with $h = 0.25$.

4. Consider the following table of data for the function $f(x)$

i	$\mathbf{x_i}$	$\mathbf{y_i}$
0	0.000	1.0000000
1	0.125	1.1108220
2	0.250	1.1979232
3	0.375	1.2663800
4	0.500	1.3196170
5	0.625	1.3600599
6	0.750	1.3895079
7	0.875	1.4093565
8	1.000	1.4207355

(a) Use the Central Difference formula to approximate $f'(0.5)$, followed by Richardson's extrapolation of the $1st$ and $2nd$ orders to improve the results. Fill out the following table:

h	$\psi_h(.)$	$\psi_h^{(1)}(.)$	$\psi_h^{(2)}(.)$
0.5	$\times$		
0.25	$\times$	$\times$	
0.125	$\times$	$\times$	$\times$

(b) Calculate the $2nd$ derivative $f''(0.5)$, using the Central Difference approximation. Use Richardson's extrapolation of the $1st$ and $2nd$ orders to improve this result.

(c) Calculate the $3rd$ derivative $f'''(1.000)$, using the Backward Difference approximation.

5. Based on the set of data of the preceding exercise, use the Forward Difference formula to approximate $f'(0)$, followed by Richardson's extrapolation of the $1st$ and $2nd$ orders. Fill out the following table:

h	$\phi_h(.)$	$\phi_h^{(1)}(.)$	$\phi_h^{(2)}(.)$
0.5	$\times$		
0.25	$\times$	$\times$	
0.125	$\times$	$\times$	$\times$

Numerical Integration

6. Approximate $I = \int_a^b f(x)\,dx$ based on the set of data given in Exercise 3, using the Midpoint Rectangular Rule.

7. • Estimate the value of $I = \int_0^1 (x^2+1)^{-1} dx$ by using the composite Midpoint Rule if the partition points are $0, 1/4, 1/2, 3/4, 1$.

- Find the relative error in this approximation.
- Obtain an upper bound on the Absolute Error of I, if 5 partition points are used.

8. The Bessel function of order 0 is defined by the equation $J_0(x) = \frac{1}{\pi}\int_0^{\pi} cos(xsin\theta)d\theta$ Approximate $J_0(1)$ by the Midpoint Rectangular Rule using 5 equally spaced partition points, then find an upper bound to the error in this approximation. Give your answer in terms of A and B, where $B = cos\sqrt{2}/2$.

9. In the Composite Midpoint Rule the nodes should be equally spaced. Establish "Composite Rectangular Rules" in case the spacing is not unique based on Upper or Lower Sums to approximate the definite integral.

10. How many equi-spaced partition points should be used, with an error $|\epsilon| \leq \frac{10^{-4}}{2}$ in the approximation of $I = \int_0^1 e^{-x^2}dx$ using
    - The Composite Midpoint Rectangular Rule
    - The Composite Trapezoid Rule

11. Compute an approximate value of $\int_0^1 (x^2+1)^{-1}dx$ by using the composite Trapezoid rule with 3 points. Next determine the error formula and numerically verify an upper bound on it.

12. Obtain an upper bound on the absolute error using 101 equally spaced points, when we compute $\int_0^6 sinx^2 dx$ by means of
    - the composite Trapezoid rule .
    - the composite Midpoint Rectangular rule.

13. How large must n be if the composite trapezoid rule is to estimate $\int_0^{\pi} sinxdx$ with error $\leq 10^{-12}$? Will the estimate be too big or too small ?

14. Prove that if a function is concave downwards, the Trapezoidal Rule underestimates the integral.

15. Approximate $\int_0^2 2^x dx$ using the composite trapezoid rule with $h = 1/2$.

16. Let $f(x) = 2^x$. Approximate $\int_0^4 f(x)dx$ by the trapezoid rule using the partition points $0, 2, 4$. Repeat by using partition points $0, 1, 2, 3, 4$. Now apply Romberg extrapolation to obtain a better approximation.

17. Consider the data given in Exercise 3. Fill in the following Tableau, using $h_0 = 2$.

h	$T(h)$	$R^1(h)$	$R^2(h)$	$R^3(h)$
h_0	$\times$			
$h_0/2 = 1$	$\times$	$\times$		
$\frac{h_0}{4} = 0.5$	$\times$	$\times$	$\times$	
$\frac{h_0}{8} = 0.25$	$\times$	$\times$	$\times$	$\times$

18. Compute $\int_0^1 (1 + x^2)^{-1} dx$ by Simpson's Rule using 3 then 5 partition points. Compare with the true solution.

19. Find an approximate value of $\int_1^2 x^{-1} dx$ using composite Simpson's Rule with $h = 0.25$. Give a bound on the error.

20. The Bessel function of order 0 is defined by the equation $J_0(x) = \frac{1}{\pi} \int_0^{\pi} cos(xsin\theta d\theta)dx$

    - Approximate $J_0(1)$ by the Trapezoid Rule using 3 equally spaced partition points, then find an upper bound to the error in this approximation. Give your answer in terms of A and B, where $A = cos 1$ and $B = cos\sqrt{2}/2$.
    - Apply Romberg extrapolation of 1st order to obtain a better approximation to $J_0(1)$.

21. In the Composite Trapezoid Rule approximating $\int_a^b f(x)dx$, the spacing need not be uniform. If $h_i = x_{i+1} - x_i$ and $a = x_0 < x_1 < ... < x_n = b$, establish the Composite Trapezoid Rule Formula, then find an Upper Bound for the error term in this approximation.
    Hint: On the interval $[x_k, x_{k+1}]$, $f(x) = \frac{d}{dx}(T_k) + \frac{1}{2}(x - x_k)(x - x_{k+1})f"(c(x))$ where $c(x) \in I$.

22. Given some sequence of n random numbers, use the Monte Carlo method to estimate $F_n = \int_0^1 4\sqrt{1 - x^2}\, dx$ as a function of n. How many trials are needed to determine F_n up to 2 decimal places ?

23. Let $f(x) = \sqrt{x}$. Use the Monte Carlo method to compute an approximation of $I = \int_0^4 f(x)\, dx$ using 10 random numbers. Find the relative error in this approximation.

24. Let $f(x) = \sqrt{x + \sqrt{x}}$. Use the Monte Carlo method to compute an approximation of $I = \int_0^4 f(x)\, dx$ using 10 random numbers.

25. Let $V = \int_0^{5/4} \int_0^{5/4} (\sqrt{4 - x^2 - y^2}) \, dy dx$.
Use the Monte Carlo simulation with successively $n = 10^2, 10^3, 10^4$, to approximate V.
Find the relatie error in each case if the exact value of V is 2.66905414.

6 Appendix: Error expression for the Mid-point rule when $h = \frac{b-a}{2^l}$

For the purpose of applying Richardson's extrapolation (41) can be used in its infinte series expansion form.. Let $h_0 = (b-a)$. Then one has for $m = (a+b)/2$, $M(h_0) = h_0 f(m)$,

$$I = M(h_0) + f^{(2)}(m)\frac{h_0^3}{24} + ... + f^{(2j)}(m)\frac{h_0^{2j+1}}{4^j(2j+1)!} + ...$$

which is equivalent to:

(60) $$I = M(h_0) + h_0 \Sigma_{j\geq 1}\gamma_j f^{(2j)}(m) h_0^{2j},$$

Similarly to (22), there exists a sequence of universal constants $\{a_i : i = 1, 2, ...\}$, such that:

(61) $$f^{(2j)}(m) = \frac{f^{(2j-1)}(b) - f^{(2j-1)}(a)}{2h_0} + \sum_{i=1}^{\infty} a_i f^{(2j+2i)}(m) h_0^{2i}.$$

Combining (60) with (61), one deduces:

(62) $$I = M(h_0) + \Sigma_{j=1}^{\infty}\mu_j h_0^{2j},$$

where:

$$\mu_j = (\sum_i^j \gamma_i^{j-i})[f^{(2j-1)}(b) - f^{(2j-1)}(a)],$$

and the sequence γ_i^l defined by the recurence relations:

(63) $$\begin{cases} \gamma_j^0 = \gamma_j, & (63.1) \\ \gamma_j^l = \sum_{i=1}^{j-1} \gamma_i^{l-1} a_{j-1},\ l \geq 1. & (63.2) \end{cases}$$

Let

$$\nu_j = \sum_i^j \gamma_i^{j-i}.$$

Then (62) is equivalent to:

(64) $$I = M(h_0) + \Sigma_{j=1}^{\infty}\nu_j (f^{(2j-1)}(b) - f^{(2j-1)}(a)) h_0^{2j}.$$

For $h = \frac{h_0}{2}$, let $I_1 = \int_a^m f(x)dx$ and $I_2 = \int_m^b f(x)dx$ with $M_1(h_0/2)$ and $M_2(h_0/2)$, respectively their approximations using the Mid-point rule. Obviously, from (64), we have successively:

$$I_1 = M_1(h_0/2) + \Sigma_{j=1}^{\infty}\nu_j (f^{(2j-1)}(m) - f^{(2j-1)}(a))(h_0/2)^{2j}$$

and

$$I_2 = M_2(h_0/2) + \Sigma_{j=1}^{\infty}\nu_j (f^{(2j-1)}(b) - f^{(2j-1)}(a))(h_0/2)^{2j}.$$

Adding up these 2 equations, lead to:

$$I = I_1 + I_2 = M_1(h_0/2) + M_2(h_0/2) + \Sigma_{j=1}^{\infty} \nu_j (f^{(2j-1)}(b) - f^{(2j-1)}(a))(h_0/2)^{2j},$$

which is equivalent to:

$$I = M(h_0/2) + \Sigma_{j=1}^{\infty} \nu_j (f^{(2j-1)}(b) - f^{(2j-1)}(a))(h_0/2)^{2j}, \tag{65}$$

i.e. (62) with h_0, replaced by $h_0/2$. This argument can be repeated proving (62) with h_0, replaced by $h_0/2^l$, $l \geq 0$. This result can be generalized to both trapezoid and Simpson's rules and is of major importance for the implementation of **Romberg Integration**.