

III

Lecture on Numerical Integration

1 Statement of the Numerical Integration Problem

In this lecture we consider the process of numerically finding the value of the definite integral:

$$I = \int_a^b f(x)dx.$$

The need for doing so arises in practical applications, because, in many instances $f(x)$ is either not known explicitly or the value of I is difficult to determine. The process is called **Numerical Integration**. We will assume that even though $f(x)$ is not explicitly known, the values of $f(x)$ at certain points in $[a, b]$ are known.

Numerical Integration Problem

Given $f(x_0), f(x_1), \dots, f(x_n)$, where $x_0 = a < x_1 < x_2 \dots < x_n = b$, compute an approximate value of $I = \int_a^b f(x)dx$

Numerical integration is very often referred to as **numerical quadrature** meaning that *it is a process of finding an area of a square whose area is equal to the area under a curve*.

We would like to obtain a quadrature formula of the following form:

$$I = \int_a^b f(x)dx \approx a_0f_0 + a_1f_1 + \dots + a_nf_n,$$

where $f_i = f(x_i)$, $i = 0, 1, \dots, n$, are given, and the coefficients a_0, a_1, \dots, a_n are to be determined.

2 Trapezoidal Rule

Since $f(x)$ is not explicitly known, the simplest thing to do will be to construct an interpolating polynomial for $f(x)$ with x_0, x_1, \dots, x_n as nodes and integrate with the interpolating

polynomial as the integral. We shall use *Lagrange's Method* to do this. The Lagrangian polynomials of different degrees will yield different rules of quadrature.

Trapezoidal Rule

$$f(x) \approx \text{Lagrange Interpolating polynomial of degree 1} \implies \text{Trapezoidal Rule}$$

In this case, there are only two interpolating points: x_0, x_1 .



The Lagrange interpolating polynomial $P_1(x)$ of degree 1 is:

$$P_1(x) = L_0(x)f_0 + L_1(x)f_1.$$

Then $I = \int_{a=x_0}^{b=x_1} f(x)dx \approx \int_{x_0}^{x_1} [L_0(x)f_0 + L_1(x)f_1]dx$

Recall that $L_0(x) = \frac{x - x_1}{x_0 - x_1}$, and $L_1(x) = \frac{x - x_0}{x_1 - x_0}$.

So, $I_T =$ trapezoidal rule approximation of I is:

$$\begin{aligned}
 I_T &= \int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 \right] dx \\
 &= \frac{f_0}{x_0 - x_1} \int_{x_0}^{x_1} (x - x_1) dx + \frac{f_1}{x_1 - x_0} \int_{x_0}^{x_1} (x - x_0) dx \\
 &= \frac{f_0}{x_0 - x_1} \left[\frac{(x - x_1)^2}{2} \right]_{x_0}^{x_1} + \frac{f_1}{x_1 - x_0} \left[\frac{(x - x_0)^2}{2} \right]_{x_0}^{x_1} = \frac{x_1 - x_0}{2} (f_0 + f_1).
 \end{aligned} \tag{2.1}$$

Let $x_1 - x_0 = h$. Then we have

Trapezoidal Rule

$$I_T = \frac{(b - a)}{2} (f_0 + f_1) = \frac{h}{2} (f(a) + f(b)).$$

2.1 Error in Trapezoidal Rule

Since the above formula only gives a crude approximation to the actual value of the integral, we need to assess the error.

To obtain an error formula for this integral approximation, recall that *the error formula for interpolation of degree n* is given by

$$E_n(x) = \frac{f^{(n+1)}(\xi(x))\Psi_n(x)}{(n+1)!},$$

where $\Psi_n(x) = (x - x_0)(x - x_1) \dots (x - x_n)$, and $a \leq \xi \leq b$ ($a \equiv x_0, b \equiv x_n$).

Since in case of the Trapezoidal rule, $n = 1$, we have

$$E_1(x) = \frac{f^{(2)}(\xi(x))\Psi_1(x)}{2!},$$

where $\Psi_1(x) = (x - x_0)(x - x_1)$.

Integrating this formula we have the following error formula for the Trapezoidal rule:

$$E_T(x) = \int_{x_0}^{x_1} \frac{f^{(2)}(\xi(x))}{2!} (x - x_0)(x - x_1) dx = \int_{x_0}^{x_1} \frac{f^{(2)}(\xi(x))}{2!} \Psi_1(x) dx. \quad (2.2)$$

We can now **simplify** the above formula by applying the **Weighted Mean Value Theorem (WMT)**.

Weighted Mean Value Theorem (WMT Theorem)

Let $g(x)$ does not change sign in (a, b) , then there exists a constant c between a and b such that

$$\int_a^b f(x)g(x)dx = f(c) \int_a^b g(x)dx.$$

To apply the WMT to (2.2), we have note that the function $\Psi_1(x) = (x - x_0)(x - x_1)$ does not change sign over $[x_0, x_1]$, because, for $x \in [x_0, x_1]$, $(x - x_0) > 0$ and $(x - x_1) < 0$. Thus, $\Psi_1(x)$ is always negative.

So, applying the above theorem to E_T , with $g(x) = \Psi(x)$ and noting that $h = x_1 - x_0$, we obtain

$$E_T = \frac{f^{(2)}(\eta)}{2!} \int_{x_0}^{x_1} (x - x_0)(x - x_1)dx = \frac{-h^3}{12} f''(\eta), \quad (2.3)$$

where $x_0 < \eta < x_1$.

Trapezoidal Rule with Error Formula

$$\int_{x_0=a}^{x_1=b} f(x)dx = \frac{(b-a)}{2}[f_0 + f_1] - \frac{(b-a)^3}{12} f''(\eta) = \frac{h}{2}[f(a) + f(b)] - \frac{h^3}{12} f''(\eta), \text{ where } a < \eta < b.$$

Exactness of Trapezoidal Rule

From the above error formula it follows that the Trapezoidal rule is exact only for straight lines. This is because, $f''(x) = 0$, when $f(x)$ is a straight line, and is *non zero*, whenever $f(x)$ is of degree 2 and higher.

2.2 Geometrical Representation of the Trapezoidal Rule

Trapezoidal rule approximates the area under the curve $y = f(x)$ from $x_0 = a$ to $x_1 = b$ by the area of the trapezoid as shown below:

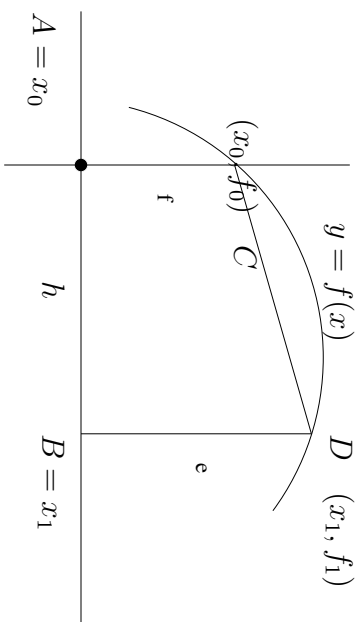


Figure 1: The Trapezoidal Rule.

Note: The area of the trapezoid $ABCD = \text{Length of the base} \times \text{average height} = h \cdot \frac{1}{2}(f_0 + f_1) = \frac{h}{2}(f_0 + f_1)$.

3 Simpson's Rule

If $f(x)$ is approximated by Lagrange interpolating polynomial of degree 2 and then integration is taken over $[a, b]$ with the interpolating polynomial as integrand, the result is *Simpson's rule*.

$$f(x) \approx \text{Lagrange Interpolating polynomial of degree 2} \implies \text{Simpson's Rule}$$

The three points of interpolation in this case are: x_0, x_1 , and x_2 .

$$\begin{array}{ccc} \times & \bullet & \times \\ x_0 = a & x_1 & x_2 = b \end{array}$$

The Lagrangian interpolating polynomial $P_2(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2$.

So,

$$I = \int_{a=x_0}^{b=x_2} f(x)dx \approx \int_{x_0}^{x_2} [L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2]dx$$

$$\text{Now, } L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)},$$

$$\text{and } L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}.$$

Let h be the distance between two consecutive points of interpolation, assumed to be equally spaced. That is, $x_1 - x_0 = h$ and $x_2 - x_1 = h$.

Substituting these expressions for $L_0(x), L_1(x)$ and $L_2(x)$ and taking integration, we obtain

Simpson's Rule:

$$I_S = \frac{h}{3}(f_0 + 4f_1 + f_2) = \frac{h}{3}(f(a) + 4f_1 + f(b))$$

Simpson's Rule

$$I_S = \frac{h}{3}(f(a) + 4f_1 + f(b))$$

3.1 Error Formula for Simpson's Rule

We have used $n = 2$ to derive Simpson's rule. So, the error formula for Simpson's Rule is given by

$$E_S = \frac{1}{3!} \int_a^b f^{(3)}(\xi(x)) \Psi_2(x) dx.$$

Since $\Psi_2(x) = (x - x_0)(x - x_1)(x - x_2)$ **does change sign** in (x_0, x_2) , we *can not apply WMT directly*. In this case, we will use a slightly different technique. The following result will be used.

Suppose that $f(x)$ changes sign over (a, b) , however $\Psi_n(x) = (x - x_0)(x - x_1) \cdots (x - x_n)$ is such that

$$\int_a^b \Psi_n(x) dx = 0.$$

Let x_{n+1} be another point such that $\Psi_{n+1}(x) = (x - x_{n+1})\Psi_n(x)$ is of one sign in (a, b) . Then $\int_a^b f(x)\Psi_n(x)dx = \frac{1}{(n+2)!} f^{(n+2)}(\eta) \int_a^b \Psi_{n+1}(x)dx$ where,

$$a < \eta < b.$$

In our case $n = 2$ and we note that

$$\int_{x_0}^{x_2} \Psi_2(x) dx = \int_{x_0}^{x_2} (x - x_0)(x - x_1)(x - x_2) dx = 0.$$

$$\left(\text{Since } x_1 = \frac{x_0 + x_2}{2}\right).$$

Now choose $x_3 = x_1$, then

$$\Psi_3(x) = (x - x_3)\Psi_2(x) = (x - x_1)(x - x_0)(x - x_1)(x - x_2) = (x - x_1)^2(x - x_0)(x - x_2).$$

Clearly, $\Psi_3(x)$ does not change sign over the interval (x_0, x_2) . So, according to the above result, the error for Simpson's rule is given by

$$\begin{aligned} E_S &= \frac{1}{4!} f^{(4)}(\eta) \int_{x_0}^{x_2} \Psi_3(x) \\ &= \frac{1}{24} f^{(4)}(\eta) \int_{x_0}^{x_2} (x - x_1)^2 (x - x_0)(x - x_2) dx \\ &= \frac{1}{24} f^{(4)}(\eta) \left(\frac{-4}{15} \right) h^5 = -\frac{h^5}{90} f^{(4)}(\eta). \end{aligned}$$

Simpson's Rule with Error Formula

$$\begin{aligned} \int_a^b f(x) dx &= \int_{a=x_0}^{b=x_2} f(x) dx = \frac{h}{3} (f_0 + 4f_1 + f_2) - \frac{h^5}{90} f^{(4)}(\eta) \\ &= \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \\ &\quad - \frac{\left(\frac{b-a}{2}\right)^5}{90} f^{(4)}(\eta), \end{aligned}$$

where $a < \eta < b$

Exactness of Simpson's Formula

It follows from the above error formula that *Simpson's rule is exact for all polynomials of degree less than or equal to 3. (note that if $f(x)$ is a polynomial of degree less than equal to 3, then $f^{(4)}(x) = 0$, and is nonzero for higher degree polynomials).*

If $f(x)$ is a polynomial of degree less than or equal to 3. Simpson's rule is exact.

Example 3.1 Consider approximating $\int_0^1 \cos x dx$ using both Trapezoidal Rule (TRAP) and Simpson's Rule (SYMS).

$$I_T = \mathbf{Trap:} \int_0^1 \cos x dx \approx 0.5(1 + 0.5403) = 0.7702$$

$$I_S = \mathbf{SYMS:} \int_0^1 \cos x dx \approx \frac{1}{6}(1 + 4 \cos(\frac{1}{2}) + \cos(1)) = 0.8418.$$

Exact value $\equiv 0.8415$ (in 4-digit arithmetic).

4 Newton's-Cotes Quadrature

- **Trapezoidal Rule** - Based on interpolating the function by a polynomial of degree 1 with the nodes: $x_0 = a$ and $x_1 = b$.

$$I_T = \frac{b-a}{2}(f(a) + f(b)).$$

- **Simpson's Rule** - Based on interpolating the function by a polynomial of degree 2 with the nodes:

$$x_0 = a, \quad x_1 = a + h = a + \frac{b-a}{2} = \frac{a+b}{2}, \quad x_2 = b.$$

$$I_S = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right].$$

These two rules are special cases of the **Closed Newton-Cotes** (CNC) rule.

An n -point **closed Newton-Cotes** rule has the $(n+1)$ nodes:

$$x_i = a + i \frac{(b-a)}{n}, \quad i = 0, 1, \dots, n.$$

$n = 1 \Rightarrow$ Trapezoidal Rule

$n = 2 \Rightarrow$ Simpson's Rule

(Note that CNC Rule includes the end points of the nodes)

The **open Newton-Cotes** has the $(n + 1)$ nodes **which do not include the end points**.

$$x_i = a + i \frac{(b - a)}{n + 2}, i = 1, 2, \dots, n.$$

A well-known example of the n -point open Newton-Cotes rule is the **midpoint rule** (with $n = 0$). Thus, **the midpoint rule is based on interpolation of $f(x)$ with a constant function**. The only node in this case is: $x_1 = \frac{a + b}{2}$.

Thus $I_M =$ Midpoint Approximation to the Integral $\int_a^b f(x)dx = (b - a)f\left(\frac{a + b}{2}\right)$.

Error Formula for the Midpoint Rule:

In this case $\Psi_0(x) = x - x_1 = x - \frac{a + b}{2}$ changes sign in (a, b) .

However, note that if we $x_0 = x_1$, then $\Psi_1(x) = (x - x_1)^2 = (x - \frac{a + b}{2})^2$ is always of the same sign. Thus, we can show as in the case of Simpson's rule that

$$E_M = f''(\eta) \frac{(b - a)^3}{24}$$

, where $a < \eta < b$

Thus

Midpoint Rule with Error Formula

$$I_M = \int_a^b f(x)dx = (b - a)f\left(\frac{a + b}{2}\right) + f''(\eta) \frac{(b - a)^3}{24}.$$

Comparing the error terms of I_M and I_T , we easily see that the midpoint rule is more accurate than the trapezoidal rule.

Example 4.1 Apply the midpoint, trapezoidal and Simpson's rule to

$$\int_1^0 e^x dx$$

$$I_M = f(0.5) = e^{0.5} = 1.6487$$

$$I_T = \frac{1}{2}(1 + e) = 1.8591$$

$$I_S = \frac{1}{6} \left(e^0 + 4e^{\frac{1}{2}} + e^1 \right) = 1.7189$$

$$I = \int_0^1 e^x dx \approx 1.7183 \text{ (correct to four decimal digits).}$$

5 The Composite Rules

Since the Trapezoidal and Simpson's rules have been derived with only 1 and 2, subintervals, respectively, these rules are not likely to give accurate results over a large interval with 1 or two subintervals/Ada.

To obtain a greater accuracy, the idea then will be to subdivide the interval $[a, b]$ into smaller intervals, apply these quadrature formulas in each of these smaller intervals and add up the results to obtain more accurate approximations.

Let's divide $[a, b]$ into n equal subintervals as follows:

$$a = x_0 < x_1 < x_2 \dots < x_{n-1} < x_n = b.$$

Let $h = \frac{b-a}{n}$ = the length of each of these subintervals.

Then $x_0 = a$, $x_1 = a + h$, $x_2 = a + 2h$, \dots , $x_n = b = a + nh$.

5.1 The Composite Trapezoidal Rule (CTR)

To obtain the Composite Trapezoidal Rule over $[a, b]$

- Divide the interval $[a, b]$ into n equal subintervals.
- Integrate $f(x)$ over each of those subintervals using the Trapezoidal rule for each subinterval.
- Add the results.

$$\begin{aligned}
 I_{CT} &= \int_{x_0=a}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \dots + \int_{x_{n-1}}^{x_n=b} f(x)dx \\
 &= \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \dots + \frac{h}{2}(f_{n-1} + f_n) \\
 &= h \left(\frac{f_0}{2} + f_1 + f_2 + \dots + f_{n-1} + \frac{f_n}{2} \right).
 \end{aligned}$$

The Composite Trapezoidal Rule

$$\begin{aligned}
 I_{CT} &= h \left[\frac{f_0}{2} + f_1 + f_2 + \dots + f_{n-1} + \frac{f_n}{2} \right] \\
 &= \frac{h}{2} [f(a) + 2f_1 + 2f_2 + \dots + 2f_{n-1} + f(b)].
 \end{aligned}$$

5.2 The Error Formula for Composite Trapezoidal Rule

The error formula for CTR is obtained by adding the individual error terms of the trapezoidal rule in each of the subintervals. Thus, the error formula for the composites trapezoidal rule, denoted by E_T^C in given by:

$$E_T^C = \frac{-h^3}{12} [f''(\eta_1) + f''(\eta_2) + \dots + f''(\eta_n)]$$

Simplification of the Error Formula.

To simplify the expression within the parenthesis, we need the following well-known result.

The Intermediate Value Theorem (IVT)

If $f(x)$ is continuous on $[a, b]$ and k is a number such that $f(a) < k < f(b)$, then there exists a number c , $a < c < b$ with the property: $f(c) = k$.

Applying the IVT and remembering that $h = \frac{b-a}{n}$, we get

$$\begin{aligned} E_{CT} &= -\frac{nh^3}{12}f''(\eta), \text{ where } \eta_1 < \eta < \eta_n. \\ &= -n \frac{(b-a)}{n} \cdot \frac{h^2}{12}f''(\eta) = -\frac{(b-a)}{12}h^2f''(\eta), \end{aligned}$$

where $a < \eta < b$.

The Composite Trapezoidal Rule With Error Formula

$$\int_{a=x_0}^{b=x_n} f(x)dx = h \underbrace{\left[\frac{f_0}{2} + f_1 + f_2 + \dots + \frac{f_n}{2} \right]}_{\text{Composite Trapezoidal Rule}} + \underbrace{\frac{b-a}{12}h^2f''(\eta)}_{\text{Error}}$$

where $a < \eta < b$.

5.3 The Composite Simpson's Rule (CSR)

Since Simpson's rule was obtained with two subintervals, in order to derive the CSR, we divide the interval $[a, b]$ into *even number of subintervals*, say $n = 2m$, where m is a positive integer and then apply Simpson's rule in each of those subintervals and finally, add up the results.

Obtaining Composite Simpson's Rule

- Divide the interval $[a, b]$ into $n = 2m$ equal subintervals: $[x_0, x_2], [x_2, x_4] \dots, [x_{n-2}, x_n]$
- Integrate $f(x)$ over each of these subintervals using Simpson's rule
- Add the results.

$$\begin{aligned}
 I_{CT} &= \int_{a=x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \dots + \int_{x_{n-2}}^{b=x_n} f(x)dx \\
 &= \frac{h}{3} [(f_0 + 4f_1 + f_2) + (f_2 + 4f_3 + f_4) + \dots + (f_{n-2} + 4f_{n-1} + f_n)] \\
 &= \frac{h}{3} [(f_0 + f_n) + 4(f_1 + f_3 + \dots + f_{n-1}) + 2(f_2 + f_4 + \dots + f_{n-2})].
 \end{aligned}$$

The Composite Simpson's Rule

$$I_{CS} = \int_{a=x_0}^{b=x_n} f(x)dx \approx \frac{h}{3} [(f_0 + f_n) + 4(f_1 + \dots + f_{n-1}) + 2(f_2 + \dots + f_{n-2})].$$

The Error in Composite Simpson's Rule

The error in composite Simpson's Rule, denoted by E_C^S , is given by

$$E_C^S = \frac{-h^5}{90} \left[f^{(4)}(\eta_1) + f^{(4)}(\eta_2) + \dots + f^{(4)}\left(\eta_n\right) \right],$$

where $x_{i-1} < \eta_{i-1} < x_{i+1}, i = 1, 2, \dots, n - 1$.

A Simplified Expression for the Error:

By using IMT, it can be shown that there exists a number η in (a, b) such that

$$\begin{aligned} E_{CS} &= \frac{-h^5}{90} \times \frac{n}{2} f^{(4)}(\eta) \\ &= \frac{-h^5 (b-a)}{180 h} f^{(4)}(\eta) = \frac{-h^4}{180} (b-a) f^{(4)}(\eta). \end{aligned}$$

(Note that $n = \frac{b-a}{h}$).

The Composite Simpson's Rule with Error Term

$$\begin{aligned} \int_a^b f(x) dx &= \frac{h}{3} [(f_0 + f_n) + 4(f_1 + \dots + f_{n-1}) + 2(f_2 + \dots + f_{n-2})] - \frac{h^4}{180} (b-a) f^{(4)}(\eta) \\ &= \underbrace{\frac{h}{3} [f(a) + f(b) + 4(f_1 + \dots + f_{n-1}) + 2(f_2 + \dots + f_{n-2})]}_{\text{Composite Simpson's Rule}} - \underbrace{\frac{h^4}{180} (b-a) f^{(4)}(\eta)}_{\text{Error}} \end{aligned}$$

Example 5.1 Let $f(x) = \begin{cases} x & \text{if } 0 \leq x \leq \frac{1}{2} \\ 1-x & \text{if } \frac{1}{2} \leq x \leq 1 \end{cases}$

(a) Trapezoidal Rule over $[0, 1]$

$$I_T = \frac{1}{2}(f(0) + f(1)) = \frac{1}{2}(0 + 0) = \boxed{0}$$

(b) Trapezoidal Rule over $\left[0, \frac{1}{2}\right]$ and $\left[\frac{1}{2}, 1\right]$:

$$\begin{aligned} I_{CT} &= \frac{1}{4}(f(0) + f(1/2)) + \frac{1}{4}\left(f\left(\frac{1}{2}\right) + f(1)\right) \\ &= \frac{1}{4}\left(0 + \frac{1}{2} + \frac{1}{2} + 0\right) = \frac{1}{4}(1) = \boxed{\frac{1}{4}} \end{aligned}$$

(c) Simpson's Rule over $[0, 1]$

$$\begin{aligned} I_S &= \frac{1}{3}\left[f(0) + 4f\left(\frac{1}{2}\right) + f(1)\right] \\ &= \frac{1}{3}\left(0 + 4\left(\frac{1}{2}\right) + 0\right) = \frac{1}{3}(2) = \boxed{\frac{2}{3}} \end{aligned}$$

5.4 Example (Application of the Error Formula)

Determine h to approximate

$$\int_{.1}^{10} \frac{1}{t e^t} dt$$

with an accuracy of $\epsilon = 10^{-3}$ using the **Composite Trapezoidal rule**.

Recall that the error formula in this case is:

$$E_{CT} = -\frac{b-a}{12} h^2 f''(\eta).$$

Let's now find the maximum value (in magnitude) of E_{CT} in the interval $[0.1, 10]$.

We then need to find $f''(\eta)$.

Now, $f(t) = \frac{1}{t e^t}$ (given)

and $f''(t) = \frac{1}{t e^t} \left(\frac{1}{t^2} + \frac{2}{t} + 1 \right)$

Thus, f'' is maximum when $t = 0.1$

and

$$\max |f''(t)| = \frac{1}{0.1 \times e^{0.1}} (100 + 20 + 1) = 1094.9$$

So, maximum value of $E_C^T = \left(\frac{9.9}{12} \right) h^2 \times 1094.9$.

Thus, to approximate h with an accuracy of $\epsilon = 10^{-3}$, h has to be such that

$$\left(\frac{9.9}{12} \right) h^2 \times 1094.9 \leq 10^{-3}.$$

That is,

$$h^2 \leq 12 \cdot 10^{-3} \times \frac{1}{9.9 \times 1094.9}$$

or

$$h \leq 0.01052 \times 10^{-7}.$$

6 Romberg Integration

The idea behind Romberg integration is to *successfully use the Trapezoidal rule with increasing intervals and stop as soon as two successive approximations agree to each other by a desired accuracy.*

The key to do that is to observe that the successive approximations can be generated recursively in terms of the previous approximations. Thus,

$$\begin{aligned} R_{11} &= \text{The Trapezoidal rule with 1 interval} \\ &= \frac{1}{2}(b-a)[f(a) + f(b)] \end{aligned} \tag{6.1}$$

(Note that $h = b - a$)

$$\begin{aligned} R_{21} &= \text{The Trapezoidal rule with 2 intervals} \\ &= \frac{b-a}{4} \left[f(a) + f(b) + 2f\left(a + \frac{b-a}{2}\right) \right] \end{aligned}$$

(Note that in this case, $h = \frac{b-a}{2}$ and the points of subdivision are:

$$x_0 = a, x_1 = a + \frac{b-a}{2}, \text{ and } x_2 = b$$

Thus,

$$R_{21} = \frac{1}{2} \left[R_{11} + (b-a)f\left(a + \frac{b-a}{2}\right) \right]. \tag{6.2}$$

This formula immediately can be generalized.

Denote $R_{k1} =$ The Trapezoidal rule with 2^{k-1} intervals

$$h_k = \frac{b-a}{2^{k-1}}, k = 1, 2, \dots$$

It can be shown [**Exercise**] that

$$R_{k1} = \frac{1}{2} \left[R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k) \right], k = 2, 3, \dots, n \tag{6.3}$$

Verify: $k = 2$.

$$\begin{aligned}
 R_{21} &= \frac{1}{2}[R_{11} + h_1 f(a + h_2)] \\
 &= \frac{1}{2} \left[R_{11} + (b - a) f \left(a + \frac{b - a}{2} \right) \right].
 \end{aligned}$$

Furthermore, one can show that R_{11} and R_{21} can be combined to compute another number R_{22} ; R_{31} and R_{21} can be combined to compute R_{32} ; and so on. The formula to do so is:

$$R_{kj} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}, \quad k = 2, 3, \dots, n; \quad j = 2, \dots, k \tag{6.4}$$

Thus, $R_{22} = R_{21} + \frac{R_{21} - R_{11}}{4 - 1} = R_{21} + \frac{R_{21} - R_{11}}{3}$.

and so on.

These numbers are called *Romberg numbers* and can be arranged in a table, similar to the divided difference table, and is known as **The Romberg Table**.

Romberg Table				
R_{11}				
R_{21}	R_{22}			
		R_{33}		
R_{31}		\vdots	\ddots	
\vdots	R_{32}	R_{42}	\ddots	
R_{n1}	R_{n2}	R_{n3}		R_{nn}

6.1 Stopping Criterion

Suppose that we would like to compute $\int_a^b f(x)$ with an accuracy of ϵ , then the iteration can be stopped as soon as

$$|R_{nn} - R_{n-1,n-1}| < \epsilon.$$

6.2 Creating the Romberg Table

Since our ultimate interest is to obtain the diagonal entries and these entries can be computed just out of two entries from the previous column, we can compute the entries Romberg Table in the following order of computations.

- Compute R_{11} and R_{21} using (6.1) and (6.2)
- Compute R_{22} out of R_{11} and R_{21} using (6.4)
- Compute R_{31} from (6.3) and R_{32} from (6.4) and then combine R_{32} with R_{22} to obtain R_{33} using (6.4) again.
- In general, compute R_{k1} from (6.3) and $R_{k,k-1}$ from (6.4) and then combine $R_{k,k-1}$ with $R_{k-1,k-1}$ to obtain R_{kk} using (6.4) again.

Example 6.1 $I = \int_1^{1.5} x^2 \ln x$ with $n = 3$

$$R_{11} = \frac{1}{2}(1.5 - 1)[f(1) + f(1.5)] = .2280741$$

$$R_{21} = \frac{1}{2}(R_{11} + (1.5 - 1)(f(1 + \frac{1.5 - 1}{2}))) = .201225$$

$$R_{22} = R_{2.1} + \frac{R_{2.1} - R_{1.1}}{4^1 - 1} = .1944945$$

$$\begin{array}{l|l} R_{11} = 0.2280741 & \\ R_{21} = 0.2012025 & R_{22} = 0.1922453 \\ R_{31} = 0.1944945 & R_{32} = 0.1922585 \quad R_{33} = 0.1922593 \end{array}$$

Exact value of I (up to five decimal figures) = 0.192259

Adaptive Quadrature

Adaptive quadrature rule is a way to adaptively adjust the value of the step-size h such that the error becomes less than a prescribed tolerance (say ϵ).

For the purpose of describing the idea of adaptive quadrature rule, we will use Simpson's rule as our ground rule of approximating the integral.

With the step-size h , that is, with the points of subdivisions as $a, a + h$, and b

$$\begin{array}{c} \text{X} \text{-----} \text{X} \text{-----} \text{X} \\ \text{a} \qquad \qquad \text{a+h} \qquad \qquad \qquad \text{b} \end{array}$$

We have the Simpson's rule approximation:

$$I_S^h = \frac{h}{3} [f(a) + 4f(a + h) + f(b)]$$

and **Error** = $E_S^h = -\frac{h^5}{90} f^{(4)}(\eta)$, where $a < \eta < b$.

Now let's use 4 intervals; that is, this time the points of subdivision are:

$$a, a + \frac{h}{2}, a + h, a + \frac{3h}{2}, b.$$

$$\begin{array}{c} \text{X} \text{-----} \text{X} \text{-----} \text{X} \text{-----} \text{X} \text{-----} \text{X} \\ \text{a} \qquad \text{a+\frac{h}{2}} \qquad \text{a+h} \qquad \text{a+\frac{3h}{2}} \qquad \text{b} \end{array}$$

Then, using *Compositive Simpson's rule* with $n = 4$, that is, with the length of each subinterval $\frac{h}{2}$, we have

$$I_S^{\frac{h}{2}} = \frac{h}{6} \left[f(a) + 4f\left(a + \frac{h}{2}\right) + f(b) \right]$$

and $E_S^{\frac{h}{2}} = -\frac{1}{16} \left(\frac{h^5}{90}\right) f^{(4)}(\bar{\eta})$,

were $a < \bar{\eta} < b$.

Now the equation is: *how ell does $I_S^{\frac{h}{2}}$ approximate I over I_S^h ?*

In this context, assuming $\eta \approx \tilde{\eta}$, it follows from the expressions of E_S^h and $E_S^{\frac{h}{2}}$ that

$$|I - I_S^{\frac{h}{2}}| \approx \frac{1}{15} |I_S^h - I_S^{\frac{h}{2}}|$$

This is a rather pleasant result; because it is easy to compute $|I_S^h - I_S^{\frac{h}{2}}|$, suppose this quantity is denoted by δ .

Then, if we choose h such that $\delta = 15\epsilon$, we see that $|E_S^{\frac{h}{2}}| < \epsilon$.