Introduction

The general problem of numerical integration may be stated as follows:

- Given a set of data points (x_0, y_0), (x_1, y_1), ..., (x_n, y_n) of a function $y = f(x)$, where $f(x)$ is not known explicitly.
- It is required to compute the value of the definite integral

$$I = \int_a^b y \, dx$$

- In this case we have to replace $f(x)$ by an interpolating polynomial $\phi(x)$ and obtain an approximate value of the definite integral by integrating $\phi(x)$.
- Thus, different integration formulae can be obtained depending upon the type of the interpolation formula used.

Introduction

Definition:

Numerical differentiation is the process of calculating the derivatives of a function from a set of given values of that function.

How to Solve:

- The problem is solved by
  - Representing the function by an interpolation formula.
  - Then differentiating this formula as many times as desired.

Differentiation for Equidistant and Non-equidistant Values

- If the function is given by equidistant values, it should be represented by an interpolation formula employing differences, such as Newton's formula.

- If the given values of the function are not equidistant, we must represent the formula by Lagrange's formula.

Numerical Differentiation

- Consider Newton's Forward difference formula, putting $u = (x - x_0)/h$, we get

$$y = y_0 + u\,\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \dots$$

- Then,

$$\frac{dy}{dx} = \frac{dy}{du}\cdot\frac{du}{dx} = \frac{dy}{du}\cdot\frac{d}{dx}\left(\frac{x}{h} - \frac{x_0}{h}\right)$$

$$= \frac{dy}{du}\cdot\frac{d}{dx}\left(\frac{x}{h}\right) - \frac{dy}{du}\cdot\frac{d}{dx}\left(\frac{x_0}{h}\right)$$

$$= \frac{dy}{du}\cdot\frac{1}{h} = \frac{1}{h}\cdot\frac{dy}{du}$$

Numerical Differentiation

- Therefore,

$$\frac{dy}{dx} = \frac{1}{h} \cdot \frac{dy}{du}$$

$$= \frac{1}{h} \cdot \frac{d}{du}\left[y_0 + u\,\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \ldots \right]$$

$$= \frac{1}{h} \cdot \left[\frac{d}{du}(y_0) + \frac{d}{du}(u\,\Delta y_0) + \frac{d}{du}\left(\frac{u(u-1)}{2!}\Delta^2 y_0 \right) + \frac{d}{du}\left(\frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 \right) + \ldots \right]$$

$$= \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \cdots \right] \quad (1.1)$$

Numerical Differentiation

For tabular values of x, the formula takes a simpler form, by setting $x = x_0$ we obtain $u = 0$ [since $u = (x - x_0)/h$] and hence (1.1) gives

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \cdots\right] \quad (1.1)$$

$$\left[\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right] \quad (1.2)$$

Numerical Differentiation: Double Derivatives

We know,

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \cdots\right] \quad (1.1)$$

Differentiating (1.1) again, we obtain,

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + \frac{6u-6}{6}\Delta^3 y_0 + \frac{12u^2-36u+22}{24}\Delta^4 y_0 + \cdots\right] \quad (1.3)$$

At $x = x_0$, u =0 and we obtain

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 \cdots\right] \quad (1.4)$$

Formulae for computing higher derivatives may be obtained by successive differentiation.

Numerical Differentiation: Higher Derivatives

Different formulae can be derived by starting with other interpolation formulae.

(a) Newton's backward difference formula gives

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \ldots\right] \quad (1.5)$$

and

$$\left[\frac{d^2 y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n \ldots\right] \quad (1.6)$$

Numerical Differentiation: Higher Derivatives

If a derivative is required near the start of a table the following formulae may be used

$$hy_0' = \left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \frac{1}{5}\Delta^5 - \frac{1}{6}\Delta^6 + \frac{1}{7}\nabla^7 - \frac{1}{8}\nabla^8 + \ldots\right]y_0 \quad (1.7)$$

$$hy_0' = \left[\Delta + \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \frac{1}{12}\Delta^4 - \frac{1}{20}\Delta^5 + \frac{1}{30}\Delta^6 - \ldots\right]y_{-1} \quad (1.7b)$$

$$h^2 y_0'' = \left[\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \frac{137}{180}\Delta^6 - \frac{7}{10}\Delta^7 + \frac{363}{560}\Delta^8 + \ldots\right]y_0 \quad (1.8)$$

Numerical Differentiation: Higher Derivatives

If a derivative is required near the end of a table the following formulae may be used

$$hy_n' = \left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \frac{1}{5}\nabla^5 + \frac{1}{6}\nabla^6 + \frac{1}{7}\nabla^7 + \frac{1}{8}\nabla^8 + \ldots\right] y_n \quad (1.9)$$

$$hy_n' = \left[\nabla - \frac{1}{2}\nabla^2 - \frac{1}{6}\nabla^3 - \frac{1}{12}\nabla^4 - \frac{1}{20}\nabla^5 - \frac{1}{30}\nabla^6 - \frac{1}{42}\nabla^7 - \frac{1}{56}\nabla^8 - \ldots\right] y_{n+1} \quad (1.9b)$$

$$h^2 y_n'' = \left[\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{5}{6}\nabla^5 + \frac{137}{180}\nabla^6 + \frac{7}{10}\nabla^7 + \frac{363}{560}\nabla^8 + \ldots\right] y_n \quad (1.10)$$

Example

From the following table of values of x and y, obtain

$$\frac{dy}{dx} \quad and \quad \frac{d^2y}{dx^2} \quad for \quad x = 1.2$$

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.953	6.0496	7.3891	9.025

Solution

The difference table is in the next slide:

Solution

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1.0	2.7183						
x_0	y_0	0.6081					
1.2	3.3201		0.1333				
		Δy_0					
		0.7351	$\Delta^2 y_0$	0.0294			
1.4	4.0552		0.1627	$\Delta^3 y_0$	0.0067		
		0.8978		0.0361	$\Delta^4 y_0$	0.0013	
1.6	4.9530		0.1988		0.0080	$\Delta^5 y_0$	0.0001
		1.0966		0.0441		0.0014	
1.8	6.0496		0.2429		0..0094		
		1.3395		0.0535			
2.0	7.3891		0.2964				
		1.6359					
2.2	9.0250						

Solution

Here $x_0 = 1.2$, $y_0 = 3.3201$ and $h = 0.2$

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.7351 - \frac{1}{2}(0.1627) + \frac{1}{3}(0.0361) - \frac{1}{4}(0.0080) + \frac{1}{5}(0.0014)\right]$$

$$= 3.3205$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1627 - 0.0361 + \frac{11}{12}(0.0080) - \frac{5}{6}(0.0014)\right]$$

$$= 3.318$$

Alternative Solution

Here $x_0 = 1.2$, $y_0 = 3.3201$ and $h = 0.2$

Then, $x_{-1} = 1.0$, $y_{-1} = 2.7183$ and $h = 0.2$

$$\left[\frac{dy}{dx}\right]_{x=1.2} = \frac{1}{0.2}\left[0.6018 + \frac{1}{2}(0.1333) - \frac{1}{6}(0.0294) + \frac{1}{12}(0.0067) - \frac{1}{20}(0.0013)\right]$$

$$= 3.3205$$

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.2} = \frac{1}{0.04}\left[0.1333 - \frac{1}{12}(0.0067) + \frac{1}{12}(0.0013)\right]$$

$$= 3.32$$

Problem

From the following table of values of x and y, obtain

$$\frac{dy}{dx} \quad for \quad x = 2.0$$

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.953	6.0496	7.3891	9.025

Answer: 7.3896

Problem

Find $\frac{d}{dx}\left(J_0\right)$ $x = 0.1$ from the following table:

x	0.0	0.1	0.2	0.3	0.4
$J_0(x)$	1.0000	0.9975	0.9900	0.9776	0.9604

Problem

The following table gives the angular displacements θ (radians) at different intervals of time t (seconds).

Calculate the angular velocity at the instant $x = 0.408$.

θ	0.052	0.105	0.168	0.242	0.327	0.408	0.489
t	0	0.02	0.04	0.06	0.08	0.10	0.12

Errors in Numerical Differentiation

In the given example,

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.953	6.0496	7.3891	9.025

$$when\ x = 1.2, \text{ then we get } \frac{dy}{dx} = 3.3205 \text{ and } \frac{d^2y}{dx^2} = 3.318$$

$$\text{But, here } y = e^x, \text{ therefore, } \frac{dy}{dx} = \frac{d}{dx}(e^x) = e^x \text{ and } \frac{d^2y}{dx^2} = e^x$$

- Therefore, here we can see with each differentiation, some error occurs in the derivatives.
- The error increases with higher derivatives.
- This is because, in interpolation the new polynomial would agree at the set of points.
- But, their slopes at these points may vary considerably.

Maximum Value of a Tabulated Function

- It is known that the maximum values of a function can be found by equating the first derivative to zero and solving for the variable.

- The same procedure can be applied to determine the maxima of a tabulated function.

- Consider Newton's forward difference formula

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \ldots$$

$$where \quad x = x_0 + uh$$

$$Then, \frac{dy}{du} = \Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \ldots$$

Maximum Value of a Tabulated Function

- For maxima, $dy/dx = 0$.
- Hence, terminating the right-hand side after the third difference (for simplicity) and equating it to zero.
- We obtain the quadratic for u.

$$c_0 + c_1 u + c_2 u^2 = 0$$

where

$$c_0 = \Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0$$

$$c_1 = \Delta^2 y_0 - \Delta^3 y_0$$

$$c_2 = \frac{1}{2}\Delta^3 y_0$$

The values of x can then be found from the relation $x = x_0 + uh$

Example

From the following table, find x, correct to two decimal places, for which y the function has the maximum value and find the value of y.

x	1.2	1.3	1.4	1.5	1.6
y	0.9320	0.9636	0.9855	0.9975	0.9996

Solution

The difference table is in the next slide:

Solution

x	y		
1.2	0.9320		
		0.0316	
1.3	0.9636		-0.0097
		0.0219	
1.4	0.9855		-0.0099
		0.0120	
1.5	0.9975		-0.0099
		0.0021	
1.6	0.9996		

Solution

Let, x_0 = 1.2 and we can terminate the formula after the second difference (since the difference is very negligible).

Now we have,

$$0.0316+(2u-1)(-0.0097)/2 = 0$$

Therefore, $u = 3.8$ and $x = x_0 + uh = 1.2+(3.8)(0.1) = 1.58$

For $x = 1.58$, we have the maximum value of y.

Using Newton's backward difference formula at $x_n = 1.6$ gives,

$y(1.58) = 1.0$ (CLASS WORK)

That is the maximum value of y in the function.

Introduction

The general problem of numerical integration may be stated as follows:

- Given a set of data points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ of a function $y = f(x)$, where $f(x)$ is not known explicitly.
- It is required to compute the value of the definite integral

$$I = \int_a^b y \, dx$$

- In this case we have to replace $f(x)$ by an interpolating polynomial $\phi(x)$ and obtain an approximate value of the definite integral by integrating $\phi(x)$.
- Thus, different integration formulae can be obtained depending upon the type of the interpolation formula used.

Numerical Integration

- Let, the interval [a, b] be divided into n equal subintervals such that $a = x_0 < x_1 < \ldots < x_n = b$.
- Then, $x_n = x_0 + nh$.
- Hence, the integral becomes $I = \int_{x_0}^{x_n} y\, dx$
- Integrating Newton's forward difference formula, we obtain

$$I = \int_{x_0}^{x_n} \left[y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots \right] dx$$

$$= \int_{x_0}^{x_0+nh} \left[y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots \right] dx$$

Numerical Integration

- Since $x = x_0 + hu$ from which we get $dx = hdu$.
- The limit of integration for x are x_0 and x_0+nh
- We know, $u = (x - x_0)/h$
- Therefore, for u, the corresponding lower limit is
  $(x_0 - x_0)/h = 0.$
- For u, the corresponding upper limit is
  $(x_n - x_0)/h = (x_0 + hn - x_0)/h = n$.
- We therefore have,

$$I = h\int_0^n \left[y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots \right] du$$

Numerical Integration

- Now,

$$I = h\int_0^n \left[y_0 + u\Delta y_0 + \frac{\Delta^2 y_0}{2}(u^2 - u) + \frac{\Delta^3 y_0}{3!}(u^3 - 3u^2 + 2u) + \cdots \right] du$$

$$= h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + (\frac{n^3}{3} - \frac{n^2}{2})\frac{\Delta^2 y_0}{2} + (\frac{n^4}{4} - n^3 + n^2)\frac{\Delta^3 y_0}{3!} + \cdots \right]$$

- Which gives on simplification

$$I = \int_{x_0}^{x_n} y\, dx = nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}.\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots \right] \qquad (1)$$

- From this general formula we can obtain different integration formulae by putting n = 1, 2, 3, ... etc.

Trapezoidal Rule

- Setting $n = 1$ in the general formula (1) and neglecting all differences above the first we obtain for the first interval $[x_0, x_1]$

$$\int_{x_0}^{x_1} y\, dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}[y_0 + y_1]$$

- For the next interval $[x_1, x_2]$, we deduce similarly … (and so on) …

$$\int_{x_1}^{x_2} y\, dx = \frac{h}{2}[y_1 + y_2]$$

- Similarly, for the last interval $[x_{n-1}, x_n]$, we have

$$\int_{x_{n-1}}^{x_n} y\, dx = \frac{h}{2}[y_{n-1} + y_n]$$

- Combining all these expressions, we obtain the rule

$$\int_{x_0}^{x_n} y\, dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + \cdots + y_{n-1}) + y_n]$$

- This rule is known as the Trapezoidal Rule.

Trapezoidal Rule: Geometric Significance

- The geometrical significance of this rule is that
  - The curve $y = f(x)$ is replaced by n straight lines joining the points (x_0, y_0) and (x_1, y_1); (x_1, y_1) and (x_2, y_2); ... (x_{n-1}, y_{n-1}), and (x_n, y_n).
  - The area bounded by the curve $y = f(x)$, within the x-coordinates $x = x_0$, and $x = x_n$, and the x-axis is then approximately equivalent to the sum of the areas of the n trapeziums obtained.

Example

Evaluate $I = \int_0^1 \frac{1}{1+x}\,dx,$

for h = 0.5, 0.25 and 0.125 using Trapezoidal rule (correct to three decimal places).

Solution

The values of x and y are tabulated below h = 0.5

x	0	0.5	1.0
y	1.0000	0.6667	0.5

Trapezoidal rule gives

$$I = \int_{x_0}^{x_n} y\,dx = \frac{h}{2}\left[y_0 + 2\left(y_1 + y_2 + \cdots + y_{n-1}\right) + y_n\right]$$

$$I = \frac{0.5}{2}\left[1.0000 + 2(0.6667) + 0.5\right] = 0.7084$$

Example (Cont.)

Solution

The values of x and y are tabulated below $h = 0.25$

x	0	0.25	0.5	0.75	1
y	1	0.8	0.6667	0.5714	0.5

Trapezoidal rule gives

$$I = \int_{x_0}^{x_n} y\, dx = \frac{h}{2}\left[y_0 + 2\left(y_1 + y_2 + \cdots + y_{n-1}\right) + y_n\right]$$

$$I = \frac{0.25}{2}\left[1 + 2(0.8 + 0.6667 + 0.5714) + 0.5\right] = 0.6970$$

Example (Cont.)

Solution

The values of x and y are tabulated below h = 0.125 (CLASS WORK)

Answer: I = 0.6941

Problem

A solid of revolution is formed by rotating about the x-axis the area between the x-axis, the lines $x = 0$ and $x = 1$, and a curve through the points with the following coordinates

x	0.00	0.25	0.50	0.75	1.00
y	1.0000	0.9896	0.9589	0.9089	0.8415

Estimate the volume of the solid formed using Trapezoidal rule, giving the answer to three decimal places.

Answer: 0.9447625

Errors of Trapezoidal Rule

The error of the trapezoidal formula can be obtained in the following way. Let $y = f(x)$ be continuous, well-behaved, and possess continuous derivatives in $[x_0, x_n]$. Expanding y in a Taylor's series around $x = x_0$, we obtain

$$\int_{x_0}^{x_1} y\,dx = \int_{x_0}^{x_1} \left[y_0 + (x - x_0)y_0' + \frac{(x-x_0)^2}{2} y_0'' + \cdots \right] dx$$

$$= hy_0 + \frac{h^2}{2} y_0' + \frac{h^3}{6} y_0'' + \cdots \tag{5.34}$$

Similarly,

$$\frac{h}{2}(y_0 + y_1) = \frac{h}{2}\left(y_0 + y_0 + hy_0' + \frac{h^2}{2} y_0'' + \frac{h^3}{6} y_0''' + \cdots \right)$$

$$= hy_0 + \frac{h^2}{2} y_0' + \frac{h^3}{4} y_0'' + \cdots \tag{5.35}$$

From (5.34) and (5.35), we obtain

$$\int_{x_0}^{x_1} y\,dx - \frac{h}{2}(y_0 + y_1) = -\frac{1}{12}h^3 y_0'' + \cdots, \tag{5.36}$$

which is the error in the interval $[x_0, x_1]$. Proceeding in a similar manner we obtain the errors in the remaining subintervals, viz., $[x_1, x_2], [x_2, x_3], \ldots$ and $[x_{n-1}, x_n]$. We thus have

$$E = -\frac{1}{12}h^3(y_0'' + y_1'' + \cdots + y_{n-1}''), \tag{5.37}$$

where E is the *total error*. Assuming that $y''(\bar{x})$ is the largest value of the n quantities on the right-hand side of (5.37), we obtain

$$E = -\frac{1}{12}h^3 n y''(\bar{x}) = -\frac{b-a}{12}h^2 y''(\bar{x}) \tag{5.38}$$

since $nh = b - a$.

Simpson's 1/3-Rule

- Setting $n = 2$ in the general formula (1) and neglecting all differences above the second we obtain for the first interval $[x_0, x_2]$

$$I = \int_{x_0}^{x_n} y\,dx = nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots\right] \quad (1)$$

$$\int_{x_0}^{x_2} y\,dx = 2h\left[y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right] = \frac{h}{3}\left[y_0 + 4y_1 + y_2\right]$$

- For the next interval $[x_2, x_4]$, we deduce similarly … (and so on) …

$$\int_{x_2}^{x_4} y\,dx = \frac{h}{3}\left[y_2 + 4y_3 + y_4\right]$$

- Finaly, for the last interval $[x_{n-2}, x_n]$, we have

$$\int_{x_{n-2}}^{x_n} y\,dx = \frac{h}{3}\left[y_{n-2} + 4y_{n-1} + y_n\right]$$

- Combining all these expressions, we obtain the rule

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{3}\left[y_0 + 4\left(y_1 + y_3 + y_5 + \cdots + y_{n-1}\right) + 2\left(y_2 + y_4 + y_6 + \cdots + y_{n-2}\right) + y_n\right]$$

- This rule is known as the Simson's 1/3 Rule (or Simpson's Rule).

Simpson's 1/3 Rule: Geometric Significance

- The geometrical significance of this rule is that
  - Replacing the curve $y = f(x)$ is by n/2 arcs of second degree polynomials or parabolas joining the points (x_0, y_0) and (x_2, y_2); (x_2, y_2) and (x_4, y_4); ... (x_{n-2}, y_{n-2}), and (x_n, y_n).
  - It should be noted that this rule requires the division of the whole range into an even number of subintervals of width h.

Example

Evaluate $I = \int_0^1 \frac{1}{1+x}\,dx,$
correct to three decimal places for h = 0.5, 0.25 and 0.125 using Simpson's 1/3 rule.

Solution

The values of x and y are tabulated below h = 0.5

x	0	0.5	1.0
y	1.0000	0.6667	0.5

Simpson's rule gives

$$I = \frac{1}{6}\left[1.0000 + 4(0.6667) + 0.5\right] = 0.6945$$

Example (Cont.)

Problem : Do the same for h = 0.25 and h = 0.125

Solution

For $h = 0.25$

Simpson's rule gives I = 0.6932

For $h = 0.125$

Simpson's rule gives I = 0.6932

Problem

Apply trapezoidal and Simpson's 1/3 rules to the integral for 10, 20, 30, 40, and 50 subintervals.

$$I = \int_0^1 \sqrt{1 - x^2}\,dx$$

Errors in Simpson's 1/3 rules

error in Simpson's rule is given by

$$\int_a^b y\,dx = \frac{h}{3}[y_0 + 4(y_1 + y_3 + y_5 + \cdots + y_{n-1})$$

$$+ 2(y_2 + y_4 + y_6 + \cdots + y_{n-2}) + y_n]$$

$$= -\frac{b-a}{180} h^4 y^{iv}(\bar{x}), \qquad (5.40)$$

where $y^{iv}(\bar{x})$ is the largest value of the fourth derivatives.

Simpson's 3/8-Rule

$$I = \int_{x_0}^{x_n} y\, dx = nh\left[y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \cdots \right] \quad (1)$$

The rule is obtained by putting $n = 3$ in the general equation (1) and neglecting all the differences above the third we have,

$$\int_{x_0}^{x_3} y\, dx = 3h\left[y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0 \right]$$

$$= 3h\left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0) \right]$$

$$= \frac{3h}{8}\left[y_0 + 3y_1 + 3y_2 + y_3 \right]$$

Similarly,

$$\int_{x_3}^{x_6} y\, dx = \frac{3h}{8}\left[y_3 + 3y_4 + 3y_5 + y_6 \right]$$

Simpson's 3/8-Rule

$$\text{And finally } \cdots\cdots\cdots\cdots$$

$$\int_{x_{n-3}}^{x_n} y\,dx = \frac{3h}{3}\left[y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right]$$

Summing up we obtain

$$\int_{x_0}^{x_n} y\,dx = \frac{3h}{8}\left[(y_0 + 3y_1 + 3y_2 + y_3) + (y_3 + 3y_4 + 3y_5 + y_6) + \cdots\cdots + (y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)\right]$$

$$= \frac{3h}{8}\left[y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + \cdots\cdots + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right]$$

This rule called Simpson's 3/8-rule, is not so accurate as Simpson's rule.

Problem

Apply trapezoidal and Simpson's 3/8 rules to the integral for 3, 6 and 12subintervals.

$$I = \int_0^3 \sqrt{1+x^2}\,dx$$

Weddle's Rule

- The rule is obtained by putting $n = 6$ in the general equation i.e., and neglecting all the differences above the sixth we have,

$$\int_{x_0}^{x_6} y\,dx = h\left[6y_0 + 18\Delta y_0 + 27\Delta^2 y_0 + 24\Delta^3 y_0 + \frac{123}{10}\Delta^4 y_0 + \frac{33}{10}\Delta^5 y_0 + \frac{41}{140}\Delta^6 y_0\right]$$

- Here the coefficient of $\Delta^6 y_0$ differs from 3/10 by the small fraction 1/140 (i.e., 3/10 – 41/140 = 1/140, which is very negligible)

- Hence if we replace this coefficient by 3/10, we commit an error of only $\frac{h}{140}\Delta^6 y_0$
- If the value of h is such that the sixth differences are small, the error committed will be negligible.

- We therefore change the last term to $(3/10)\Delta^6 y_0$

Weddle's Rule

- Then replace all differences by their values in terms of the given y's. The result reduces down to

$$\int_{x_0}^{x_6} y\,dx = \frac{3h}{10}\left[y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6\right]$$

Similarly,

$$\int_{x_6}^{x_{12}} y\,dx = \frac{3h}{10}\left[y_6 + 5y_7 + y_8 + 6y_9 + y_{10} + 5y_{11} + y_{12}\right]$$

- Adding all such expressions as these from x_0 to x_n, where n is now a multiple of six, we get Weddle's Rule

$$\int_{x_0}^{x_n} y\,dx = \frac{3h}{10}\begin{bmatrix} y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + 2y_6 + \\ 5y_7 + y_8 + 6y_9 + y_{10} + 5y_{11} + 2y_{12} + \ldots \\ + 2y_{n-6} + 5y_{n-5} + y_{n-4} + 6y_{n-3} + y_{n-2} + 5y_{n-1} + y_n \end{bmatrix}$$

Weddle's Rule: More

- Weddle's rule is more accurate, in general than Simpson's rule,
- It requires at least seven consecutive values of the function.
- The geometric meaning of Weddle's Rule is that we replace the graph of the function by n/6 arcs of fifth-degree polynomials.

Example

Compute the value of the definite integral for $h = 0.2$ using Weddle's rule

$$\int_{4}^{5.2} \ln x dx$$

Solution

The values of this function is computed for each point of subdivision.

x	$\ln x$
4.0	1.3863
4.2	1.4351
4.4	1.4816
4.6	1.5261
4.8	1.5686
5.0	1.6094
5.2	1.6487

By Weddle's rule we get

I=3(0.2)[1.3863+5(1.4351)+1.4816+6(1.5261)+1.5686+5(1.6094)+1.6487]/10

=1.827858

Problem

Compute the value of the definite integral for h = 0.1 using Weddle's rule

$$I = \int_{0.2}^{1.4} \left(\sin x - \ln x + e^{x}\right) dx$$

Answer: 4.05095

Romberg Integration

$$I = \int_a^b y\,dx$$

and evaluate it by the trapezoidal rule (5.33) with two different subintervals of widths h_1 and h_2 to obtain the approximate values I_1 and I_2, respectively. Then Eq. (5.38) gives the errors E_1 and E_2 as

$$E_1 = -\frac{1}{12}(b-a)h_1^2 y''(\bar{x}) \tag{5.45}$$

and

$$E_2 = -\frac{1}{12}(b-a)h_2^2 y''(\bar{\bar{x}}). \tag{5.46}$$

Since the term $y''(\bar{\bar{x}})$ in (5.46) is also the largest value of $y''(x)$, it is reasonable to assume that the quantities $y''(\bar{x})$ and $y''(\bar{\bar{x}})$ are very nearly the same. We therefore have

$$\frac{E_1}{E_2} = \frac{h_1^2}{h_2^2}$$

and hence

$$\frac{E_2}{E_2 - E_1} = \frac{h_2^2}{h_2^2 - h_1^2}.$$

Since $E_2 - E_1 = I_2 - I_1$, this gives

$$E_2 = \frac{h_2^2}{h_2^2 - h_1^2}(I_2 - I_1). \tag{5.47}$$

We therefore obtain a new approximation I_3 defined by

$$I_3 = I_2 - E_2 = \frac{I_1\,h_2^2 - I_2\,h_1^2}{h_2^2 - h_1^2}, \tag{5.48}$$

which, in general, would be closer to the actual value—provided that the errors decrease monotonically and are of the same sign.

If we now set

$$h_2 = \frac{1}{2} h_1 = \frac{1}{2} h$$

Eq. (5.48) can be written in the more convenient form

$$I\left(h, \frac{1}{2}h\right) = \frac{1}{3}\left[4I\left(\frac{1}{2}h\right) - I(h)\right], \qquad (5.49)$$

where $I(h) = I_1$,

$$I\left(\frac{1}{2}h\right) = I_2 \quad \text{and} \quad I\left(h, \frac{1}{2}h\right) = I_3.$$

With this notation the following table can be formed

$I(h)$			
	$I\left(h, \frac{1}{2}h\right)$		
		$I\left(h, \frac{1}{2}h, \frac{1}{4}h\right)$	
$I\left(\frac{1}{2}h\right)$			$I\left(h, \frac{1}{2}h, \frac{1}{4}h, \frac{1}{8}h\right)$
	$I\left(\frac{1}{2}h, \frac{1}{4}h\right)$		
$I\left(\frac{1}{4}h\right)$		$I\left(\frac{1}{2}h, \frac{1}{4}h, \frac{1}{8}h\right)$	
	$I\left(\frac{1}{4}h, \frac{1}{8}h\right)$		
$I\left(\frac{1}{8}h\right)$			

Example 5.10 Use Romberg's method to compute

$$I = \int_0^1 \frac{1}{1+x}\,dx,$$

correct to three decimal places.

We take $h = 0.5$, 0.25 and 0.125 successively and use the results obtained in the previous example. We therefore have

$$I(h) = 0.7084, \quad I\left(\frac{1}{2}h\right) = 0.6970, \quad \text{and} \quad I\left(\frac{1}{4}h\right) = 0.6941$$

Hence, using (5.49), we obtain

$$I\left(h, \frac{1}{2}h\right) = 0.6970 + \frac{1}{3}(0.6970 - 0.7084) = 0.6932.$$

$$I\left(\frac{1}{2}h, \frac{1}{4}h\right) = 0.6941 + \frac{1}{3}(0.6941 - 0.6970) = 0.6931$$

Finally,

$$I\left(h, \frac{1}{2}h, \frac{1}{4}h\right) = 0.6931 + \frac{1}{3}(0.6931 - 0.6932) = 0.6931.$$

The table of values is therefore

0.7084		
	0.6932	
0.6970		0.6931
	0.6931	
0.6941		

An obvious advantage of this method is that the accuracy of the computed value is known at each step.

Romberg Integration

- This method can be used to improve the approximate results obtained by the finite difference methods such as trapezoidal method.

- Let T_n be the approximation of the integral $I = \int_a^b y\,dx$, using trapezoid rule with 2^n subintervals.

- Let $I_{1,1} = T_{1.}$ (here, I is calculated with 2^1 segments)

- Calculated $I_{1,n}$, $I_{2,n}$ ..., $I_{n,n}$ as follows:

  - Set $I_{1,n+1} = T_{n+1}$ (i.e., $I_{1,2} = T_2$, calculated with 2^2 segments, $I_{1,3} = T_3$, calculated with 2^3 segments, $I_{1,4} = T_4$, calculated with 2^4 segments)

  - Next, for $j = 2, 3, \ldots, n$

$$I_{j,k} = I_{j-1,k+1} + \frac{I_{j-1,k+1} - I_{j-1,k}}{4^{j-1} - 1}, \quad j \geq 2$$

Romberg Integration

We have,

$$I_{j,k} = I_{j-1,k+1} + \frac{I_{j-1,k+1} - I_{j-1,k}}{4^{j-1} - 1}, \quad j \geq 2$$

- The index j represents the order of interpolation.
- For example, $j = 1$ represents the values obtained from the regular Trapezoidal rule.
- The index k represents the more or less accurate estimate of the integral.
- The value of the integral with $k + 1$ index is more accurate than with k index.
- With this notation the following table can be formed.

Romberg Integration

We have,

$$I_{j,k} = I_{j-1,k+1} + \frac{I_{j-1,k+1} - I_{j-1,k}}{4^{j-1} - 1}, \quad j \ge 2$$

With this notation the following table can be formed.

$$\begin{tikzcd}
I_{1,1} \arrow[dr] & & & \\
& I_{2,1} \arrow[dr] & & \\
I_{1,2} \arrow[ur] \arrow[dr] & & I_{3,1} \arrow[dr] & \\
& I_{2,2} \arrow[ur] \arrow[dr] & & I_{4,1} \\
I_{1,3} \arrow[ur] \arrow[dr] & & I_{3,2} \arrow[ur] & \\
& I_{2,3} \arrow[ur] & & \\
I_{1,4} \arrow[ur] & & &
\end{tikzcd}$$

An advantage of this method is that the accuracy of the computed value is known at each step.

Romberg Integration

We have,

$$I_{j,k} = I_{j-1,k+1} + \frac{I_{j-1,k+1} - I_{j-1,k}}{4^{j-1} - 1}, \quad j \geq 2$$

For j =2, k = 1,

$$I_{2,1} = I_{1,2} + \frac{I_{1,2} - I_{1,1}}{4^{2-1} - 1} = I_{1,2} + \frac{I_{1,2} - I_{1,1}}{3}$$

For j = 3, k = 1,

$$I_{3,1} = I_{2,2} + \frac{I_{2,2} - I_{2,1}}{4^{3-1} - 1} = I_{2,2} + \frac{I_{2,2} - I_{2,1}}{15}$$

Example

Use Romberg method to compute the following integral correct to three decimal places.

$$I = \int_0^1 \frac{1}{1+x}\,dx,$$

Use 2, 4 and 8-segment Trapezoidal rule results.

Example: Solution

Here, we have to calculate I using $2 = 2^1$, $4 = 2^2$ and $8 = 2^3$ intervals. Therefore,

- $I_{1,1} = T_1$, that is calculate I using Trapezoidal rule with $2^1 = 2$ intervals.

- $I_{1,2} = T_2$, that is calculate I using Trapezoidal rule with $2^2 = 4$ intervals.

- $I_{1,3} = T_3$, that is calculate I using Trapezoidal rule with $2^3 = 8$ intervals.

With this notation the following table can be formed.

$$
\begin{tikzcd}
I_{1,1} \arrow[dr] & & \\
& I_{2,1} \arrow[dr] & \\
I_{1,2} \arrow[ur] \arrow[dr] & & I_{3,1} \\
& I_{2,2} \arrow[ur] & \\
I_{1,3} \arrow[ur] & &
\end{tikzcd}
$$

Example: Solution

Using Trapezoidal Rule, we get [Class Work]

$$I_{1,1} = 0.7084, \quad I_{1,2} = 0.6970, \quad I_{1,3} = 0.6941$$

Now,

$$I_{j,k} = I_{j-1,k+1} + \frac{I_{j-1,k+1} - I_{j-1,k}}{4^{j-1} - 1}, \quad j \geq 2$$

$$I_{2,1} = I_{1,2} + \frac{I_{1,2} - I_{1,1}}{4^{2-1} - 1} = I_{1,2} + \frac{I_{1,2} - I_{1,1}}{3} = 0.6970 + \frac{1}{3}(0.6970 - 0.7084) = 0.6932$$

$$I_{2,2} = I_{1,3} + \frac{I_{1,3} - I_{1,2}}{4^{2-1} - 1} = I_{1,3} + \frac{I_{1,3} - I_{1,2}}{3} = 0.6941 + \frac{1}{3}(0.6941 - 0.6970) = 0.6931$$

$$I_{3,1} = I_{2,2} + \frac{I_{2,2} - I_{2,1}}{4^{3-1} - 1} = I_{2,2} + \frac{I_{2,2} - I_{2,1}}{15} = 0.6931 + \frac{1}{15}(0.6931 - 0.6932) = 0.6931$$

Solution (Cont.)

The table of values is therefore

0.7084		
	0.6932	
0.6970		0.6931
	0.6931	
0.6941		

Therefore, $I = 0.6931$

Home Work

Compute the values of

$$I = \int_0^1 \frac{1}{1+x^2}\,dx,$$

by using the trapezoidal rule with h=0.5, 0.25 and 0.125. Then obtain a better estimate by using Romberg's method.