6

Numerical Differentiation and Numerical Integration

In this chapter we shall be concerned with the problems of numerical differentiation and integration. We shall derive the formula to compute the following when only tabulated values of the function are known but the explicitly nature of the function is not known. Such scenario occurs in engineering in case of experimental data:

- $\frac{dy}{dx}$, $\frac{d^2y}{dx^2}$, ... for any value of x in $[x_0, x_n]$, and
- $\int_{x_0}^{x_n} y\,dx$

6.1 Numerical Differentiation

The general method for deriving the numerical differentiation formulae is to differentiate the interpolating polynomial. Hence, corresponding to each of the Interpolating formula derived, we may derive a formula for the derivative.

6.1.1 Newton's forward difference formulae

The Newton's forward difference formula is:

$$\begin{aligned} y_n(x) = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + ... \\ + \frac{u(u-1)(u-2)...(u-(n-1))}{n!}\Delta^n y_0 \end{aligned} \tag{6.1}$$

where, $x = x_0 + uh$ and $h = x_{i+1} - x_i$. Differentiating 6.1 with respect to x,

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + ...\right] \tag{6.2}$$

Differentiating 6.2 with respect to x, we get,

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + \frac{6u-6}{6}\Delta^3 y_0 + \frac{12u^2-36u+22}{24}\Delta^4 y_0 + ...\right] \tag{6.3}$$

These formulae are used for *non-tabular* values of x. For tabular values of x, the formulae take simpler form. For $x = x_0$, we have $u = 0$, and using this we can find the relations of $\left[\frac{dy}{dx}\right]_{x=x_0}$ *and* $\left[\frac{d^2y}{dx^2}\right]_{x=x_0}$ which is in a simpler form.

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\Delta\, y_n - \frac{1}{2}\Delta^2\, y_n + \frac{1}{3}\Delta^3\, y_n - ...\right] \tag{6.4}$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\Delta^2\, y_n - \Delta^3\, y_n + \frac{11}{12}\Delta^4\, y_n - \frac{5}{6}\Delta^5\, y_n + ...\right] \tag{6.5}$$

6.1.2 Newton's backward difference formula

In a similar way, different formulae can be derived by starting with other interpolation formulae. Thus, Newton's backward difference formula gives

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla\, y_n + \frac{1}{2}\nabla^2\, y_n + \frac{1}{3}\nabla^3\, y_n + ...\right] \tag{6.6}$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2\, y_n + \nabla^3\, y_n + \frac{11}{12}\nabla^4\, y_n + \frac{5}{6}\nabla^5\, y_n + ...\right] \tag{6.7}$$

Remark. If the x-values of the data points are equally spaced then it is common to use Newton's interpolation.

6.1.3 Exercise

Find the dy/dx and d^2y/dx^2 at $x = 1.2,\ x = 1.6,\ x = 2.2$ from the data:
$(1, 2.7183),\ (1.2, 3.3201),\ (1.4, 4.0522),\ (1.6, 4.9530),\ (1.8, 6.0496),\ (2.0, 7.3891),\ (2.2, 9.0250).$

6.2 Numerical Integration

The general problem of numerical integration may be stated as: Given a set of data points of a function $y = f(x)$, where $f(x)$ is not known explicitly, it is required compute the value of the definite integral

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

As with the case of numerical differentiation, one replaces $f(x)$ by an interpolating polynomial $\phi(x)$ and obtains, on integration, an approximate value of the definite integral. Thus, different integration formulae can be obtained depending upon the type of the interpolation formula used. Approximating y by Newton's forward difference formula, we obtained

$$I = \int_{x_0}^{x_n} \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\,\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\,\Delta^3 y_0 + ...\right] dx$$

Since $x = x_0 + ph$, $dx = hdp$. When $x = x_0$, $p = 0$ and $x = x_n$, $p = n$. Then,

$$I = \int_0^n \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2}\,\Delta^2 y_0 + \frac{p(p-1)(p-2)}{6}\,\Delta^3 y_0 + ...\right] h\, dp$$

Integrating we get,

$$I = h\left[py_0 + \frac{p^2}{2}\,\Delta y_0 + \left(\frac{p^3}{3} - \frac{p^2}{2}\right)\frac{\Delta^2 y_0}{2} + \left(\frac{p^4}{4} - p^3 + p^2\right)\frac{\Delta^3\, y_0}{6} + ...\right]_0^n$$
$$= nh\left[y_0 + \frac{n}{2}\,\Delta y_0 + \left(\frac{2n^2 - 3n}{12}\right)\Delta^2\, y_0 + \left(\frac{n^3 - 4n^2 + 4n}{24}\right)\Delta^3\, y_0 + ...\right] \tag{6.8}$$

This relation 6.8 is considered to be a general formula in the variable n. For a particular value of n we get a particular formula. For example for $n = 1$ we get the famous Trapezoidal rule and for $n = 2$ and $n = 3$ we get Simpson's 1/3 rule and Simpson's 3/8 rule respectively.

6.2.1 Trapezoidal Rule

Setting $n = 1$ in the general formula 6.8, all differences higher than the first order will become zero and we obtained
$\displaystyle\int_{x_0}^{x_1} y\,dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}\,(y_0 + y_1)$. Similarly we can obtain

$\int_{x_1}^{x_2} y\,dx, ...\int_{x_{n-1}}^{n} y\,dx$. Then we have,

$$\int_{x_0}^{x_n} y\,dx = \int_{x_0}^{x_1} y\,dx + \int_{x_1}^{x_2} y\,dx + ... + \int_{x_{n-1}}^{x_n} y\,dx$$
$$= \frac{h}{2}\,(y_0 + y_1) + \frac{h}{2}\,(y_1 + y_2) + ... + \frac{h}{2}\,(y_{n-1} + y_n)$$
$$= \frac{h}{2}\,\{y_0 + 2(y_1 + y_2 + ... + y_{n-1}) + y_n\} \tag{6.9}$$

Question: Illustrate the trapezoidal method geometrically.

6.2.2 Simpson's 1/3-Rule

Setting $n = 2$ in the general formula 6.8, all differences higher than the second will become zero and we obtained
$\displaystyle\int_{x_0}^{x_2} y\,dx = 2h\left[y_0 + \Delta\, y_0 + \frac{1}{6}\Delta^2\, y_0\right] = \frac{h}{3}\,(y_0 + 4y_1 + y_2)$. Similarly we can obtain

$\int_{x_2}^{x_4} y\,dx, ...\int_{x_{n-2}}^{n} y\,dx$. Then we have,

$$\int_{x_0}^{x_n} y\,dx = \int_{x_0}^{x_2} y\,dx + \int_{x_2}^{x_4} y\,dx + ... + \int_{x_{n-2}}^{x_n} y\,dx$$
$$= \frac{h}{3}\,(y_0 + 4y_1 + y_2) + \frac{h}{3}\,(y_2 + 4y_3 + y_4) + ... + \frac{h}{3}\,(y_{n-2} + 4y_{n-1} + y_n)$$
$$= \frac{h}{3}\,\{y_0 + 4(y_1 + y_3 + ... + y_{n-1}) + 2(y_2 + y_4 ... + y_{n-2}) + y_n\} \tag{6.10}$$

Remark. It should be noted that this rule requires the division of the whole range into an even number of sub-intervals of width h.

6.2.3 Simpson's 3/8-Rule

Setting $n = 3$ in the general formula 6.8, all differences higher than the third will become zero and we obtained

$$\int_{x_0}^{x_3} y\,dx = 3h\left[y_0 + \frac{3}{2}\Delta\, y_0 + \frac{3}{4}\Delta^2\, y_0 + \frac{1}{8}\Delta^3\, y_0\right] = \frac{3h}{8}\,(y_0 + 3y_1 + 3y_2 + y_3).$$

Similarly we can obtain

$\int_{x_3}^{x_6} y\,dx, ... \int_{x_{n-3}}^{n} y\,dx$. Then we have,

$$\begin{aligned}\int_{x_0}^{x_n} y\,dx &= \int_{x_0}^{x_3} y\,dx + \int_{x_3}^{x_6} y\,dx + ... + \int_{x_{n-3}}^{x_n} y\,dx \\ &= \frac{3h}{8}\,(y_0 + 3y_1 + 3y_2 + y_3) + \frac{3h}{8}\,(y_3 + 3y_4 + 3y_5 + y_6) + ... + \frac{3h}{8}\,(y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n) \\ &= \frac{3h}{8}\,\{y_0 + 3(y_1 + y_2 + y_4 + y_5 + ... + y_{n-1}) + 2(y_3 + y_6 ... + y_{n-3}) + y_n\}\end{aligned} \tag{6.11}$$

6.2.4 Exercise

1. For the given (x, y) data points: Evaluate $\int_0^2 ydx$ using the trapezoidal rule. $(0.0, 0.399)$, $(0.5, 0.352)$, $(1.0, 0.242)$, $(1.5, 0.129)$, $(2.0, 0.054)$.

2. Evaluate using Simpson's 1/3 rule:

   (a) $\displaystyle\int_1^3 \frac{1}{x}\,dx$ with 8 stripes.

   (b) $\displaystyle\int_0^{\pi/2} \sqrt{sinx}\,dx$ with $h = \pi/12$.

   (c) $\displaystyle\int_3^7 x^2 logx\,dx$ with $h = 1$.

   (d) $\displaystyle\int_0^1 e^{-x^2}\,dx$ with $h = 0.1$

3. Evaluate using Simpson's 3/8 rule: $\displaystyle\int_0^1 \frac{dx}{1+x}$ with $h = 1/6$.

4. Compute the values of $I = \displaystyle\int_0^1 \frac{dx}{1+x^2}$ using the trapezoidal rule with $h = 0.5,\ 0.25,\ 0.125$. Then obtain a better estimate using **Romberg's method**.

5. Compute $I\left(\frac{\pi}{4}\right),\ I\left(\frac{\pi}{8}\right),\ I\left(\frac{\pi}{8}, \frac{\pi}{4}\right)$ for : $I = \displaystyle\int_0^{\pi/4} cos^2 x\,dx.$

6. Using Trapezoidal rule and Simpson's 1/3 rule evaluate the double integral

$$\int_2^2 \int_0^4 (x^2 - xy + y^2)\,dx\,dy.$$

6.2.5 Boole's and Weddle's Rules, *Extra material*

To incorporate the fourth order difference as well we need 5 data points $x_0, ..., x_4$ and we need to integrate from x_0 to x_4. Then we obtain Boole's formula:

$$\int_{x_0}^{x_4} y\,dx = \frac{2h}{45}\left(7y_0 + 32y_1 + 12y_2 + 32y_3 + 7y_4\right) \tag{6.12}$$

If we incorporate differences u to six order then we obtain Weddle's formula as follows:

$$\int_{x_0}^{x_6} y\,dx = \frac{3h}{10}\left(y_0 + 5y_1 + y_2 + 6y_3 + y_4 + 5y_5 + y_6\right) \tag{6.13}$$

6.2.6 Romberg Integration

This method improves the approximation obtained from the other methods. Here we describe the Romberge method to improve the results obtained from the Trapezoidal method.

Suppose the integral $\displaystyle\int_a^b y\,dx$ is evaluated by the Trapezoidal rule with two different subintervals of widths h_1 and h_2, to obtain the approximate values I_1 and I_2, respectively. Romberg's method uses this two approximations: I_1 and I_2 to obtain the next better approximations which is given by

$$I_3 = \frac{I_1 h_2^2 - I_2 h_1^2}{h_2^2 - h_1^2} \tag{6.14}$$

6.2.7 Gaussian Quadrature

The methods in the previous sections are based upon the values of function a equally-spaced points of the interval. Gauss derived a formula for which the points in the interval **need not be equally spaced**. The Gaussian formula is expressed as:

$$\int_{-1}^{1} F(u)\,du = \sum_{i=1}^{n} W_i\,F(u_i) \tag{6.15}$$

where W_i and u_i are called the *weights* and *abscissae*, respectively. It can be shown that the u_i are the zeros of the $(n+1)^{th}$ **Legendre** polynomial $P_{n+1}(u)$ which can be generated usingthe recurrence relation:

$$(n+1)\,P_{n+1}(u) = (2n+1)\,u\,P_n(u) - n\,P_{n-1}(u)$$

where $P_0(u) = 1$ and $P_1(u) = u$. It can also be shown that corresponding weights W_i are given by

$$W_i = \int_{-1}^{1} \prod_{j=0, j\neq i}^{n} \frac{u - u_j}{u_i - u_j}\,du$$

However the weights and the abscissae are extensively tabulated for different values of n. We list the weights and the abscissae for values of n up to $n = 6$.

Change of Limits In the general case, the limits of the integral have to be changed to that of 6.15 by means of the following variable transformation:

$$x = \frac{1}{2}\,u(b-a) + \frac{1}{2}\,(a+b)$$

Table 5.1 Abscissae and Weights for Gaussian Integration

n	$\pm u_i$	W_i
2	0.57735 02692	1.0
3	0.0	0.88888 88889
	0.77459 66692	0.55555 55556
4	0.33998 10436	0.65214 51549
	0.86113 63116	0.34785 48451
5	0.0	0.56888 88889
	0.53846 93101	0.47862 86705
	0.90617 98459	0.23692 68851
6	0.23861 91861	0.46791 39346
	0.66120 93865	0.36076 15730
	0.93246 95142	0.17132 44924

6.2.8 Exercise

1. Derive the Gauss quadrature formula for $n = 2$ and apply it to evaluate the integral $\displaystyle\int_{-1}^{1} \frac{dx}{1+x^2}$.

2. Use the three point Gauss formula to evaluate the integral $\displaystyle\int_{0}^{1} \frac{dx}{1+x}$.

6.3 Double Integration

Formulae for the evaluation of double integral can be obtained by repeatedly applying the trapezoidal and Simpson's rules derived earlier.

6.3.1 Trapezoidal Rule

$$I = \int_{y_j}^{y_{j+1}} \int_{x_i}^{x_{i+1}} f(x, y)\, dx\, dy$$

where, $x_{i+1} = x_i + h$ and $y_{j+1} = y_j + k$. By repeated application of trapezoidal rule to we get,

$$\begin{aligned}
I &= \frac{h}{2} \int_{y_j}^{y_{j+1}} [f(x_i, y) + f(x_{i+1}, y)]\, dx\, dy \\
&= \frac{hk}{4} [f(x_i, y_j) + f(x_{i+1}, y_j) + f(x_i, y_{j+1}) + f(x_{i+1}, y_{j+1})]\, dx\, dy \qquad (6.16) \\
&= \frac{hk}{4} [f_{i,j} + f_{i+1,j} + f_{i,j+1} + f_{i+1,j+1}]\, dx\, dy
\end{aligned}$$

6.3.2 Simpson's Rule

$$I = \int_{y_{j-1}}^{y_{j+1}} \int_{x_{i-1}}^{x_{i+1}} f(x, y)\, dx\, dy$$

where, $x_{i+1} = x_i + h$ and $y_{j+1} = y_j + k$. By repeated application of Simpson's rule to we get,

$$I = \frac{h}{3}\int_{y_{j-1}}^{y_{j+1}} \left[f(x_{i-1}, y) + 4f(x_i, y) + f(x_{i+1}, y)\right] dx\, dy$$

$$= \frac{hk}{9}\left[f(x_{i-1}, y_{j-1}) + 4f(x_{i-1}, y_j) + f(x_{i-1}, y_{j+1})\right.$$

$$\left.4\{f(x_i, y_{j-1}) + 4f(x_i, y_j) + f(x_i, y_{j+1})\} + f(x_{i+1}, y_{j-1}) + 4f(x_{i+1}, y_j) + f(x_{i+1}, y_{j+1})\right] \tag{6.17}$$

Numerical double integration

Evaluate:
$I = \int_a^b \int_c^d f(x, y) dxdy = \int_0^2 \int_0^1 e^{x+y} dxdy$

Given: $a = 0, b = 2, c = 0, d = 1$, $f(x, y) = e^{x+y}$. **Let us choose** $n = 4$ **such that** $h = \frac{b-a}{n} = \frac{2-0}{4} = 0.5$ **and** $k = \frac{d-c}{n} = \frac{1-0}{4} = 0.25$ **The corresponding functional value table is:**

x

f(x,y)	0	0.5	1	1.5	2
0	1.0000	1.6487	2.7183	4.4817	7.3891
0.25	1.2840	2.1170	3.4903	5.7546	9.4877
0.5	1.6487	2.7183	4.4817	7.3891	12.1825
0.75	2.1170	3.4903	5.7546	9.4877	15.6426
1	2.7183	4.4817	7.3891	12.1825	20.0855

y

Now, the solution is
$I = \int_0^2 \int_0^1 e^{x+y} dxdy = \frac{h}{2}\frac{k}{2}$**[sum of all multiples of corresponding elements of functional value table and multiplication table]**

Multiplication table (Trapezoidal rule):

x

×	1	2	2	2	1
1	1	2	2	2	1
2	2	4	4	4	2
2	2	4	4	4	2
2	2	4	4	4	2
1	1	2	2	2	1

y

$\therefore I = \left(\frac{0.5}{2}\right)\left(\frac{0.25}{2}\right)[1 \times 1 + 1.6487 \times 2 + 2.7183 \times 2 + \cdots + 20.0855 \times 1] = 11.2643$

Multiplication table (Simpson's rule):

x

×	1	4	2	4	1
1	1	4	2	4	1
4	4	16	8	16	4
2	2	8	4	8	2
4	4	16	8	16	4
1	1	4	2	4	1

y

$\therefore I = \left(\frac{0.5}{3}\right)\left(\frac{0.25}{3}\right)[1 \times 1 + 1.6487 \times 4 + 2.7183 \times 2 + \cdots + 20.0855 \times 1] = 10.9821$

Exercise: Evaluate
$\int_{-2}^{2} \int_0^4 (x^2 - xy + y^2) dxdy$

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