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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:

- $\frac{dy}{dx}, \frac{d^2y}{dx^2}, \ldots$ 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:

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

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

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

Differentiating 6.2 with respect to x, we get,

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

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.

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

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

and

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

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,

$$\begin{aligned} I &= h\left[py_0 + \frac{p^2}{2}\Delta y_0 + \left(\frac{p^3}{3} - \frac{p^2}{2}\right)\frac{\Delta^2 y_0}{2} + \left(\frac{p^4}{4} - p^3 + p^2\right)\frac{\Delta^3 y_0}{6} + ...\right]_0^n \\ &= nh\left[y_0 + \frac{n}{2}\Delta y_0 + \left(\frac{2n^2 - 3n}{12}\right)\Delta^2 y_0 + \left(\frac{n^3 - 4n^2 + 4n}{24}\right)\Delta^3 y_0 + ...\right] \end{aligned} \tag{6.6}$$

This relation 6.6 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 6.6, all differences higher than the first will become zero and we obtained
$\int_{x_0}^{x_1} y\,dx = h\left[y_0 + \frac{1}{2}\Delta y_0\right] = h\left[y_0 + \frac{1}{2}(y_1 - y_0)\right] = \frac{h}{2}\,(y_0 + y_1)$. Similarly we can obtain

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

$$\begin{aligned}
\int_{x_0}^{x_n} y\,dx &= \int_{x_0}^{x_1} y\,dx + \int_{x_1}^{x_2} y\,dx + ... + \int_{x_{n-1}}^{x_n} y\,dx \\
&= \frac{h}{2}\,(y_0 + y_1) + \frac{h}{2}\,(y_1 + y_2) + ... + \frac{h}{2}\,(y_{n-1} + y_n) \\
&= \frac{h}{2}\,\{y_0 + 2(y_1 + y_2 + ... + y_{n-1}) + y_n\} \qquad (6.7)
\end{aligned}$$

6.2.2 Simpson's 1/3-Rule

Setting $n = 2$ in the general formula 6.6, all differences higher than the second will become zero and we obtained
$\int_{x_0}^{x_2} y\,dx = 2h\left[y_0 + \Delta\,y_0 + \frac{1}{6}\Delta^2\,y_0\right] = \frac{h}{3}\,(y_0 + 4y_1 + y_2)$. Similarly we can obtain

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

$$\begin{aligned}
\int_{x_0}^{x_n} y\,dx &= \int_{x_0}^{x_2} y\,dx + \int_{x_2}^{x_4} y\,dx + ... + \int_{x_{n-2}}^{x_n} y\,dx \\
&= \frac{h}{3}\,(y_0 + 4y_1 + y_2) + \frac{h}{3}\,(y_2 + 4y_3 + y_4) + ... + \frac{h}{3}\,(y_{n-2} + 4y_{n-1} + y_n) \\
&= \frac{h}{3}\,\{y_0 + 4(y_1 + y_3 + ... + y_{n-1}) + 2(y_2 + y_4 ... + y_{n-2}) + y_n\} \qquad (6.8)
\end{aligned}$$

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 6.6, 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,

$$\int_{x_0}^{x_n} y\,dx = \int_{x_0}^{x_3} y\,dx + \int_{x_3}^{x_6} y\,dx + ... + \int_{x_{n-3}}^{x_n} y\,dx$$
$$= \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3) + \frac{3h}{8}(y_3 + 3y_4 + 3y_5 + y_6) + ... + \frac{3h}{8}(y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n)$$
$$= \frac{3h}{8}\{y_0 + 3(y_1 + y_2 + y_4 + y_5 + ... + y_{n-1}) + 2(y_3 + y_6... + y_{n-3}) + y_n\} \tag{6.9}$$

6.2.4 Exercise

1. Find, from the data, the area bounded by the curve and the x-axis:
   $(7.47, 1.93),\ (7.48, 1.95),\ (7.49, 1.98),\ (7.50, 2.01),\ (7.51, 2.03),\ (7.52, 2.06)$
2. Find the volume of solid of revolution formed by rotating about the x-axis the area between the x-axis, the line $x = 0$ and $x = 1$, and a curve through the points:
   $(0, 1),\ (0.25, 0.9896),\ (0.5, 0.9589),\ (0.75, 0.9089),\ (1, 0.8415).4$
3. Integrate $I = \displaystyle\int_0^{1.5} \frac{e^x + x}{sinx + 1}\,dx$.
4. Evaluate: $I = \displaystyle\int_0^1 \frac{1}{1+x}\,dx$ using $h = 0.125$.

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,

$$I = \frac{h}{2}\int_{y_j}^{y_{j+1}} [f(x_i, y) + f(x_{i+1}, y)]\,dx\,dy$$
$$= \frac{hk}{4}[f(x_i, y_j) + f(x_{i+1}, y_j) + f(x_i, y_{j+1}) + f(x_{i+1}, y_{j+1})]\,dx\,dy \tag{6.10}$$
$$= \frac{hk}{4}[f_{i,j} + f_{i+1,j} + f_{i,j+1} + f_{i+1,j+1}]\,dx\,dy$$

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,

$$I = \frac{h}{3}\int_{y_{j-1}}^{y_{j+1}} [f(x_{i-1}, y) + 4f(x_i, y) + f(x_{i+1}, y)]\, dx\, dy$$
$$= \frac{hk}{9}[f(x_{i-1}, y_{j-1}) + 4f(x_{i-1}, y_j) + f(x_{i-1}, y_{j+1})$$
$$4\{f(x_i, y_{j-1}) + 4f(x_i, y_j) + f(x_i, y_{j+1})\} + f(x_{i+1}, y_{j-1}) + 4f(x_{i+1}, y_j) + f(x_{i+1}, y_{j+1})] \tag{6.11}$$

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:**

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

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):

×	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

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

Multiplication table (Simpson's rule):

×	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

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

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

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