DIFFERENTIATION

NUMERICAL DIFFERENTIATION

- When we have to differentiate a function given by a set of tabulated values or when a complicated function is involved, numerical differentiation is used.
- The principle behind numerical differentiation is "*we find a suitable interpolation polynomial passing through the given data points and then the polynomial is differentiated analytically as required*".

DERIVATIVES FOR EQUALLY SPACED DATA

- 1. Newton Forward Differentiation

Let (x_i, y_i), i = 0, 1, 2, …. n be the given data points and $x_i = x_0 + ih$.

Assume $p = \frac{x - x_0}{h}$.

Then Newton forward interpolation formula is:

$$y_x = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots$$

Differentiating this polynomial, we get

Newton's Forward Differentiation Formulae

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-6p+2}{6}\Delta^3 y_0 + \frac{4p^3-18p^2+22p-6}{24}\Delta^4 y_0 + \frac{5p^4-40p^3+105p^2-100p+24}{120}\Delta^5 y_0 + \cdots\right]$$

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \frac{6p^2-18p+11}{12}\Delta^4 y_0 + \frac{2p^3-12p^2+21p-10}{12}\Delta^5 y_0 + \cdots\right]$$

Differentiating

In particular at $x = x_0$, we have p = 0.

Then we have

$$\left.\frac{dy}{dx}\right|_{x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0 - \cdots\right]$$

$$\left.\frac{d^2y}{dx^2}\right|_{x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \cdots\right]$$

Newton's Backward Differentiation Formulae

$$\frac{dy}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{(2p+1)}{2}\nabla^2 y_n + \frac{(3p^2+6p+2)}{6}\nabla^3 y_n + \frac{(4p^3+18p^2+22p+6)}{6}\nabla^4 y_n + \cdots\right]$$

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\nabla^2 y_n + (p+1)\nabla^3 y_n + \frac{6p^2+18p+11}{12}\nabla^4 y_n + \cdots\right]$$

Particular case

In particular, when x = x_0, we get p = 0.

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

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

Example

Find the first two derivatives at x = 1.1 from the following data:

x:	1	1.2	1.4	1.6	1.8	2.0
y:	0.0000	0.1280	0.5440	1.2960	2.4320	4.0000

Solution

The difference table is:

x	y	Δy	Δ^2y	Δ^3y	Δ^4y
1	0.0				
		0.1280			
1.2	0.1280		0.2880		
		0.4160		0.0480	
1.4	0.5440		0.3360		0
		0.7520		0.0480	
1.6	1.2960		0.3840		0
		1.1360		0.0480	
1.8	2.4320		0.4320		
		1.5680			
2.0	4.0000				

$p = \frac{x - x_0}{h}$ = 0.5 and h = 0.2

Applying Newton's forward differentiation formula

$$\left.\frac{dy}{dx}\right|_{1.1} = 0.630$$

$$\left.\frac{d^2y}{d^2x}\right|_{1.1} = 6.60$$

Example

The following table gives the displacement in metres at different times. Find the velocities and accelerations at t = 1.8 s.

t:	0	0.5	1.0	1.5	2.0
s:	0	8.75	30.00	71.25	140.00

Solution

h = 0.5,

$p = \frac{t - t_n}{h}$ = - 0.4

The difference table is:

t	s	∇s	∇^2s	∇^3s	∇^4s
0	0				
		8.75			
0.5	8.75		12.50		
		21.25		7.50	
1.0	30.00		20.00		0
		41.25		7.50	
1.5	71.25		27.50		
		68.75			
2.0	140.00				

Applying Newton's backward differentiation formula

$$\left.\frac{ds}{dt}\right|_{x=1.8} = 143.2$$

$$\left.\frac{d^2s}{dt^2}\right|_{x=1.8} = 128$$

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UNEQUAL INTERVALS

For unequally spaced data, Lagrange's interpolation formula may be differentiated.

Example

Find the first derivative at x = 2 for the function given by the data

x	1	1.5	2.0	3.0
y	0	0.4057	0.69315	1.09861

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Solution

Lagrange interpolation polynomial is:

$y_x = \frac{(x-1.5)(x-2)(x-3)}{(1-1.5)(1-2)(1-3)}$ x 0 + $\frac{(x-1)(x-2)(x-3)}{(1.5-1)(1.5-2)(1.5-3)}$ x 0.4057

+ $\frac{(x-1)(x-1.5)(x-3)}{(2-1)(2-1.5)(2-3)}$ x 0.69315

+ $\frac{(x-1)(x-1.5)(x-2)}{(3-1)(3-1.5)(3-2)}$ x 1.09861

Differentiating and substituting for x as 2.

$$\left.\frac{dy}{dx}\right|_{x=2} = 0.48815$$

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NUMERICAL INTEGRATION

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PRELIMINARIES

We use numerical integration when the function f(x) may not be integrable in closed form or even in case of closed form integrable functions the integrand may be complicated or the function is known only at a finite number of points.

Basic Idea

The function f(x) is being approximated by a polynomial using interpolation which can be easily integrated.

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Numerical Integration

Geometrically $\int_a^b f(x)dx$ represents the area formed by the curve y = f(x) and x – axis between the ordinates x = a and x = b.

Let the interval [a, b] be subdivided into sub intervals each of length h.

Then $x_i = x_0 + ih$, i = 1, 2, …, n,

$x_0 = a$ and $h = \frac{b-a}{n}$.

Let $y_i = f(x_i)$, i = 1, 2, …, n.

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NEWTON-COTES GENERAL INTEGRATION FORMULA

Integrating the Newton forward interpolation polynomial of degree ≤ n, we get

$$\int_a^b f(x)dx = h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \ldots\right]$$

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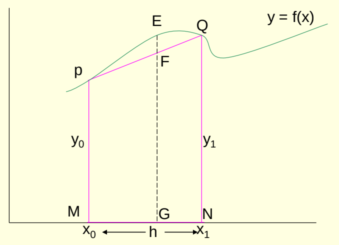
Special Case - I

For n = 1: Trapezoidal Rule



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General Form of Trapezoidal rule

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

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Special Case - II

For n = 2: Simpson's 1/3 Rule

Assume n to be an even integer.

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\,[\,(y_0 + y_n) + 4\,(y_1 + y_3 + \Lambda + y_{n-1}) + 2\,(y_2 + y_4 + \Lambda + y_{n-2})]$$

$$= \frac{h}{3}\,[(\text{sum of end ordinates}) + 4\,(\text{ sum of odd ordinates}) + 2\,(\text{sum of even ordinates})\,]$$

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Special Case - III

For n = 3 : Simpson's 3/8th Rule

Assume n to be a multiple of 3.

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

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Example

Evaluate $\int_1^2 \frac{1}{x}dx$ using

(a) Trapazoidel rule
(b) Simpson's rule and
(c) Simpson's rule and compare the values.
Divide the range into 6 sub intervals.

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Solution

x	f(x)
1	1
$\frac{7}{6}$	0.8571
$\frac{8}{6}$	0.7500
$\frac{9}{6}$	0.6667
$\frac{10}{6}$	0.6000
$\frac{11}{6}$	0.5455
2	0.5000

Trapezoidal rule

$$\int_{x_0}^{x_n} f(x)dx = 0.6949$$

Simpsons 1/3rd rule

$$\int_{x_0}^{x_n} f(x)dx = 0.6932$$

Simpsons 3/8th rule

$$\int_{x_0}^{x_n} f(x)dx = 0.6932$$

Exact Value = 0.6931

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GAUSSIAN QUADRATURE

In Gaussian quadrature sampling points and the weights have been optimized. In Newton-Cotes formulae we choose (n+1) equally spaced points x_i in the interval of integration. These formulae gives exact values if the integrand is a polynomial of degree < n.

Gauss showed that by choosing the (n+1) points suitably, the formula can be made exact when the integrand is a polynomial of degree < (2n+1).

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Using the linear transformation,

$$x = \frac{b-a}{2}t + \frac{a+b}{2}$$

the integral $\int_a^b F(x)dx$ can be transformed into

$$\int_{-1}^{1} f(t)dt.$$

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GAUSSIAN QUADRATURE FORMULA

One Point

$$\int_{-1}^{1} f(t)dt = 2\,f(0)$$

Two Points

$$\int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Three Points

$$\int_{-1}^{1} f(t)dt = \frac{8}{9} f(0) + \frac{5}{9}\left[f\left(-\sqrt{3/5}\right) + f\left(\sqrt{3/5}\right)\right]$$

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Example

Evaluate $\int_0^1 \frac{dx}{1+x}$ by Gaussian quadrature formula with one point, two points and three points.

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Solution

Put $x = \frac{t+1}{2}$, $dx = \frac{1}{2}t$

One point:	0.6667
Two points:	0.6923
Three points:	0.693122
Exact value:	0.693147

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