Chapter 4

Numerical Integration and Differentiation

Fatemeh Baharifard

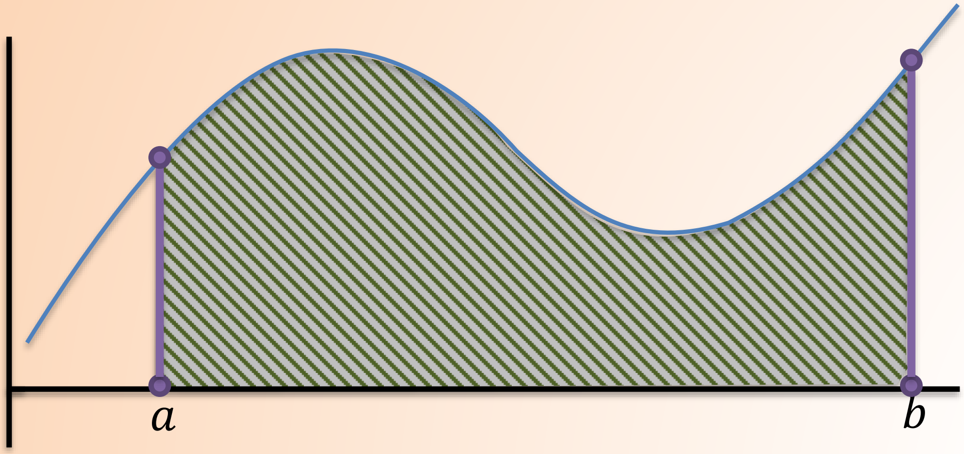
- **Integration**
  - Rectangular Method
  - Midpoint Method
  - Trapezoidal Method
  - Simpson’s Method
    - Simpson 1/3
    - Simpson 3/8
  - Romberg Method
  - Gauss-Legendre Method
- **Differentiation**

Integration

Definition

$$\int_a^b f(x)dx = F(b) - F(a) \quad | \quad F(x) = \int f(x)dx$$

$\int_a^b f(x)dx$ is the area under the curve, bounded between a and b.



Integration

Definition

- Given some points ($x_i s$ and corresponding $f(x_i)$ s), we need to calculate $\int_{x_0}^{x_n} f(x)dx$; interpolation might be one approach.

Or

- Given a function $f(x)$ where it's hard to find its integral, we make a polynomial by finding some x_is and $f(x_i)$s and apply interpolation afterwards.

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Or

- Given a function $f(x)$ where it's hard to find its integral, we make a polynomial by finding some x_is and $f(x_i)$s and apply interpolation afterwards.

But other solutions in such cases are:

NUMERICAL INTEGRATION

Integration | Differentiation

- Integration
  - Rectangular Method
  - Midpoint Method
  - Trapezoidal Method
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    - Simpson 1/3
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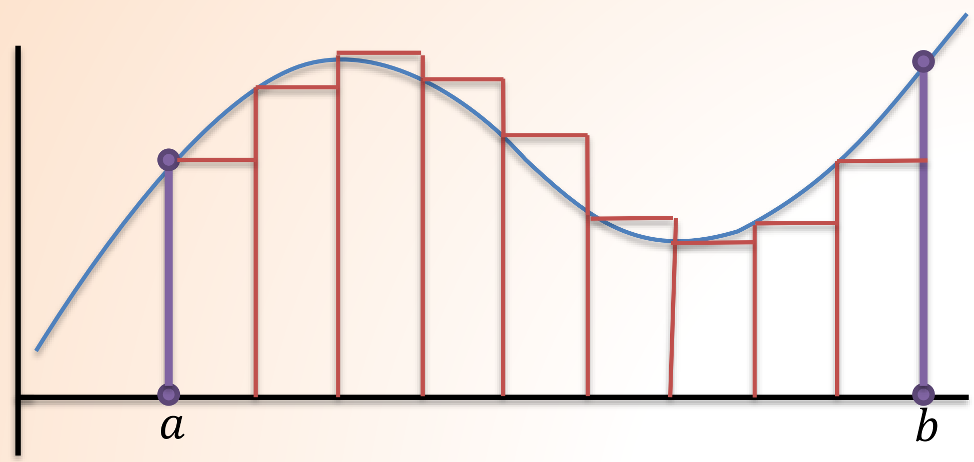
Rectangular Method

We divide the interval $[a,b]$ into n subintervals with equal lengths and find the integral by the summation of the rectangular area.

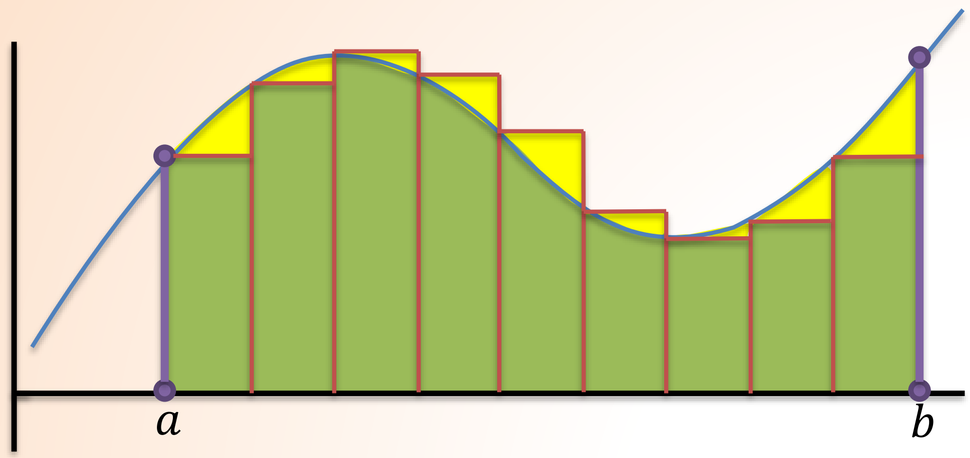
The length of the i^{th} rectangle is $f(x_i)$ and its width is $\boldsymbol{h = \frac{b-a}{n}}$

So we have:



Rectangular Method

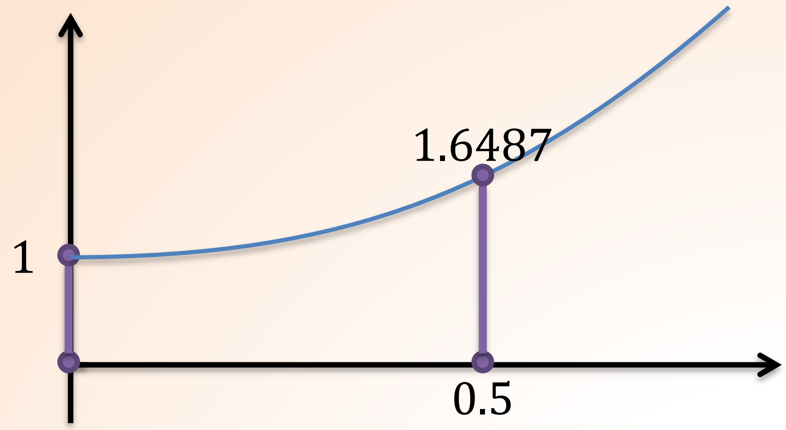
$$\int_a^b f(x)\ dx = h[f_0 + f_1 + f_2 + \cdots + f_{n-2} + f_{n-1}]$$



An Example

Compute the given integral using Rectangular method for $h = 0.5$, $h = 0.25$, $h = 0.1$.

$$\int_0^{0.5} e^x dx$$

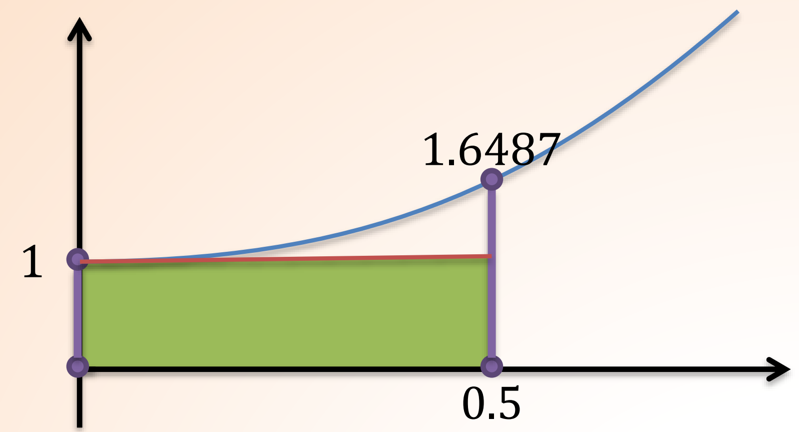


An Example

Compute the given integral using Rectangular method for $\boxed{h = 0.5,}$ $h = 0.25$, $h = 0.1$.

$$\int_0^{0.5} e^x dx$$

x_i	0	1
f_i	1	1.6487



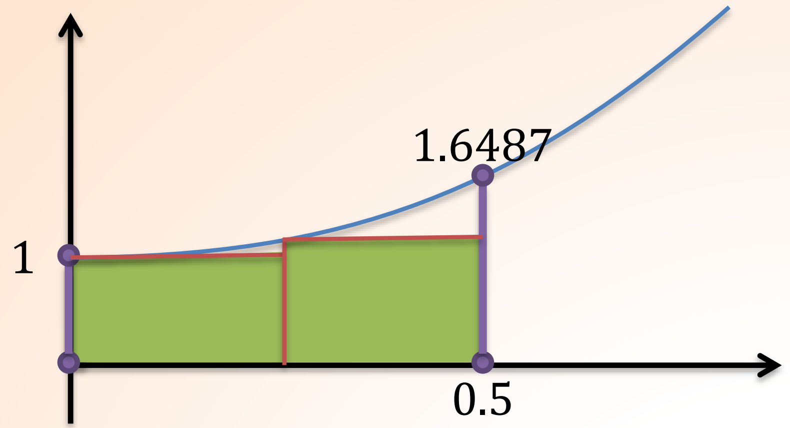
$$\Rightarrow \int_0^{0.5} e^x dx = 0.5 \times 1 = 0.5$$

An Example

Compute the given integral using Rectangular method for $h = 0.5$, $\boxed{h = 0.25}$, $h = 0.1$.

$$\int_0^{0.5} e^x dx$$

x_i	**0**	**0.25**	**0.5**
f_i	1	1.2840	1.6487



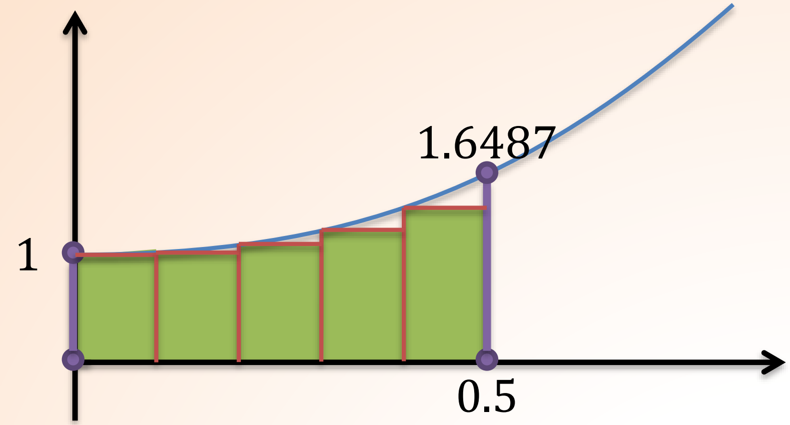
$$\Rightarrow \int_0^{0.5} e^x dx = 0.25(1 + 1.2840) = 0.571$$

An Example

Compute the given integral using rectangular method for $h = 0.5$, $h = 0.25$, $\boxed{h = 0.1}$

$$\int_0^{0.5} e^x dx$$

x_i	$\mathbf{0}$	$\mathbf{0.1}$	$\mathbf{0.2}$	$\mathbf{0.3}$	$\mathbf{0.4}$	$\mathbf{0.5}$
f_i	1	1.1052	1.2214	1.3499	1.4918	1.6487



$$\Rightarrow \int_0^{0.5} e^x dx = 0.1(f_0 + f_1 + f_2 + f_3 + f_4) = 0.61683$$

Rectangular Method

We can reduce the error in calculation by using smaller h. but for very small amounts of h, it leads to huge calculations. As a result, propagation error outweighs the error of the method itself.

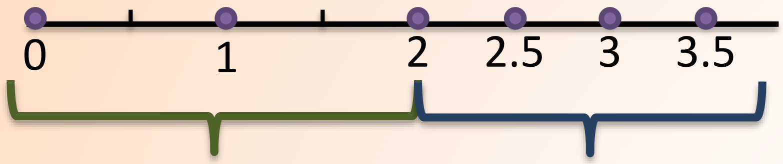
An Example:

h	Answer
1	23.1213179
0.1	21.5709612
0.01	21.5943221
0.001	21.5943776
0.0001	21.5964293

Rectangular Method

This method is very slow and its error is high.

If the space between x_is are different, we can divide the overall interval, then calculate the integral for all intervals, for example:



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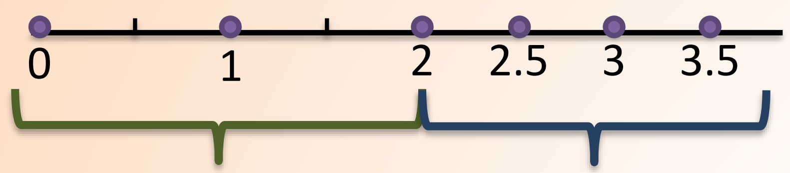

$$\int_0^{3.5} f(x) = \int_0^{2} f(x) + \int_2^{3.5} f(x)$$

Integration | Differentiation

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  - Midpoint Method
  - Trapezoidal Method
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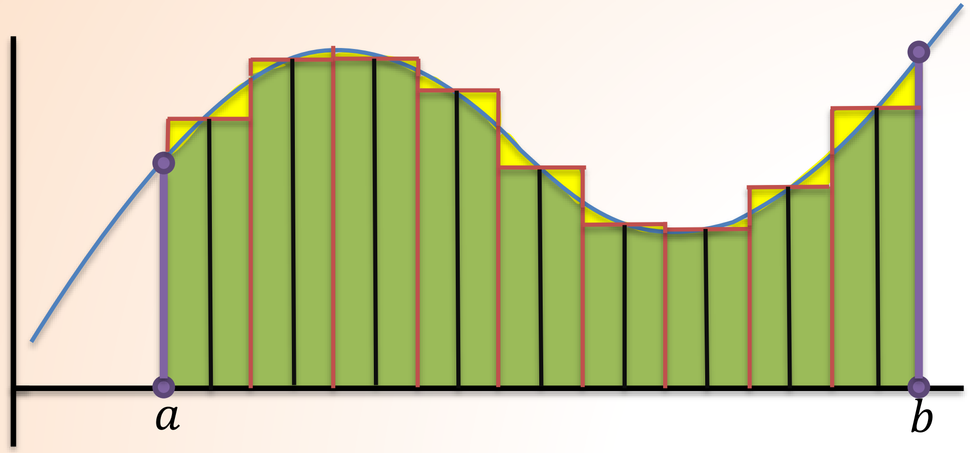
  - Gauss-Legendre Method

Midpoint Method

This method is similar to rectangular method. The only difference is that the midpoints of the intervals indicate the lengths of the rectangles. So:

$$\int_a^b f(x)\ dx = M(h) = h[f(x_0 + \frac{h}{2}) + f(x_1 + \frac{h}{2}) + \cdots + f(x_{n-1} + \frac{h}{2})]$$

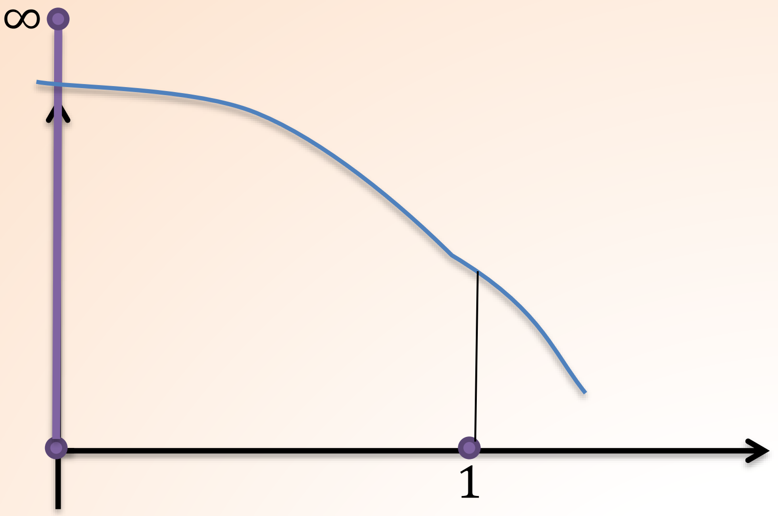


An Example

Compute the given integral using Midpoint method for:

$$h = 0.2$$

$$\int_0^1 \frac{\sin(x)}{x} dx$$



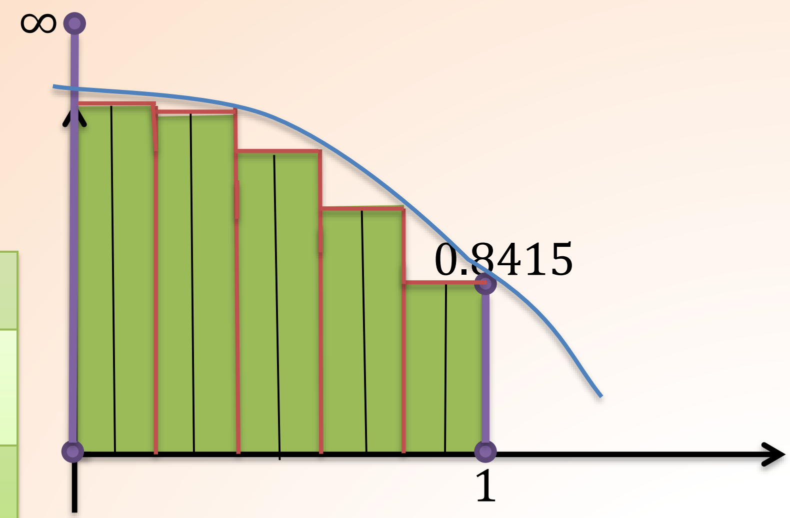
An Example

Compute the given integral using Midpoint method for:

$$h = 0.2$$

$$\int_0^1 \frac{\sin(x)}{x}dx \rightarrow f(x) = \frac{\sin(x)}{x}$$

x_i	0	0.2	0.4	0.6	0.8
$x_i + \frac{h}{2}$	0.1	0.3	0.5	0.7	0.9
$f(x_i + \frac{h}{2})$	0.9983	0.9851	0.9689	0.9203	0.8704



$$\Rightarrow \int_0^1 \frac{\sin(x)}{x}dx = 0.2(f_{0.1} + f_{0.3} + f_{0.5} + f_{0.7} + f_{0.9}) = 0.9466$$

Midpoint Method

The Error is:

$$E[M(h)] = \frac{b-a}{24} h^2 f''(z) \mid z \in [a,b]$$

- This method is used in case the value of $f(x)$ in the start point of interval is unknown, e.g. $\int_0^1 \frac{e^x}{x}$.
- For linear polynomials, this method gives an exact answer.

Integration

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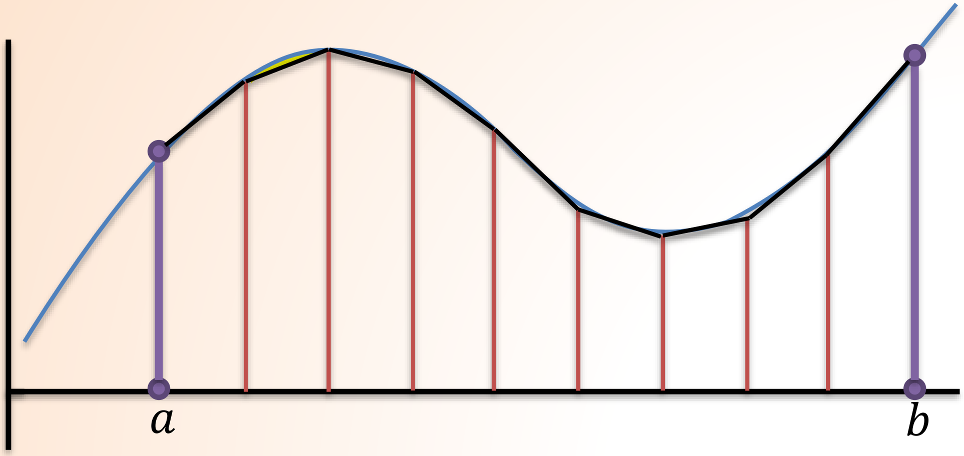
Trapezoidal Method

We divide the interval $[a,b]$ into n subintervals with equal lengths and find the integral by summing the areas of the trapezoids.

So:

$$\int_a^b f(x)\ dx = T(h) = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n]$$



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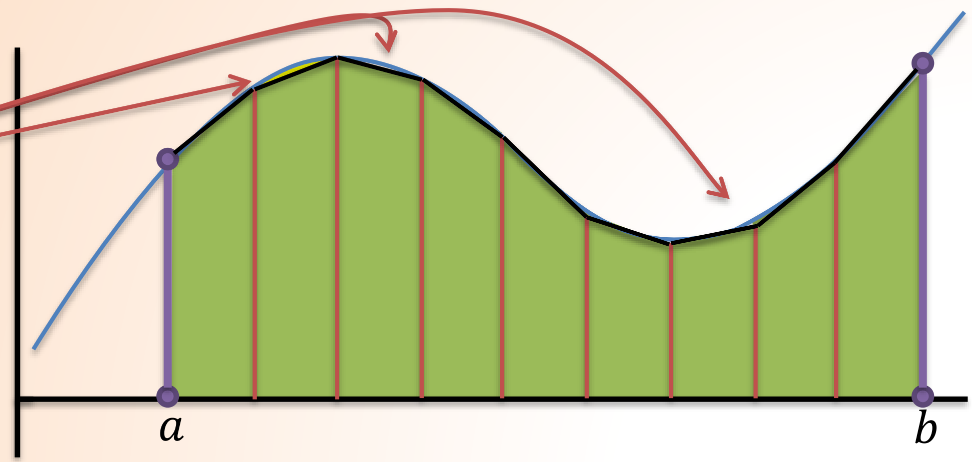
So:

$$\int_a^b f(x)\ dx = T(h) = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n]$$

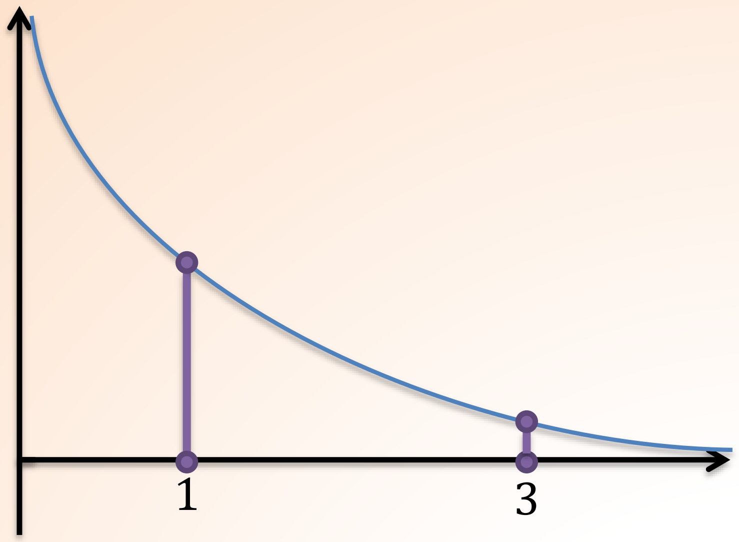
Believe it or not, there still exists errors!



An Example

Compute the given integral using Trapezoidal method for $h = 1, h = 0.5$.

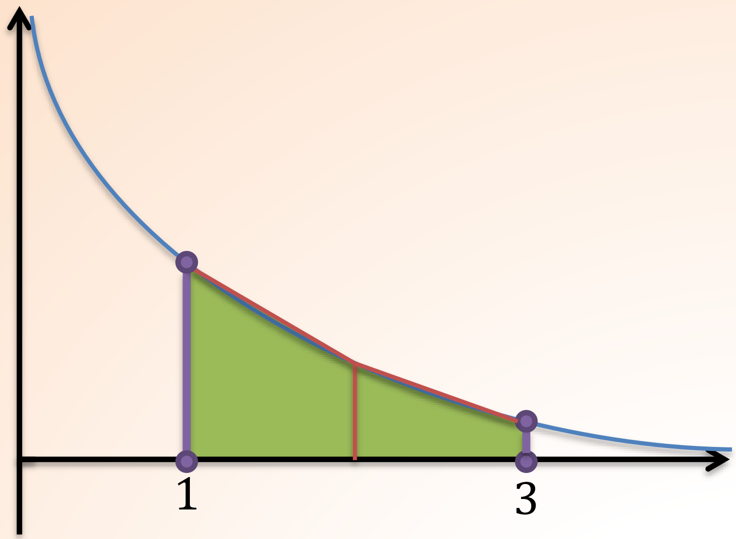
$$\int_1^3 \frac{1}{x^2} dx$$



An Example

Compute the given integral using Trapezoidal method for $\boxed{h = 1,}\ h = 0.5$.

$$\int_1^3 \frac{1}{x^2} dx$$



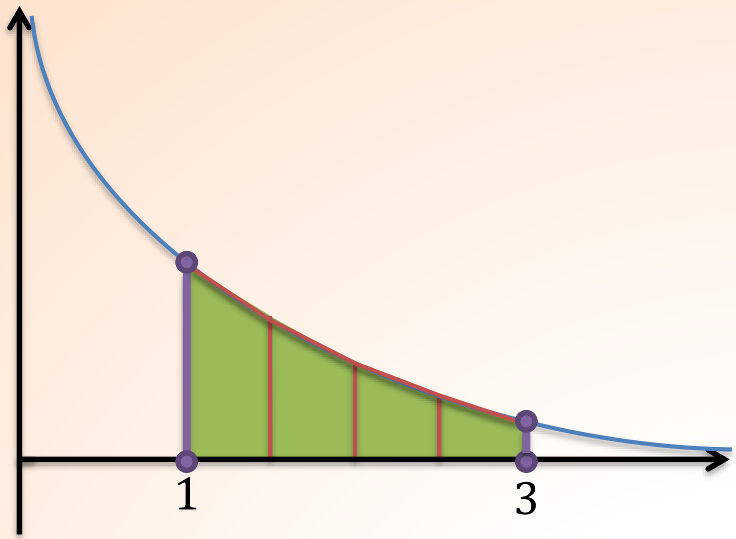
x_i	**1**	**2**	**3**
f_i	1	0.25	0.1111

$$\Rightarrow \int_1^3 \frac{1}{x^2} dx = \frac{1}{2}(f_0 + 2f_1 + f_2) = 0.8056$$

An Example

Compute the given integral using Trapezoidal method for $h = 1$, $\boxed{h = 0.5}$

$$\int_1^3 \frac{1}{x^2} dx$$



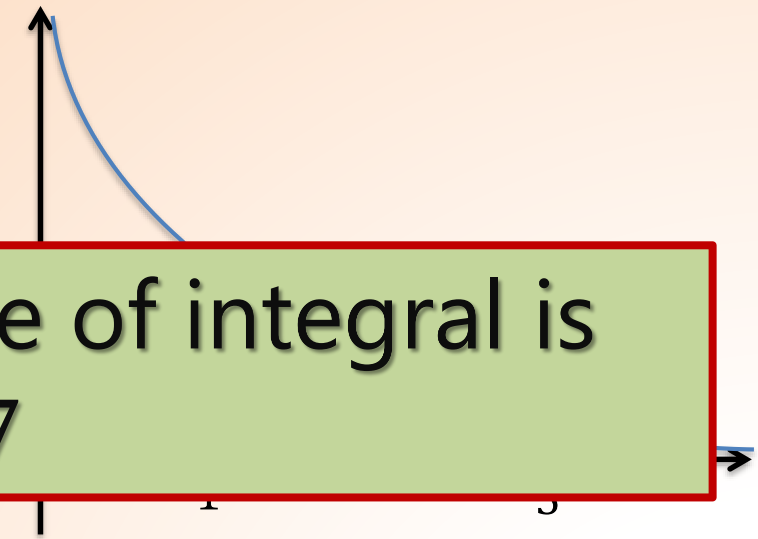
x_i	1	1.5	2	2.5	3
f_i	1	0.4444	0.25	0.16	0.1111

$$\Rightarrow \int_1^3 \frac{1}{x^2} dx = \frac{0.5}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4) = 0.705$$

An Example

Compute the given integral using Trapezoidal method for $h = 1$, $\boxed{h = 0.5}$

$$\int_1^3 \frac{1}{x^2} dx$$



While the actual value of integral is 0.66667

$$\Rightarrow \int_1^3 \frac{1}{x^2} dx = \frac{0.5}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4) = 0.705$$

Trapezoidal Method

The Error is:

$$E[T(h)] = \frac{b-a}{12} h^2 f''(z) \mid z \in [a,b]$$

To make the error less than ε, the following condition is required:

$$h = \sqrt{\frac{12\varepsilon}{(b-a)m_2}}, m_2 = max|f''(x)|, x \in [a,b]$$

The error is proportional to h^2, therefore no error exists for linear $f(x)$s.

An Example

Determine h such that error of computing the following integral using Trapezoidal method becomes less than 10^{-6}.

$$\int_0^7 cosx dx$$

An Example

Determine h such that error of computing the following integral using Trapezoidal method becomes less than 10^{-6}.

$$\int_0^7 cosxdx \Rightarrow f(x) = cosx \Rightarrow f'(x) = -sinx \Rightarrow f''(x) = -cosx$$

Since $-1 \le -cosx \le 1 \Longrightarrow M_2 = 1$

$$h = \sqrt{\frac{12\varepsilon}{(b-a)m_2}} = \sqrt{\frac{12 \times 10^{-6}}{(7-0) \times 1}} = 0.001309$$

$$\Rightarrow n > \frac{7-0}{0.001309} = 5347$$

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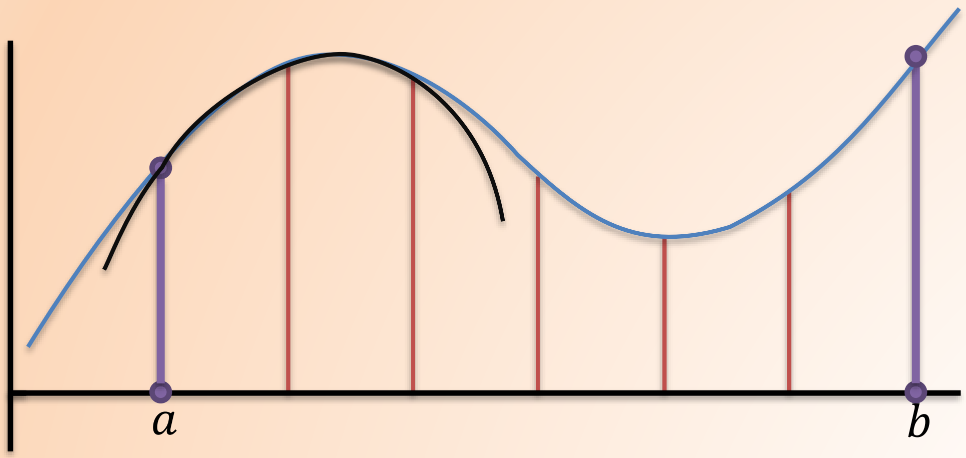
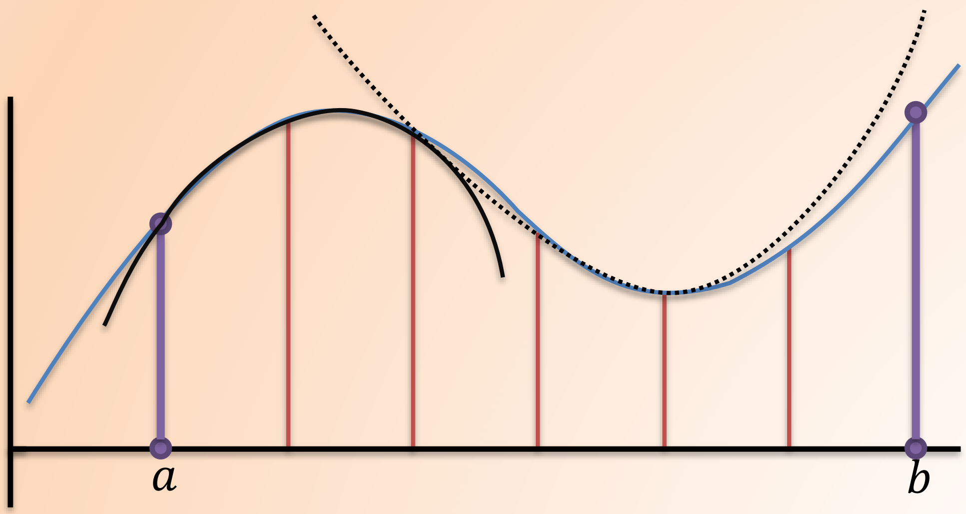
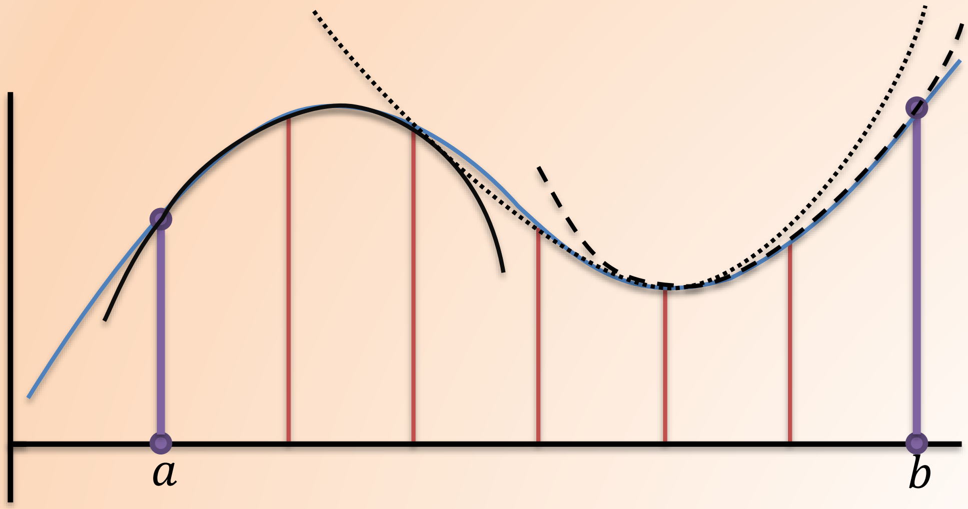
Simpson’s Method



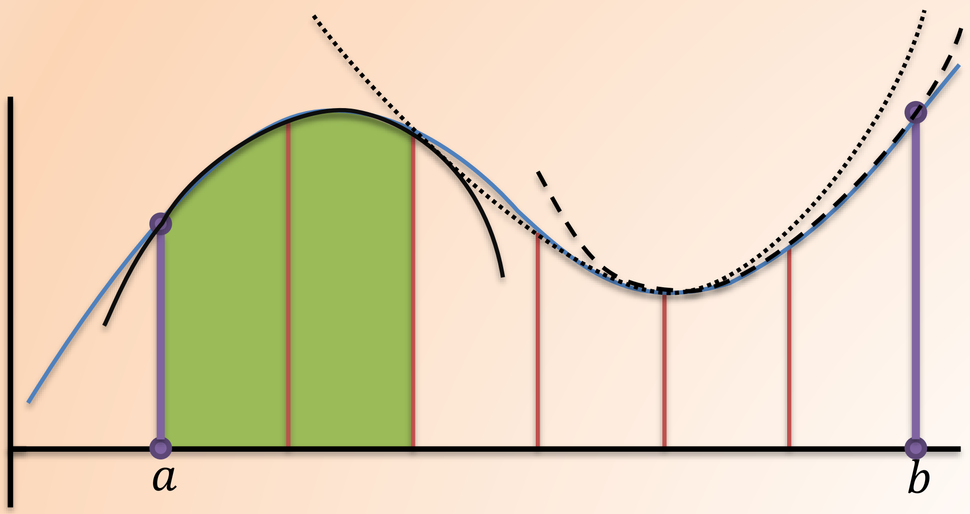
Simpson's Method



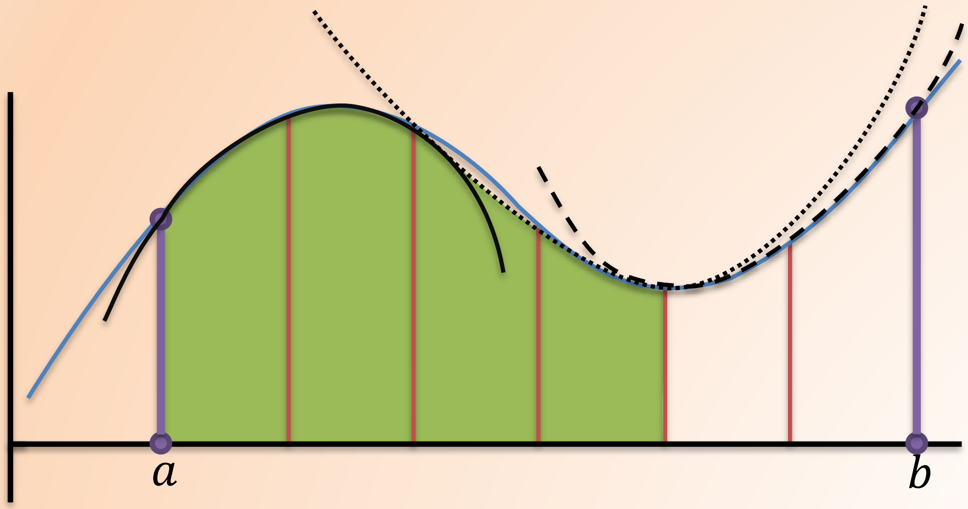
Simpson's Method



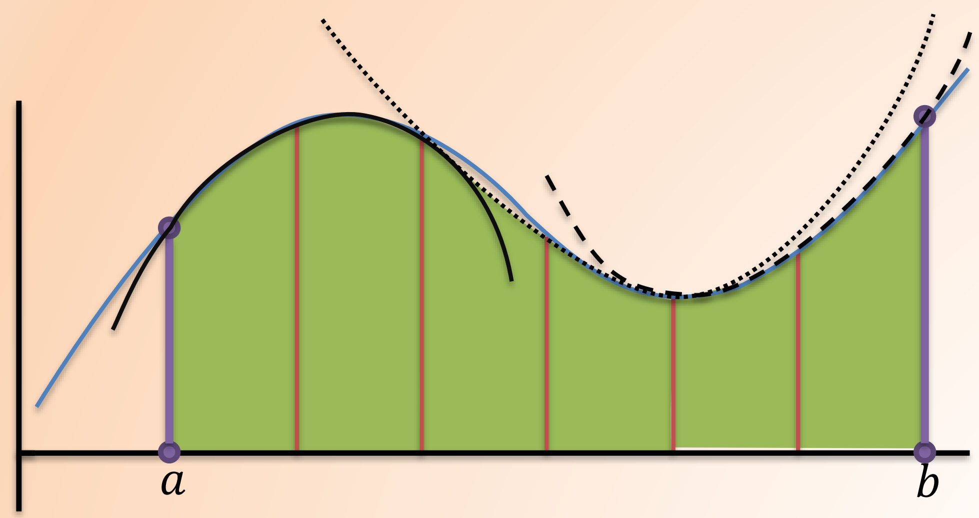
Simpson’s Method



Simpson’s Method

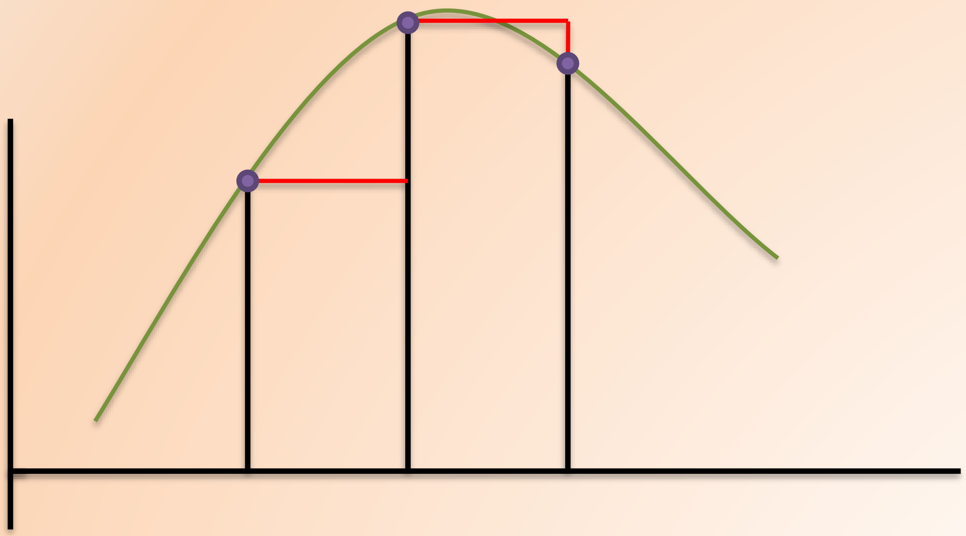


Simpson’s Method



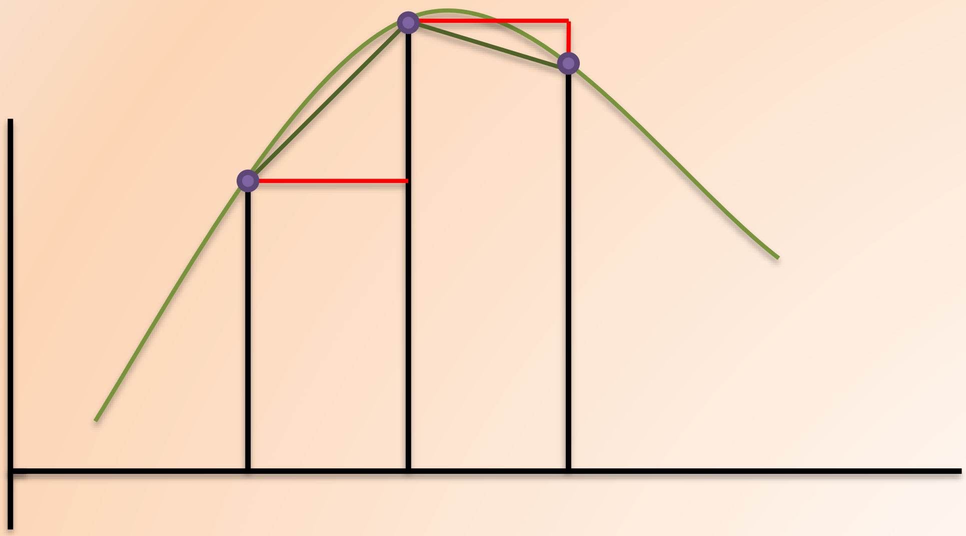
Simpson’s Method

Rectangular



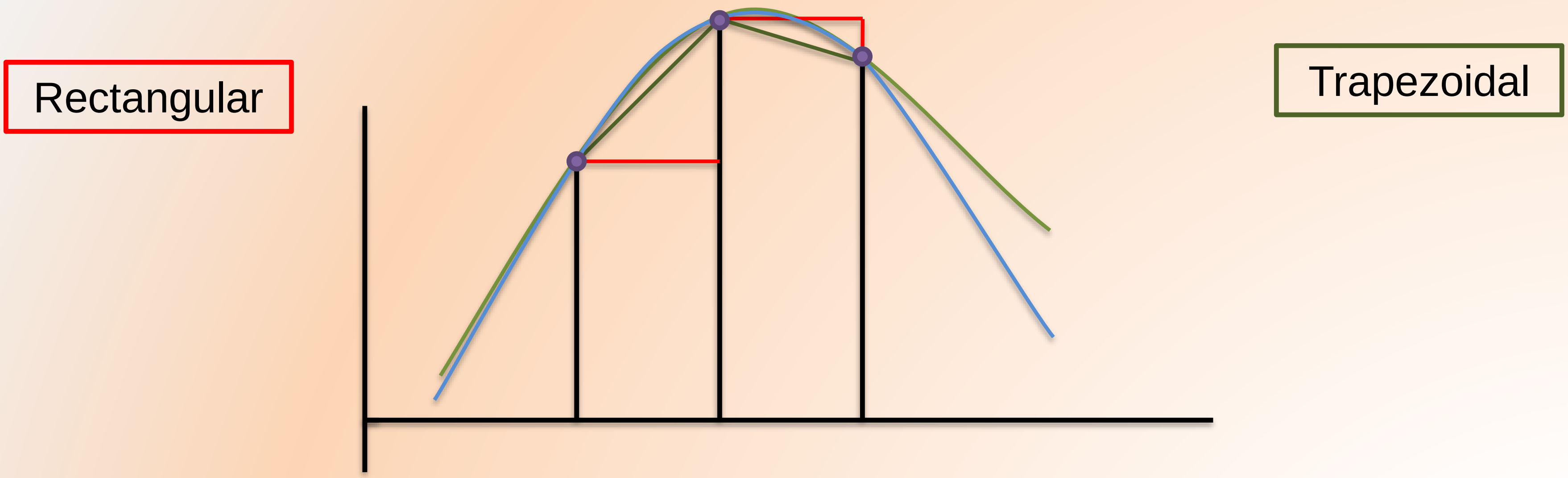
Simpson's Method

Rectangular



Trapezoidal

Simpson's Method



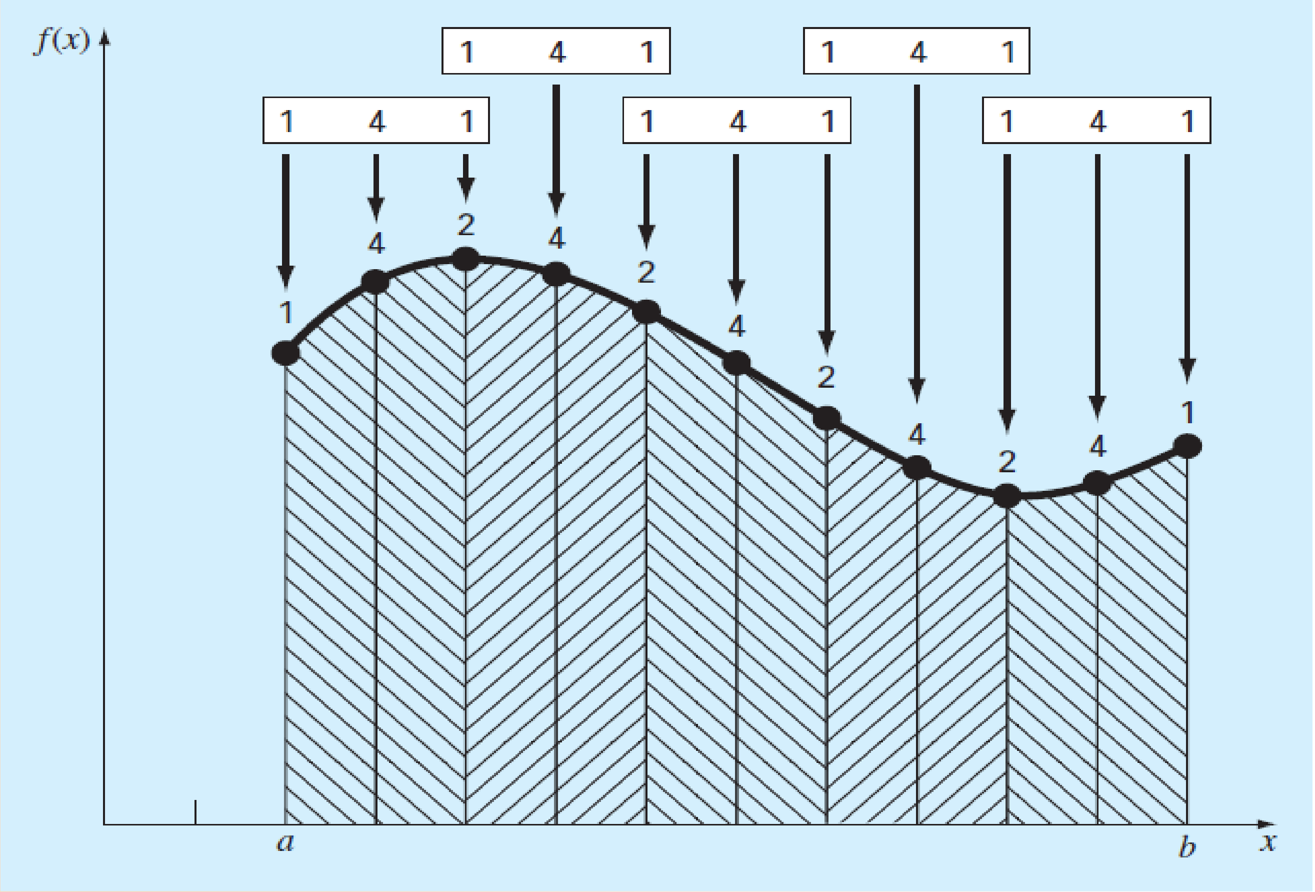
Simpson's 1/3 rule passes a parabolic interpolated curve through each three adjacent nodes.

Simpson's Method

$$I = \int_{x_0}^{x_2} \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx$$

$$I = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

Simpson's Method



Simpson's Method

Simpson's 1/3 rule implies that n is even .Therefore:

$$\int_a^b f(x)\ dx \cong S_{1/3}(h) = \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{n-2} + 4f_{n-1} + f_n\right]$$

The Error is:

$$E[S_{1/3}(h)] = \frac{b-a}{180} h^4 f^{(4)}(z) \mid z \in [a,b]$$

Simpson's Method

To make the error be less than ε, the following condition is needed:

$$h = \sqrt[4]{\frac{180\varepsilon}{(b-a)m_4}}\,, m_4 = max\left|f^{(4)}(x)\right|, x \in [a, b]$$

The error is proportional to h^4, so no error exists for cubic, parabolic and linear $f(x)$s.

Simpson's Method

Simpson's 3/8 rule passes a third degree polynomial through each four adjacent nodes.

$$\int_a^b f(x)\ dx = S_{3/8}(h) =$$

$$\frac{3h}{8}\left[f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n\right]$$

Simpson's 3/8 rule implies n is divisible by 3.

The Error is:

$$E[S_{3/8}(h)] = \frac{b-a}{80} h^4 f^{(4)}(z) \mid z \in [a,b]$$

An Example

Compute the given integral using Simpson 1/3 and 3/8 methods for $h = 0.1$.

$$\int_0^{0.6} \frac{cosx}{1+x^2}dx$$

An Example

Compute the given integral using Simpson $\boxed{1/3}$ and 3/8 methods for $h = 0.1$.

$$\int_0^{0.6} \frac{cosx}{1+x^2}dx$$

x_i	0	0.1	0.2	0.3	0.4	0.5	0.6
f_i	1	0.985153	0.942372	0.876455	0.794018	0.702066	0.606864

$$\Rightarrow \int_0^{0.6} \frac{cosx}{1+x^2}dx$$

$$= S_{1/3}(0.1) = \frac{0.1}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + f_6) = 0.511144$$

An Example

Compute the given integral using Simpson 1/3 and $\boxed{3/8}$ methods for $h = 0.1$.

$$\int_0^{0.6} \frac{cosx}{1+x^2}dx$$

x_i	0	0.1	0.2	0.3	0.4	0.5	0.6
f_i	1	0.985153	0.942372	0.876455	0.794018	0.702066	0.606864

$$\Rightarrow \int_0^{0.6} \frac{cosx}{1+x^2}dx$$

$$= S_{3/8}(0.1) = \frac{0.1 \times 3}{8}(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + f_6) = 0.511148$$

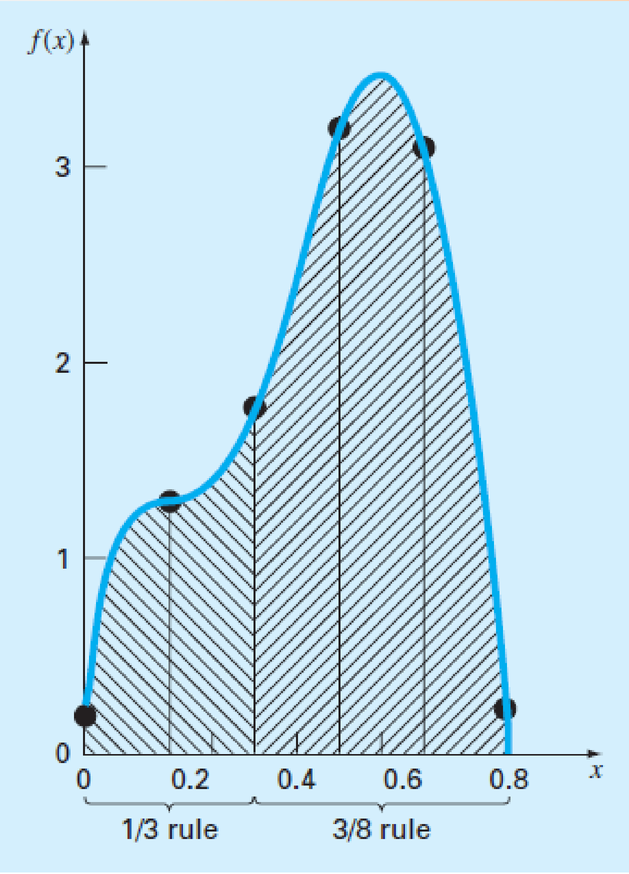
Customized Simpson

Knowing that the number of points ‘n’ should be divisible by 2 and 3 respectively in Simpson 1/3 and Simpson 3/8 methods, we introduce a customized simpson in which there are no restrictions for ‘n’:

Having divided the interval to two subintervals, it integrates on the first and second subintervals using Simpson 1/3 and Simpson 3/8, respectively.

To lower the total error, as much length as possible should be assigned to Simpson 1/3 method.

Customized Simpson



(b) The data needed for a five-segment application ($h = 0.16$) are

$$
\begin{array}{ll}
f(0) = 0.2 & f(0.16) = 1.296919 \\
f(0.32) = 1.743393 & f(0.48) = 3.186015 \\
f(0.64) = 3.181929 & f(0.80) = 0.232
\end{array}
$$

The integral for the first two segments is obtained using Simpson's 1/3 rule:

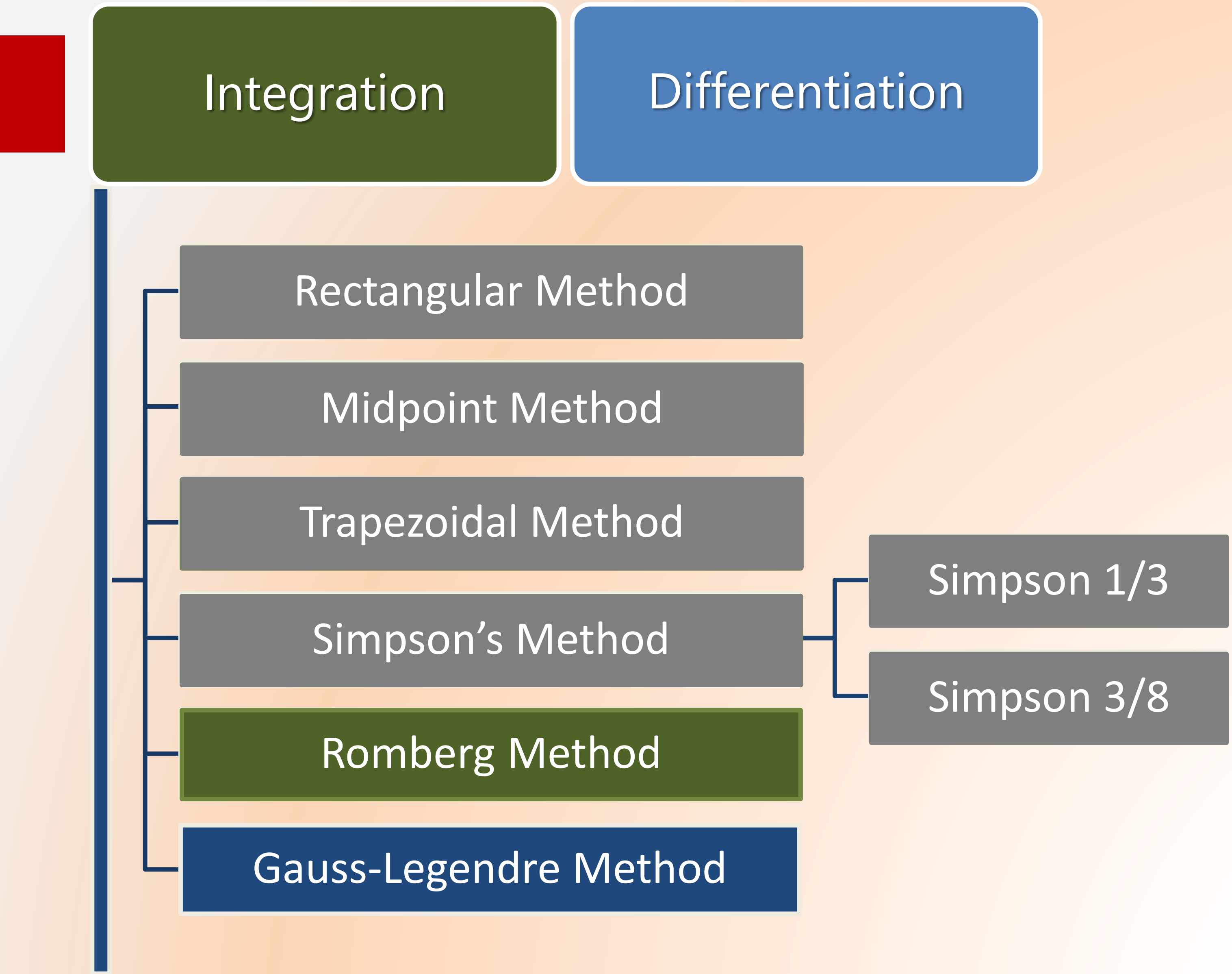
$$I = 0.32\frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237$$

For the last three segments, the 3/8 rule can be used to obtain

$$I = 0.48\frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8} = 1.264754$$

The total integral is computed by summing the two results:

$$I = 0.3803237 + 1.264754 = 1.645077$$


Integration
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Romberg Method

Romberg method is a method for combining the results of different h values for a specific method to improve the accuracy of the answer using Richardson extrapolation concept.

It is usually based on Trapezoidal method.

Romberg Method

In this method:

$$h_0 = b - a$$

$$h_1 = \frac{h_0}{2}$$

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

$$\vdots$$

$$h_P = \frac{h_{P-1}}{2}$$

Romberg Method

$$T(h_0, h_1) = \frac{4T(h_1) - T(h_0)}{4 - 1}$$

$$T(h_0, h_1, h_2) = \frac{4^2 T(h_1, h_2) - T(h_0, h_1)}{4^2 - 1}$$

$$\vdots$$

$$T(h_0, h_1, \dots, h_p) = \frac{4^p T(h_1, \dots, h_p) - T(h_0, \dots, h_{p-1})}{4^p - 1}$$

Romberg Method

h_i	
h_0	
h_1	
h_2	
…	
h_p	

Romberg Method

h_i	Trapezoidal Rule	
h_0	$T(h_0)$	
h_1	$T(h_1)$	
h_2	$T(h_2)$	
…	…	
h_p	$T(h_p)$	

Romberg Method

h_i	Trapezoidal Rule	
h_0	$T(h_0)$	
h_1	$T(h_1)$	$T(h_0, h_1)$
h_2	$T(h_2)$	$T(h_1, h_2)$
…	…	…
h_p	$T(h_p)$	$T(h_{p-1}, h_p)$

Romberg Method

h_i	Trapezoidal Rule		
h_0	$T(h_0)$		
h_1	$T(h_1)$	$T(h_0, h_1)$	
h_2	$T(h_2)$	$T(h_1, h_2)$	$T(h_0, h_1, h_2)$
…	…	…	…
h_p	$T(h_p)$	$T(h_{p-1}, h_p)$	$T(h_{p-2}, h_{p-1}, h_p)$

Romberg Method

h_i	Trapezoidal Rule				
h_0	$T(h_0)$				
h_1	$T(h_1)$	$T(h_0, h_1)$			
h_2	$T(h_2)$	$T(h_1, h_2)$	$T(h_0, h_1, h_2)$		
…	…	…	…	…	
h_p	$T(h_p)$	$T(h_{p-1}, h_p)$	$T(h_{p-2}, h_{p-1}, h_p)$	…	$T(h_0, h_1, \dots, h_p)$

An Example

Compute the given integral using Romberg method.

$$\int_0^1 x^4 dx$$

An Example

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h_i	Trapezoidal Rule	1^{st} Level	2^{nd} Level
1	0.5		
0.5	$\frac{9}{32}$	$\frac{5}{24}$	
0.25	$\frac{113}{512}$	$\frac{77}{384}$	$\frac{1}{5}$

An Example

Compute the given integral using Romberg method.

$$\int_0^1 x^4 dx$$

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0.5	$\frac{9}{32}$	$\frac{5}{24}$	
0.25	$\frac{113}{512}$	$\frac{77}{384}$	$\frac{1}{5}$

$$\int_0^1 x^4 dx = \left.\frac{x^5}{5}\right|_0^1 = \frac{1}{5} - 0 = \frac{1}{5}$$

Romberg Method

$R(j,0)$ is found by Trapezoidal Rule with:

$$h = \frac{b-a}{2^k}$$

Termination condition is:

$$|R(k,k) - R(k-1,k-1)| < \varepsilon$$

The error is proportional to h^{2p+2} (p is number of steps), so no error exists for $f(x)s$ from degrees $2p + 1$ or lower.

Richardson Extrapolation

Richardson extrapolation is a simple method for improving the accuracy of certain numerical procedures.

Suppose that:

$$G = g(h) + ch^p$$

Where c and p are constants.

Let $h = h_1$. Substituting for h in the above equation yields:

$$G = g(h_1) + c{h_1}^p$$

Resubstituting h using $h = h_2$, therefore:

$$G = g(h_2) + c{h_2}^p$$

Richardson Extrapolation

Eliminating c and solving for G, we obtain:

$$G = \frac{(h_1/h_2)^p g(h_2) - g(h_1)}{(h_1/h_2)^p - 1}$$

which is the Richardson Extrapolation formula.

Richardson Extrapolation

Eliminating c and solving for G, we obtain:

$$G = \frac{(h_1/h_2)^p g(h_2) - g(h_1)}{(h_1/h_2)^p - 1}$$

which is the Richardson Extrapolation formula. It is common practice to use $h_2 = h_1/2$, in which case the equation becomes:

$$G = \frac{2^p g(h_1/2) - g(h_1)}{2^p - 1}$$

Richardson Extrapolation

$$I = I(h) + E(h)$$ ⇒ $$I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

$$E \cong -\frac{b-a}{12} h^2 \bar{f}''$$ ⇒ $$\frac{E(h_1)}{E(h_2)} \cong \frac{h_1^2}{h_2^2}$$

$$E(h_1) \cong E(h_2)\left(\frac{h_1}{h_2}\right)^2$$ ⇒ $$I(h_1) + E(h_2)\left(\frac{h_1}{h_2}\right)^2 = I(h_2) + E(h_2)$$ ⇒

$$E(h_2) = \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}$$

$$I = I(h_2) + E(h_2)$$ ⇒ $$I = I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}[I(h_2) - I(h_1)]$$ ⇒

$$I = \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1)$$

Richardson Extrapolation

$$I = \int_a^b f(x)dx = T(h) + a_{۲}h^{۲} + a_{۴}h^{۴} + a_{۶}h^{۶} + \dots$$

$$I = \int_a^b f(x)dx = T\left(\frac{h}{۲}\right) + a_{۲}\left(\frac{h^{۲}}{۴}\right) + a_{۴}\left(\frac{h^{۴}}{۱۶}\right) + \dots$$

$$۴I - I = ۴T\left(\frac{h}{۲}\right) - T(h) - \frac{۳a^{۴}h^{۴}}{۴} + \dots$$

$$I = \frac{۴T(\frac{h}{۲}) - T(h)}{۳} - \frac{a^{۴}h^{۴}}{۴} + \dots$$

Richardson Extrapolation

$$I = \int_a^b f(x)dx = T(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots$$

$$I = \int_a^b f(x)dx = T\left(\frac{h}{2}\right) + a_2\left(\frac{h^2}{4}\right) + a_4\left(\frac{h^4}{16}\right) + \dots$$

$$4I - I = 4T\left(\frac{h}{2}\right) - T(h) - \frac{3a_4 h^4}{4} + \dots$$

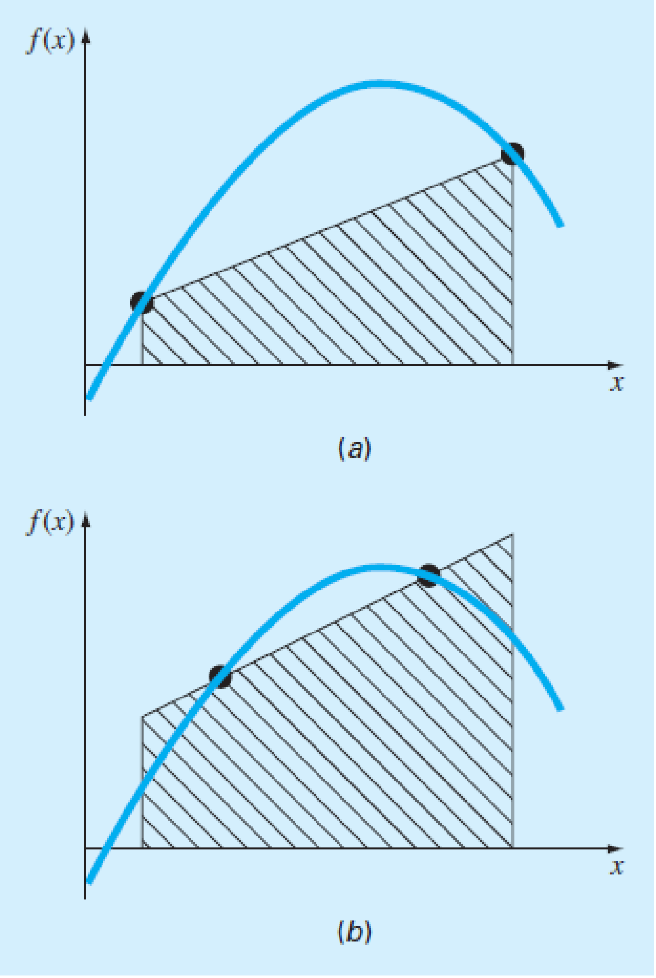
$$I = \frac{4T(\frac{h}{2}) - T(h)}{3} - \frac{a_4 h^4}{4} + \dots$$

Integration

Differentiation

- Rectangular Method
- Midpoint Method
- Trapezoidal Method
- Simpson's Method
  - Simpson 1/3
  - Simpson 3/8
- Romberg Method
- **Gauss-Legendre Method**

Gauss-Legendre Integration



Gauss-Legendre Integration

The lengths of subintervals are <u>not</u> equal in this method.

$$\int_{-1}^{1} f(x)dx = \sum_{i=0}^{n} w_i f(x_i)$$

They should be calculated such that the error of any polynomials of degree $(2n+1)$ or lower becomes zero.

Gauss-Legendre Integration

When $n = 0$, the method is precise for 1-degree $f(x)$s, so:

$$\int_{-1}^{1} f(x)\,dx = w_0 f_0$$

$$\int_{-1}^{1} x^0\,dx = 2 \rightarrow w_0 f_0 = 2 \rightarrow w_0 = 2$$

$$\int_{-1}^{1} x\,dx = 0 \rightarrow w_0 f_0 = 0 \rightarrow x_0 = 0$$

Gauss-Legendre Integration

And when $n = 1$ the method is precise for $f(x)$s with degree of 0, 1, 2 and 3, so

$$\left.\begin{array}{r} f(x) = 1 \;\rightarrow \int_{-1}^{1} 1 \; dx = 2 = \; w_0 + w_1 \\ f(x) = x \;\rightarrow \int_{-1}^{1} x \; dx = 0 = \; w_0 x_0 + w_1 x_1 \\ f(x) = x^2 \;\rightarrow \int_{-1}^{1} x^2 \; dx = \frac{2}{3} = \; w_0 {x_0}^2 + w_1 {x_1}^2 \\ f(x) = x^3 \rightarrow \int_{-1}^{1} x^3 \; dx = 0 = \; w_0 {x_0}^3 + w_1 {x_1}^3 \end{array}\right\}$$

Gauss-Legendre Integration

And when $n = 1$ the method is precise for $f(x)$s with degree of 0, 1, 2 and 3, so

$$\left.\begin{aligned}
f(x) = 1 &\rightarrow \int_{-1}^{1} 1\ dx = 2 = w_0 + w_1 \\
f(x) = x &\rightarrow \int_{-1}^{1} x\ dx = 0 = w_0 x_0 + w_1 x_1 \\
f(x) = x^2 &\rightarrow \int_{-1}^{1} x^2\ dx = \frac{2}{3} = w_0 {x_0}^2 + w_1 {x_1}^2 \\
f(x) = x^3 &\rightarrow \int_{-1}^{1} x^3\ dx = 0 = w_0 {x_0}^3 + w_1 {x_1}^3
\end{aligned}\right\} \rightarrow \begin{cases} w_0 = 1 \\ w_1 = 1 \\ x_0 = -\dfrac{1}{\sqrt{3}} \\ x_1 = \dfrac{1}{\sqrt{3}} \end{cases}$$

An Example

Compute the given integral using Gauss-Legendre method.

$$\int_{-1}^{1} \frac{dx}{x+2}$$

$$= 1 \times \frac{1}{\frac{1}{\sqrt{3}}+2} + 1 \times \frac{1}{\frac{-1}{\sqrt{3}}+2} = 1.09091$$

Gauss-Legendre Integration

All these integrals are defined in the interval $[-1, 1]$. For a general integration in the interval $[a, b]$, the following change of variable is needed:

$$x = \frac{b-a}{2}t + \frac{b+a}{2} \Rightarrow dx = \frac{b-a}{2}\,dt$$

An Example

Compute the given integral using 2-point Gauss-Legendre method.

$$\int_0^4 x^4 dx$$

$$= \int_{-1}^{1} \left(\frac{4-0}{2}t + \frac{4+0}{2}\right)^4 \times \frac{4-0}{2} dt = 2\int_{-1}^{1} (2t+2)^4 dt$$

$$= 2\left[\left(2\frac{1}{\sqrt{3}} + 2\right)^4 + \left(2\frac{-1}{\sqrt{3}} + 2\right)^4\right] = 199.11$$

Gauss-Legendre Integration

For m-point Gauss-Legendre method $(m = n + 1)$, $w_i s$ and $x_i s$ are calculated using this recursive equations system ($x_i s$ are the roots of $P_m(x)$, and $P_m{}'(x_i)$ is the derivative of $P_m(x)$):

$$\begin{cases} P_0(x) = 1 \\ P_1(x) = x \\ \vdots \\ P_m(x) = \dfrac{1}{m}[(2m-1)xP_{m-1}(x) - (m-1)P_{m-2}(x)] \end{cases}$$

$$w_i = \frac{2}{(1 - x_i{}^2)(P_m{}'(x_i))^2}$$

An Example

Compute $w_i s$ and $x_i s$ in Legendre polynomial using Gauss-Legendre method for m = 2 .

$$\begin{cases} P_0(x) = 1 \\ P_1(x) = x \\ P_2(x) = \frac{1}{2}(2 \times 2 - 1)x \times x - (2-1) \times 1 = \frac{1}{2}(3x^2 - 1) \end{cases}$$

An Example

Compute $w_i s$ and $x_i s$ in Legendre polynomial using Gauss-Legendre method for m = 2 .

$$\begin{cases} P_0(x) = 1 \\ P_1(x) = x \\ P_2(x) = \frac{1}{2}(2 \times 2 - 1)x \times x - (2 - 1) \times 1 \end{cases} = \frac{1}{2}(3x^2 - 1)$$

$$\Rightarrow x_i = \pm \frac{1}{\sqrt{3}}$$

$$\Rightarrow w_1 = \frac{2}{(1 - \frac{1}{3})(3)} = 1 \ , w_2 = \frac{2}{(1 - \frac{1}{3})(3)} = 1$$

Integration

Differentiation

- Forward Differencing Method
- Backward Differencing Method
- Central Differencing Method
- Richardson Extrapolation Method
- Derivatives by Interpolation

Numerical Differentiation

Numerical differentiation is used when given x_is and $f(x_i)$s and $f'(x)$ is needed or it is hard to achieve the derivative of $f(x)$.

We have roundoff error and interpolation error

Forward Finite Difference

Forward Taylor series expansions:

$$x_{i+1} = x_i + h$$

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h + O(h^2)$$

$$\boxed{f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)}$$

Forward Finite Difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \cdots$$

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f''(x_i)h^2 + \cdots$$

$$\boxed{f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)}$$

Forward Finite Difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$\boxed{f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)}$$

Numerical Differentiation

3 point rule:

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

$$\xrightarrow{Error} \quad Ef_i' = \frac{h^2}{3} f^{(3)}(z)\ , z \in [x_i, x_{i+2}]$$

Forward Finite Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Backward Finite Difference

Backward Taylor series expansions:

$$x_{i-1} = x_i - h$$

$$f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(x_i) + \cdots$$

$$f'(x_i) \simeq \frac{f(x_i) - f(x_{i-1})}{h} = \frac{f_i - f_{i-1}}{h}$$

$$\boxed{f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)}$$

Backward Finite Difference

First Derivative | Error

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} \qquad O(h)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} \qquad O(h^2)$$

Second Derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} \qquad O(h^2)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3} \qquad O(h)$$

$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3} \qquad O(h^2)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4} \qquad O(h)$$

$$f''''(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4} \qquad O(h^2)$$

Central Finite Difference

$$f(x_{i+۱}) = f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^۲}{۲!}f''(x_i) + \frac{h^۳}{۳!}f'''(x_i) + \cdots$$

$$f(x_{i-۱}) = f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^۲}{۲!}f''(x_i) - \frac{h^۳}{۳!}f'''(x_i) + \cdots$$

$$f(x_{i+۱}) - f(x_{i-۱})$$

$$\boxed{f'(x_i) \simeq \frac{f(x_{i+۱}) - f(x_{i-۱})}{۲h} = \frac{f_{i+۱} - f_{i-۱}}{۲h}}$$

Central Finite Difference

$$f(x_{i+1}) = f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^۲}{۲!}f''(x_i) + \frac{h^۳}{۳!}f'''(x_i) + \cdots$$

$$f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^۲}{۲!}f''(x_i) - \frac{h^۳}{۳!}f'''(x_i) + \cdots$$

$$f(x_{i+1}) + f(x_{i-1})$$

$$\boxed{f''(x_i) \simeq \frac{f(x_{i-1}) - ۲f(x_i) + f(x_{i+1})}{h^۲} = \frac{f_{i-1} - ۲f_i + f_{i+1}}{h^۲}}$$

Central Finite Difference

Central differencing with an error of $O(h^2)$:

$$f_i{}' = \frac{f_{i+1} - f_{i-1}}{2h} \xrightarrow{Error} Ef_i{}' = \frac{h^2}{6} f^{(3)}(z)\,, z \in [x_{i-1}, x_{i+1}]$$

$$f_i{}'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \xrightarrow{Error} Ef_i{}'' = \frac{h^2}{12} f^{(4)}(z)\,, z \in [x_{i-1}, x_{i+1}]$$

$$f_i{}''' = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2h^3} \xrightarrow{Error} O(h^2)$$

$$f_i{}^{(4)} = \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4} \xrightarrow{Error} O(h^2)$$

Central Finite Difference

Another central differencing method with an error of $O(h^4)$:

$$f_i{}' = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} \xrightarrow{Error} Ef_i{}' = \frac{h^4}{30} f^{(5)}(z)\ , z \in [x_{i-2}, x_{i+2}]$$

$$f_i{}'' = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12h^2} \xrightarrow{Error} O(h^4)$$

$$f_i{}^{(3)} = \frac{-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3}}{8h^3} \xrightarrow{Error} O(h^4)$$

$$f_i{}^{(4)} = \frac{-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3}}{6h^4} \xrightarrow{Error} O(h^4)$$

Central Finite Difference

First Derivative — Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \qquad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3} \qquad O(h^2)$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \qquad O(h^2)$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4} \qquad O(h^4)$$

An Example

Consider the following table. Compute $f'(0.1)$ and $f''(0.1)$ using central differencing method of order $O(h^4)$.

x_i	0	0.05	0.10	0.15	0.20
f_i	1	1.0513	1.1052	1.1618	1.2214

$$f'(0.1) = \frac{1}{12 \times 0.05}[-1.2214 + 8(1.1618) - 8(1.0513) + 1]$$

$$= 0.1043$$

$$f''(0.1) = \frac{1}{12(0.05)^2}[-1.2214 + 16(1.1618) - 30(1.1052) + 16(1.0513) - 1]$$

$$= 0.07333$$

An Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Compute $f'(0.5)$ with h=0.25.

x_i	0	0.25	0.5	0.75	1
f_i	1.2	1.1035156	0.925	0.6363281	0.2

The forward difference of accuracy $O(h^2)$ is computed as

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375$$

An Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Compute $f'(0.5)$ with h=0.25.

x_i	0	0.25	0.5	0.75	1
f_i	1.2	1.1035156	0.925	0.6363281	0.2

The backward difference of accuracy $O(h^2)$ is computed as

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125$$

An Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Compute $f'(0.5)$ with h=0.25.

x_i	0	0.25	0.5	0.75	1
f_i	1.2	1.1035156	0.925	0.6363281	0.2

The centered difference of accuracy $O(h^4)$ is computed as

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125$$

Exact value: f'(0.5)=-0.9125

Numerical Differentiation

A common pitfall is that smaller h lead to smaller errors but, it is <u>not</u> always true because of large amount of calculations. So, it is recommended to use methods with higher orders of accuracy.

An Example

$f(x) = e^{-x}, f''(1) = ?$ $h = 0.64$

$$f''(1) = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \longrightarrow O(h^2)$$

x_i	0.36	1	1.64
f_i	0.697676	0.367879	0.193980

$\Rightarrow f''(1) = 0.380610$

An Example

$$f(x) = e^{-x},$$
$$f''(1) = ?$$

h_i	6-digits Mantissa	8-digits Mantissa
0.64	0.380610	0.3860911
0.32	0.371035	0.37102939
0.16	0.368711	0.36866484
0.08	0.368281	0.36807656
0.04	0.36875	0.36783195
0.02	0.37	0.3679
0.01	0.38	0.3679
0.005	0.40	0.3676
0.0025	0.48	0.3680
0.00125	1.28	0.3712

An Example

$f(x) = e^{-x},$
$f''(1) = ?$

$f''(1) = e^{-1} = 0.367\,879\,44$

h_i	6-digits Mantissa	8-digits Mantissa
0.64	0.380610	0.3860911
0.32	0.371035	0.37102939
0.16	0.368711	0.36866484
0.08	**0.368281**	0.36807656
0.04	0.36875	0.36783195
0.02	0.37	**0.3679**
0.01	0.38	0.3679
0.005	0.40	0.3676
0.0025	0.48	0.3680
0.00125	1.28	0.3712

Richardson Extrapolation

Richardson extrapolation is a simple method for improving the accuracy of certain numerical procedures.

Suppose that:

$$G = g(h) + ch^p$$

Where c and p are constants.

Let $h = h_1$. Substituting for h in the above equation yields:

$$G = g(h_1) + c{h_1}^p$$

Resubstituting h using $h = h_2$, therefore:

$$G = g(h_2) + c{h_2}^p$$

Richardson Extrapolation

Eliminating c and solving for G, we obtain:

$$G = \frac{(h_1/h_2)^p g(h_2) - g(h_1)}{(h_1/h_2)^p - 1}$$

which is the Richardson Extrapolation formula. It is common practice to use $h_2 = h_1/2$, in which case the equation becomes:

$$G = \frac{2^p g(h_1/2) - g(h_1)}{2^p - 1}$$

An Example

$f(x) = e^{-x}, f''(1) =?$ $h = 0.64$

$$f''(1) = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \longrightarrow O(h^2)$$

x_i	0.36	1	1.64
f_i	0.697676	0.367879	0.193980

$\Rightarrow f''(1) = 0.380610$

An Example

$f(x) = e^{-x}$,
$f''(1) = 0.36787944$

$g(h_1) = 0.380\,610 \qquad g(h_1/2) = 0.371\,035$

$E(h) = \mathcal{O}(h^2) = c_1 h^2 + c_2 h^4 + c_3 h^6 + \cdots.$

substitute $p = 2$ and $h_1 = 0.64$

$$G = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1}$$

$$G = \frac{2^2 \times \ 0.371035 - 0.380610}{2^2 - 1} = 0.367843$$

h_i	6-digits Mantissa	8-digits Mantissa
0.64	0.380610	0.3860911
0.32	0.371035	0.37102939
0.16	0.368711	0.36866484
0.08	0.368281	0.36807656
0.04	0.36875	0.36783195
0.02	0.37	0.3679
0.01	0.38	0.3679
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An Example

$f(x) = e^{-x}$,
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$$G = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1}$$

$$G = \frac{2^2 \times\ 0.371035 - 0.380610}{2^2 - 1} = 0.367843$$

Derivatives by Interpolation

$$P(x) = f_i + s\Delta f_i + \frac{s(s-١)}{٢!}\Delta^{٢} f_i + \frac{s(s-١)(s-٢)}{٣!}\Delta^{٣} f_i + \cdots$$
$$+ \frac{s(s-١)\cdots(s-k+١)}{k!}\Delta^{k} f_i$$

$$x = x_i + sh \text{ و } x_{i+١} - x_i = h$$

$$f'(x) = \frac{df(x)}{dx} \simeq \frac{dP(x)}{dx} = \frac{dP(x)}{ds} \cdot \frac{ds}{dx}$$

$$f'(x) \simeq \frac{١}{h}[\Delta f_i + (s - \frac{١}{٢})\Delta^{٢} f_i + \frac{٣s^{٢} - ۶s + ٢}{۶}\Delta^{٣} f_i + \cdots]$$

Derivatives by Interpolation

$$f'(x) \simeq \frac{1}{h}\left[\Delta f_i + \left(s - \frac{1}{2}\right)\Delta^2 f_i + \frac{3s^2 - 6s + 2}{6}\Delta^3 f_i + \cdots\right]$$

$$f'(x_i) = f'_i \simeq \frac{1}{h}\left[\Delta f_i - \frac{1}{2}\Delta^2 f_i + \frac{1}{3}\Delta^3 f_i - \cdots\right]$$

$$\boxed{f'_i \simeq \frac{1}{h}\Delta f_i = \frac{f_{i+1} - f_i}{h}}$$

$$\boxed{f'_i \simeq \frac{1}{h}\left[\Delta f_i - \frac{1}{2}\Delta^2 f_i\right] = \frac{2 f_{i+1} - \frac{1}{2} f_{i+2} - \frac{3}{2} f_i}{h}}$$

Derivatives by Interpolation

$$f''(x) = \frac{d^{۲} f(x)}{dx^{۲}} \simeq \frac{d^{۲} P(x)}{dx^{۲}} \simeq \frac{۱}{h^{۲}} \frac{d^{۲} P(x)}{ds^{۲}} = \frac{۱}{h^{۲}} [\Delta^{۲} f_i + (s - ۱)\Delta^{۳} f_i + \cdots]$$

$$f''(x_i) = f_i'' \simeq \frac{۱}{h^{۲}} [\Delta^{۲} f_i - \Delta^{۳} f_i + \frac{۱۱}{۱۲} \Delta^{۴} f_i - \cdots]$$

$$\boxed{f_i'' \simeq \frac{۱}{h^{۲}} \Delta^{۲} f_i = \frac{f_{i+۲} - ۲ f_{i+۱} + f_i}{h^{۲}}}$$

An Example

مثال،

x	۱,۳	۱,۵	۱,۷	۱,۹	۲,۱
$f(x)$	۳,۶۶۹	۴,۴۸۲	۵,۴۷۴	۶,۶۸۶	۸,۱۶۶

$f'(۱,۳)$

با استفاده از تمام نقاط جدول

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
۱,۳	۳,۶۶۹				
		۰,۸۱۳			
۱,۵	۴,۴۸۲		۰,۱۷۹		
		۰,۹۹۲		۰,۰۴۱	
۱,۷	۵,۴۷۴		۰,۲۲۰		۰,۰۰۷
		۱,۲۱۲		۰,۰۴۸	
۱,۹	۶,۶۸۶		۰,۲۶۸		
		۱,۴۸۰			
۲,۱	۸,۱۶۶				

$$h = ۰,۲ \Rightarrow f'(۱,۳) = \frac{1}{۰,۲}\left(۰,۸۱۳ - \frac{۰,۱۷۹}{۲} + \frac{۰,۰۴۱}{۳} - \frac{۰,۰۰۷}{۴}\right) = ۳,۶۷۷$$

$$f'(۱,۷) = \frac{1}{۰,۲}\left(۱,۲۱۲ - \frac{۰,۲۶۸}{۲}\right) = ۵,۳۹۰$$

فرمول سه نقطه‌ای $\quad f'(۱,۷) = \frac{-۸,۱۶۶ + ۴(۶,۶۸۸) - ۳(۵,۴۷۴)}{۰,۴} = ۵,۳۹۰$

Derivatives of Inequality Space Data

For example, you can fit a second-order Lagrange polynomial to three adjacent points (x_0, y_0), (x_1, y_1), and (x_2, y_2). Differentiating the polynomial yields:

$$f'(x) = f(x_0)\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$


Any questions?