Numerical Methods in Engineering

3- NUMERICAL DIFFERENTIATION AND INTEGRATION

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Numerical Differentiation

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- Why numerical differentiation?

1. The source function is not known.
2. The source function is too complicated to differentiate.

Equidistance Differentiation

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- Using Taylor series expansion:

$$f(x+h)=f(x)+hf'(x)+\frac{1}{2!}h^2f''(x)+\frac{1}{3!}h^3f'''(x)+\cdots$$

$$\Rightarrow \frac{f(x+h)-f(x)}{h}=f'(x)+\boxed{\frac{1}{2!}hf''(x)}+\frac{1}{3!}h^2f'''(x)+\cdots$$

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

$$\Rightarrow \frac{f(x)-f(x-h)}{h}=f'(x)-\boxed{\frac{1}{2!}hf''(x)}+\frac{1}{3!}h^3f'''(x)-\cdots$$

$$\frac{f(x+h)-f(x-h)}{2h}=f'(x)+\boxed{\frac{1}{3!}h^2f'''(x)}-\cdots$$

Equidistance Differentiation

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Forward Difference Estimation:

$$f'(x)\approx\frac{f(x+h)-f(x)}{h} \qquad E=\mathcal{O}(h)$$

Backward Difference Estimation:

$$f'(x)\approx\frac{f(x)-f(x-h)}{h} \qquad E=\mathcal{O}(h)$$

Central Difference Estimation:

$$f'(x)\approx\frac{f(x+h)-f(x-h)}{2h} \qquad E=\mathcal{O}\left(h^2\right)$$

Equ. Dis. Differentiation; Richardson's Method

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- Is used to improve the accuracy of differentiation
- Using Central Difference Approximation:

$$\phi(h) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right]$$

$$= f'(x) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots$$

$$\phi\left(\frac{h}{2}\right) = f'(x) + \frac{1}{4} a_2 h^2 + \frac{1}{16} a_4 h^4 + \frac{1}{64} a_6 h^6 + \cdots$$

Equ. Dis. Differentiation; Richardson's Method

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$$\phi(h) - 4\phi\left(\frac{h}{2}\right) = -3f'(x) + \frac{3}{4} a_4 h^4 + \frac{5}{16} a_6 h^6 + \cdots$$

$$\frac{4\phi(h/2) - \phi(h)}{3} = f'(x) + \mathcal{O}\left(h^4\right)$$

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}$$

$$\boxed{E = \tfrac{h^4}{30} f^{(5)}(c)}$$

MATLAB Homework (Error)

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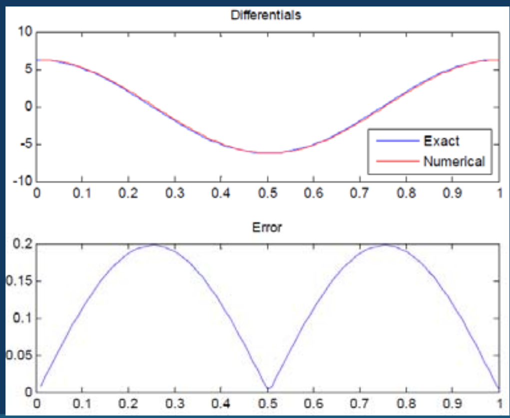
- Plot the differentiation error by MATLAB for the first derivative of *sin x*



Homework

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- For:

$$\psi(h)=\frac{1}{2h}\left[f(x+h)-f(x-h)\right]$$

- Show that:

$$\psi(h)=f'(x)+\frac{h^2}{3!}f'''(x)+\frac{h^4}{5!}f^{(5)}(x)+\frac{h^6}{7!}f^{(7)}(x)+\cdots$$

$$\frac{8\left[\psi(h)-\psi(h/2)\right]}{h^2}=f'''(x)+O\left(h^2\right)$$

Equu. Dis. Differentiation (Example)

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- Comparing Methods; Show that for

$$f(\theta)=cos(\theta)\,, \quad \theta=0.8, \quad h=0.01$$

we have:

Method	Forward	Bckward	Central	Richardson
Error	-0.0048	0.0049	$1.6667e-5$	$3.3332e-10$

Equ. Dis. Differentiation (Example)

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$$f'(x)\approx\frac{f(x+h)-f(x)}{h}\rightarrow -0.0048$$

$$f'(x)\approx\frac{f(x)-f(x-h)}{h}\rightarrow 0.0049$$

$$f'(x)\approx\frac{f(x+h)-f(x-h)}{2h}\rightarrow 1.6667E-5$$

$$f'(x)\approx\frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h}$$

$$\rightarrow 3.3332E-10$$

Equ. Dis. Differentiation: 2nd Derivative

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$$f(x+h)-f(x-h)=2f(x)+h^2 f''(x)+\cdots$$

$$f''(x)=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}+\frac{1}{2}h^2 f^{(4)}(x)$$

$$f''(x)\approx\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

MATLAB Homework (Error)

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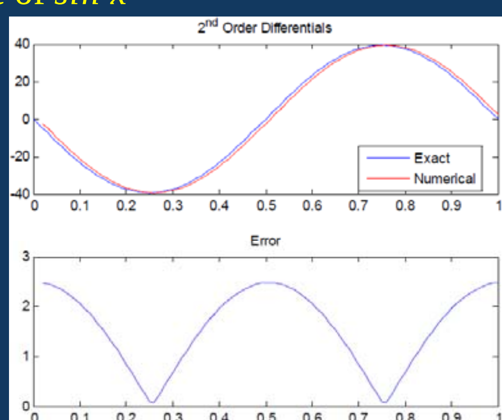
- Plot the differentiation error by MATLAB for the 2nd derivative of *sin x*



Non Equidistance Differentiation

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1. First establish an interpolating formula
   - Newton
   - Lagrange
   - Spline
2. Then differentiate the function

Lagrangian Differentiation (Example)

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- For three points: $(x_{k-1}, f_{k-1}),\ (x_k, f_k),\ (x_{k+1}, f_{k+1})$

$$f(x) = f_{k-1}\frac{(x-x_k)(x-x_{k+1})}{(x_{k-1}-x_k)(x_{k-1}-x_{k+1})} + f_k\frac{(x-x_{k-1})(x-x_{k+1})}{(x_k-x_{k-1})(x_k-x_{k+1})} + f_{k+1}\frac{(x-x_{k-1})(x-x_k)}{(x_{k+1}-x_{k-1})(x_{k+1}-x_k)}$$

- Now for equidistance data: $x_{k+1} - x_k = x_k - x_{k-1} = h$

Lagrangian Differentiation (Example)

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$$f(x) = f_{k-1}\frac{(x-x_k)(x-x_{k+1})}{2h^2} - f_k\frac{(x-x_{k-1})(x-x_{k+1})}{h^2} + f_{k+1}\frac{(x-x_{k-1})(x-x_k)}{2h^2}$$

$$f'(x) = f_{k-1}\frac{(x-x_k)+(x-x_{k+1})}{2h^2} - f_k\frac{(x-x_{k-1})+(x-x_{k+1})}{h^2} + f_{k+1}\frac{(x-x_{k-1})+(x-x_k)}{2h^2}$$

Lagrangian Differentiation (Example)

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$$f'(x_k) = f_{k-1}\frac{(x_k-x_{k+1})}{2h^2} - f_k\frac{(x_k-x_{k+1})}{h^2} - f_k\frac{(x_k-x_{k-1})}{h^2} + f_{k+1}\frac{(x_k-x_{k-1})}{2h^2}$$

$$f'(x_k) = f_{k-1}\frac{(-h)}{2h^2} - f_k\frac{(-h)}{h^2} - f_k\frac{(h)}{h^2} + f_{k+1}\frac{(h)}{2h^2}$$

$$f'(x_k) = \frac{f_{k+1} - f_{k-1}}{2h}$$

Two Dimensional Differentiation

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- Gradient:

$$\frac{\partial f}{\partial x} \approx \frac{f(x+h,y)-f(x,y)}{h} \qquad \frac{\partial f}{\partial y} \approx \frac{f(x,y+h)-f(x,y)}{h}$$

$$\frac{\partial f}{\partial x} \approx \frac{f(x,y)-f(x-h,y)}{h} \qquad \frac{\partial f}{\partial y} \approx \frac{f(x,y)-f(x,y-h)}{h}$$

$$\frac{\partial f}{\partial x} \approx \frac{f(x+h,y)-f(x-h,y)}{2h} \qquad \frac{\partial f}{\partial y} \approx \frac{f(x,y+h)-f(x,y-h)}{2h}$$

Numerical Integratgion

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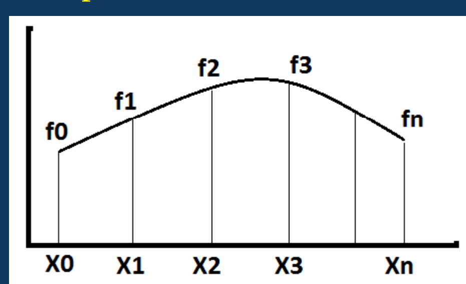
Why numerical integration?

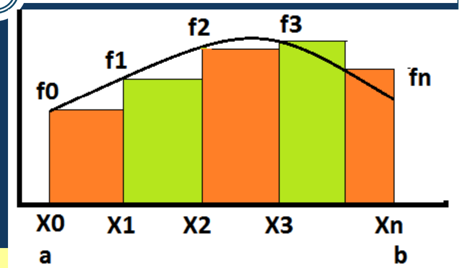
$$I = \int_a^b f(x)dx$$

- *f(x)* is not available.
- Analytical integration is not possible or is too complicated



Numerical Integration

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} f_i(x_{i+1} - x_i)$$

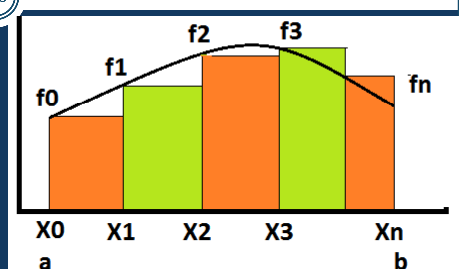


$$\int_a^b f(x)dx = f_0(x_1 - x_0) + f_1(x_2 - x_1) + \ldots + f_{n-1}(x_n - x_{n-1})$$

$$= h\left(f_0 + f_1 + \ldots + f_{n-1}\right) = h\sum_{i=0}^{n-1} f_i \quad ; h = (b-a)/n$$

Numerical Integration

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} f_{i+1}(x_{i+1} - x_i)$$



$$\int_a^b f(x)dx = f_1(x_1 - x_0) + f_2(x_2 - x_1) + \ldots + f_n(x_n - x_{n-1})$$

$$= h\left(f_1 + f_2 + \ldots + f_n\right) = h\sum_{i=1}^{n} f_i \quad ; h = (b-a)/n$$

Numerical Integration

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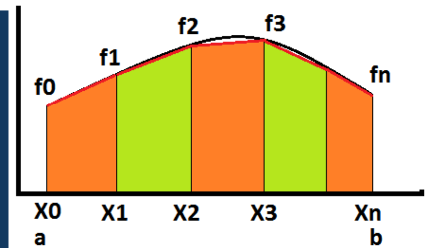
$$\int_a^b f(x)dx$$

$$= \sum_{i=0}^{n-1} (f_i + f_{i+1})(x_{i+1} - x_i)/2$$



$$\int_a^b f(x)dx = \sum_{i=0}^{n-1} (f_i + f_{i+1})h/2 = \left(f_0 + 2f_1 + \ldots + 2f_{n-1} + f_n\right)h/2$$

$$= (h/2)(f_0 + f_n + 2\sum_{i=1}^{n-1} f_i)$$

????????Method

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- Maximum error estimation
- *If* $a < \xi < b$ *then*

$$E = -\frac{(b-a)h^2}{12} f''(\xi)$$

?????????? Method (Example)

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- Determine ***n*** for integration of the following function so that the integration error is less than 10^(-10)

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

$$f(x)=\frac{1}{1+x},\quad f'(x)=-\frac{1}{(1+x)^2},\qquad f''(x)=\frac{2}{(1+x)^3}$$

$$f''(\xi)\le 2,\ \xi\in[0,1]$$

$$E=-\frac{(b-a)h^2}{12}f''(\xi)\rightarrow -\frac{(1-0)}{12}\left(\frac{1-0}{n}\right)^2 f''(\xi)=-\frac{f''(\xi)}{12n^2}$$

$$\frac{2}{12n^2}\le 1\times 10^{-10}\rightarrow n\ge\sqrt{\frac{1}{6}}\times 10^6$$

Simpson's Method (3points)

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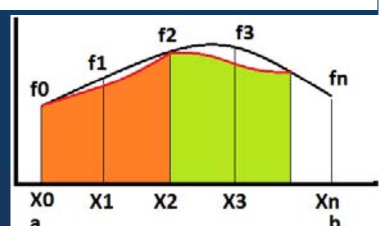
- For 3 points:



$$(x_0,x_1,x_2)\qquad h=\frac{x_2-x_0}{2}$$

$$\int_{x_0}^{x_2} f(x)dx\approx\int_{x_0}^{x_2}\left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f_0+\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f_1+\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f_2\right]dx$$

$$\int_{x_0}^{x_2} f(x)dx\approx\frac{h}{3}(f_0+4f_1+f_2)\qquad E=-\frac{h^5}{90}f^{(4)}(c)$$

Simpson's Method (3points)

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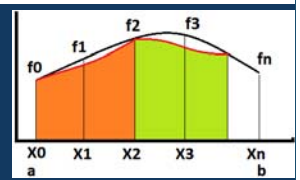

$(x_0, x_1, \cdots, x_n)$ $h = \frac{x_n - x_0}{n}$

$$I = \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) + \cdots + \frac{h}{3}(f_{n-2} + 4f_{n-1} + f_n)$$

$$I = \frac{h}{3}\left[f_0 + f_n + 4\sum_{i=1,3,\cdots}^{n-1} f_i + 2\sum_{i=2,4,\cdots}^{n-2} f_i\right] \qquad E = -\frac{(b-a)h^4}{180} f^{(4)}(\alpha)$$

- ***n=2k** is a necessity*

Num. Methods: 4-Differentiation & Integration

Simpson's Method (4points)

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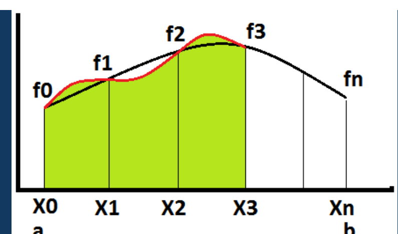
- For four points

(x_0, x_1, x_2, x_3)

$$I = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

$$E \approx \frac{3h^5}{80} f^{(4)}(c)$$



$$\int_a^b f(x)dx = \frac{3h}{8}\left(f_0 + f_n + 3\sum_{i=1,4,7,..}^{n-2}(f_i + f_{i+1}) + 2\sum_{i=3,6,9,..}^{n-3} f_i\right)$$

- ***n=3k** is a necessity*

Num. Methods: 4-Differentiation & Integration

Integral Estimation Using Polynomial

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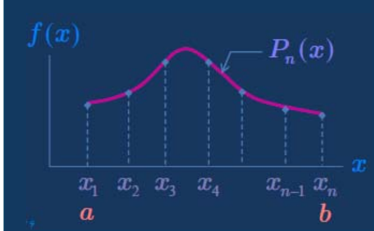
- Fit a polynomial to tabulated data
  Then use it to analytically evaluate the integral
- For example by Lagrange's method:

$$P_{n-1}(x)=\sum_{i=1}^{n} f(x_i)\ell_i(x)$$



$$I=\int_a^b P_{n-1}(x)dx$$

$$=\sum_{i=1}^{n} f(x_i)\int_a^b \ell_i(x)dx=\sum_{i=1}^{n} A_i f(x_i)$$

$$A_i=\int_a^b \ell_i(x)dx$$

Gauss Integration Method

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- For $n+1$ data: $\{(x_i,f_i)\}_{i=0}^{n}$

$$\int_a^b f(x)dx=\sum_{i=0}^{n} A_i f_i,\quad x_0\le a<b\le x_n$$

- Use the following $n+1$ equations to evaluate Ai , i=0,1,...,n

$$\left.\begin{aligned} f=1 &\Rightarrow \int_a^b f(x)dx=b-a=\sum_{i=0}^{n} A_i \\ f=x &\Rightarrow \int_a^b f(x)dx=\frac{b^2-a^2}{2}=\sum_{i=0}^{n} A_i x_i \\ &\vdots \\ f=x^n &\Rightarrow \int_a^b f(x)dx=\frac{b^{n+1}-a^{n+1}}{n+1}=\sum_{i=0}^{n} A_i x_i^n \end{aligned}\right\}\Rightarrow \{A_i\}_{i=0}^{n}$$

Gauss Integration (Example)

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$$\{(1,0.3679),(2,0.0183),(3,1.2341\times10^{-4})\}$$

$$I=\int_{1.25}^{2.3} e^{-x^2}\,dx \qquad a=1.25 \quad b=2.3$$

$$\left.\begin{aligned} A_0+A_1+A_2&=1.05\\ A_0+2A_1+3A_2&=1.8637\\ A_0+4A_1+9A_2&=3.4046 \end{aligned}\right\} \Rightarrow \begin{cases} A_0=0.1930\\ A_1=0.9002\\ A_2=-0.0433 \end{cases}$$

$$I\approx A_0f_0+A_1f_1+A_2f_2=0.0875$$

Gauss Two-point Integration

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- Gauss Formula: $$\int_{-1}^{+1} f(t)dt=f\left(-\frac{1}{\sqrt{3}}\right)+f\left(\frac{1}{\sqrt{3}}\right)$$
- For a general integral like: $$\int_a^b f(x)dx$$

Change the variable from ***x*** to ***t*** and then use the Gauss two-point formula

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

Gauss Two-point Integration

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$$\int_a^b f(x)dx$$

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

$$\int_a^b f(x)dx=\frac{b-a}{2}\int_{-1}^{+1} f\left[\frac{(b-a)t+(b+a)}{2}\right]dt$$

$$\int_a^b f(x)dx \approx \frac{(b-a)}{2}\left\{f\left[\frac{-(b-a)/\sqrt{3}+(b+a)}{2}\right]+f\left[\frac{(b-a)/\sqrt{3}+(b+a)}{2}\right]\right\}$$

Integration (Two-point Example)

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- 1) $I=\int_0^{\pi/2} sin(x)dx$
- Analytic al solution; *I=1*
- ???????

$$\frac{sin(0)+sin(\pi/2)}{2}\left(\frac{\pi}{2}-0\right)=\frac{\pi}{4}\approx 0.785398$$

- Gauss two-point method:

$$\frac{\pi}{4}\left\{sin\left[\frac{\pi}{4\sqrt{3}}+\frac{\pi}{4}\right]+sin\left[-\frac{\pi}{4\sqrt{3}}+\frac{\pi}{4}\right]\right\}\approx 0.998473$$

Integration (Two-point Example)

33

- 2) $$I=\int_0^1 \frac{dx}{1+x^2}$$
- Analytic al solution; $I=tan^{-1}(x)\Big|_0^1=\frac{\pi}{4}\approx 0.7854$
- ???????

$$I=\frac{1}{2}(1+0.5)\approx 0.7500$$

- Gauss two-point method:

$$\int_0^1 f(x)dx\approx\frac{1}{2}\left\{f\left[\frac{-1/\sqrt{3}+1}{2}\right]+f\left[\frac{1/\sqrt{3}+1}{2}\right]\right\}=0.7869$$

0.211 0.789

Gauss Three-point Integration

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- Gauss Formula:

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

- For a general integral like: $$\int_a^b f(x)dx$$

Change the variable from ***x*** to ***t*** and then use the Gauss two-point formula

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

Gauss Three-point Integration

35

$$I=\int_a^b f(x)dx=\frac{(b-a)}{2}\int_{-1}^{1} f\left[\frac{(b-a)t+(b+a)}{2}\right]dt$$

$$I=\int_a^b f(x)dx\cong\frac{(b-a)}{18}\left\{5f\left(\frac{b+a}{2}-\sqrt{\frac{3}{5}}\frac{b-a}{2}\right)\right.$$

$$\left.+8f\left(\frac{b+a}{2}\right)+5f\left(\frac{b+a}{2}+\sqrt{\frac{3}{5}}\frac{b-a}{2}\right)\right\}$$

Integration (Three-point Example)

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$$I=\int_0^1 x\sin(x)dx$$

- Analytic al solution:

$$I=\int_0^1 x\sin(x)dx=[-x\cos(x)+\sin(x)]_0^1\cong 0.30117$$

- Simpson's method

$$I=\int_0^1 x\sin(x)dx\cong\frac{1}{6}\left[\sin(1)+4\left(\frac{1}{2}\right)\sin\left(\frac{1}{2}\right)+0\sin(0)\right]\cong 0.30005$$

- Gauss three-point method:

$$I=\int_0^1 x\sin(x)dx\cong\frac{1}{18}\{5(0.1127)\sin(0.1127)$$

$$+8(0.5)\sin(0.5)+5(0.8873)\sin(0.8873)\}\cong 0.30117$$