ME 310

Numerical Methods

Integration

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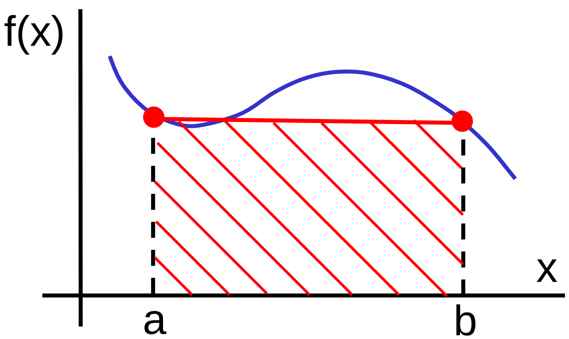
Newton-Cotes Integration Formulas

Idea: Replace a complicated function or a tabulated data with an approximating (interpolating) function.

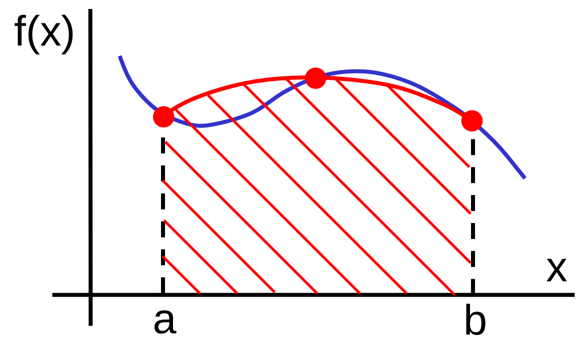
$$\mathbf{I} = \int_a^b \mathbf{f(x)\,dx} \approx \int_a^b \mathbf{f_n(x)\,dx}$$

where $f_n(x)$ is an n^{th} order interpolating polynomial.

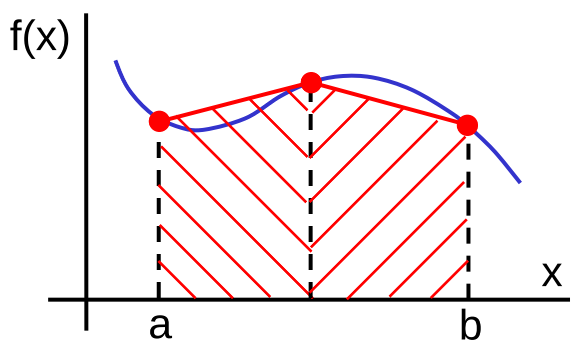
1^{st} order polynomial



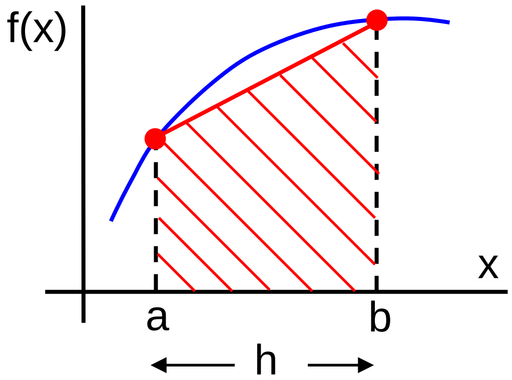
2^{nd} order polynomial



1^{st} order with multiple segments



Trapezoidal Rule:



$$I \approx \frac{f(a)+f(b)}{2}\underbrace{(b-a)}_{h} \quad = \quad \textbf{Average height} * \textbf{width}$$

All Newton-Cotes formulas can be written in the form "Average height * width". Different formulas will have different expressions for average height.

Newton-Cotes formulas can be derived by integrating Newton's Interpoating Polynomials. Newton-Gregory version can be used for equispaced data points. These derivations also provide an estimate for the truncation error.

- Newton's Divided Difference Interpolating Polynomials

$$f_n(x) = f(x_0) + (x - x_0)\, f[x_1, x_0] + (x - x_0)(x - x_1)\, f[x_2, x_1, x_0] + \ldots$$
$$+ (x - x_0)(x - x_1) \cdots (x - x_{n-1})\, f[x_n, x_{n-1}, \ldots, x_1, x_0]$$

- Newton-Gregory Formula

$$f_n(x) = f(x_0) + \Delta f(x_0)\, \alpha + \Delta^2 f(x_0)\, \alpha(\alpha - 1) / 2! + \ldots + \Delta^n f(x_0)\, \alpha(\alpha - 1) \cdots (\alpha - n + 1) / n! + R_n$$

where $\alpha = (x - x_0) / h$, $R_n = f^{(n+1)}(\xi)\, h^{n+1}\, \alpha(\alpha - 1) \cdots (\alpha - n) / (n+1)!$

and $\Delta f^n(x_0)$ is the n^{th} forward difference.

Derivation of the Trapezoidal Rule using Newton-Gregory Formula:

$$I = \int_a^b \left[\underbrace{f(a) + \Delta f(a)\alpha}_{1^{st} \text{ order N-G formula}} + \underbrace{\frac{f''(\xi)}{2}\alpha(\alpha-1)h^2}_{\text{Remainder term}} \right] dx$$

Change integration limits from x to α.

$$\alpha = \frac{x-a}{h}, \qquad dx = h d\alpha, \qquad \int_{x=a}^{x=b} dx \rightarrow \int_{\alpha=0}^{\alpha=1} h\, d\alpha$$

$$I = \int_{\alpha=0}^{1} \left[f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha-1)h^2 \right] h\, d\alpha$$

$$I = h\int_0^1 \left(f(a) + \Delta f(a)\alpha\right) d\alpha + h^3 \int_0^1 \frac{f''(\xi)}{2}\alpha(\alpha-1)\, d\alpha$$

$$I = h\left[f(a)\alpha + \underbrace{\Delta f(a)}_{f(b)-f(a)} \frac{\alpha^2}{2} \right]_0^1 + h^3 \left[\frac{f''(\xi)}{2}\left(\frac{\alpha^3}{3} - \frac{\alpha^2}{2}\right) \right]_0^1$$

$$I = \underbrace{h\frac{f(a)+f(b)}{2}}_{\text{Trapezoidal Rule}} \underbrace{- \frac{1}{12} f''(\xi)\, h^3}_{\text{Truncation Error } (E_t)}$$

- Trapezoidal Rule is first order accurate. It can integrate linear polynomials exactly.

Error Estimation for the Trapezoidal Rule:

$$I = h\,\frac{f(a)+f(b)}{2} - \frac{1}{12}\,f''(\xi)\,h^3$$

- Usually $f''(\xi)$ in the error term can not be evaluated since ξ is not known.
- If the function f is known than $f''(\xi)$ can be approximated with an average 2**nd** derivative

$$f''(\xi) \approx \overline{f''(x)} = \frac{\int_a^b f''(x)\,dx}{b-a} \quad \rightarrow \quad E_a = -\frac{h^3}{12}\,\overline{f''(x)}$$

Example 35: Integrate $f(x)= e^x$ from a=1.5 to a=2.5 using the Trapezoidal Rule. Estimate the error.

True value is $e^{2.5} - e^{1.5} = 7.700805$

Using the trapezoidal rule:

$a = 1.5$, $b = 2.5$, $h = 2.5 - 1.5 = 1.0$

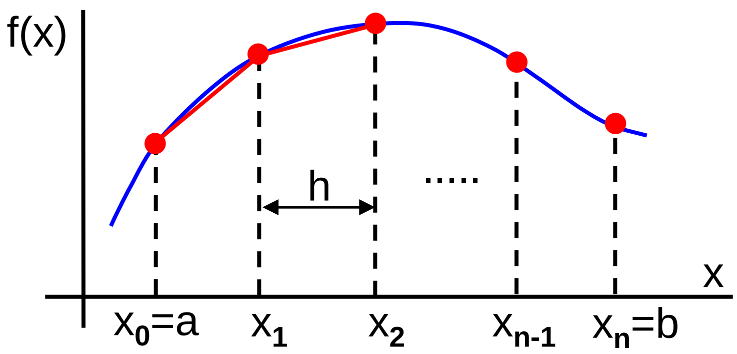
$$I \approx h\,\frac{f(a)+f(b)}{2} = 1.0\,\frac{e^{1.5}+e^{2.5}}{2} = 8.332092$$

$E_t = - 0.631287$, $\varepsilon_t = - 8.2\ \%$

Estimated error:

$$E_a \approx -\frac{h^3}{12}\,\frac{\int_a^b f''(x)\,dx}{b-a} = -\frac{1^3}{12}\,\frac{\int_{1.5}^{2.5} e^x\,dx}{1.0} = -0.641734$$

Multiple application of the Trapezoidal Rule:



In general we have n+1 points and n intervals (segments).

If the points are equispaced $h = (b-a)/n$

$$I = \int_a^b f(x)\,dx = \int_{x0}^{x1} f(x)\,dx + \int_{x1}^{x2} f(x)\,dx + \ldots + \int_{x(n-1)}^{xn} f(x)\,dx$$

$$I \approx h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \ldots + h\frac{f(x_{n-1})+f(x_n)}{2}$$

$$I \approx \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right] = (b-a)\left[\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}\right]$$

- The last equation is again of the form “Width * Average height”

Error Estimation for the Multiple Application of the Trapezoidal Rule:

- Add the individual errors for each interval $\rightarrow$ $$E_t = -\frac{h^3}{12}\sum_{i=1}^{n} f''(\xi_i) = -\frac{(b-a)^3}{12\,n^3}\sum_{i=1}^{n} f''(\xi_i)$$

- Use a single ξ for the entire interval $\rightarrow$ $$\sum_{i=1}^{n} f''(\xi_i) = n\,f''(\xi)$$

$$E_t = -\frac{(b-a)^3}{12\,n^2}\,f''(\xi) = -\frac{(b-a)\,h^2}{12}\,f''(\xi)$$

- This is of order h^2. Compare it with the true error of the single application of the Trapezoidal Rule which was of order h^3.

- Similar to the single application of the trapezoidal rule, if the function f is known than $f''(\xi)$ can be approximated with an average 2^{nd} derivative

$$f''(\xi) \approx \overline{f''(x)} = \frac{\int_a^b f''(x)\,dx}{b-a} \quad \rightarrow \quad E_a = -\frac{(b-a)^3}{12\,n^2}\,\overline{f''(x)}$$

Example 36: Integrate f(x)= e^x from a=1.5 to a=2.5 using the Trapezoidal Rule. Use a step size of 0.25. True value of the integral is 7.700805.

a = 1.5, b = 2.5, h = 0.25 than we have n=4 intervals.

$$I \approx (b-a)\left[\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_1)}{2n}\right] = (2.5-1.5)\left[\frac{e^{1.5} + 2\,(e^{1.75}+e^{2}+e^{2.25}) + e^{2.5}}{2\,(4)}\right]$$

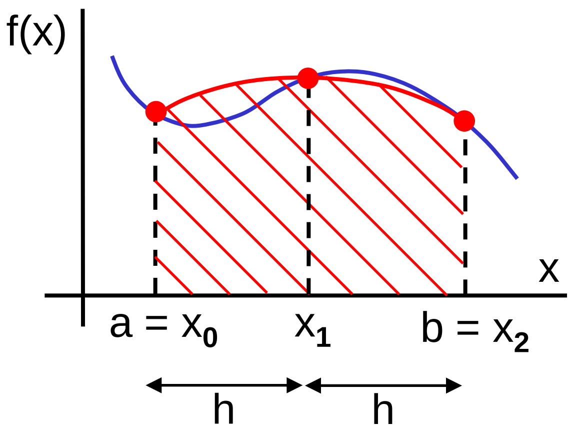
$I \approx 7.740872$, E_t = - 0.040067, ε_t = - 0.5 %

Estimated error: $$E_a = -\frac{(b-a)^3}{12\,n^2}\,\overline{f''(x)} = -\frac{(1.0)^3}{12\,(4)^2}\,\frac{\int_{1.5}^{2.5} f''(x)\,dx}{(1.0)} = -0.040108$$

Note that the calculation of E_a requires the evaluation of the same integral that the question asks for. Of course the integral in E_a can laso be calculated numerically. This approach also gives

$$E_a = -\frac{(1.0)^3}{12\,(4)^2}\,\frac{7.740872}{(1.0)} = -0.040317$$

Simpson's 1/3 Rule:



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

$$I \approx (b-a)\,\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$$

This can be derived using the second order Newton-Gregory formula

$$I = \int_{x0}^{x2} \left[\underbrace{f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha-1)}_{2^{nd}\ \text{order Newton-Gregory}} + \underbrace{\frac{\Delta^3 f(x_0)}{6}\alpha(\alpha-1)(\alpha-2)}_{\text{This term will vanish}} + \text{Remainder} \right] dx$$

where the remainder is $\quad \dfrac{\Delta^4 f(x_0)}{24}\alpha(\alpha-1)(\alpha-2)(\alpha-3)h^4$

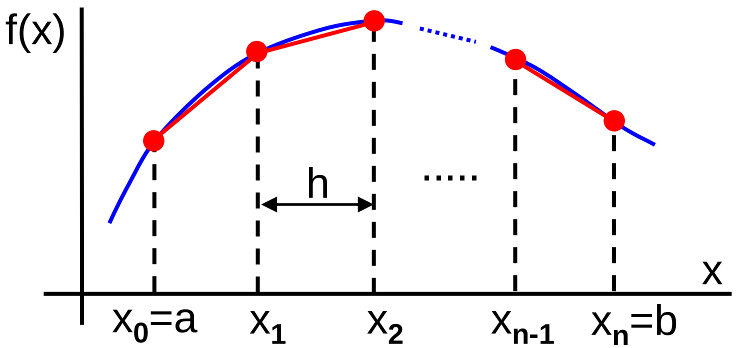
The derivation yields (see page 597 for details)

$$I = \underbrace{\frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right]}_{\text{Simpson's 1/3 Rule}} \underbrace{-\frac{1}{90} f^{(4)}(\xi)\,h^5}_{\text{Truncation Error }(E_t)}$$

$$E_a = -\frac{h^5}{90}\bar{f}^{(4)}(x) = -\frac{(b-a)^5}{2880}\bar{f}^{(4)}(x)$$

- Simpson's 1/3 Rule uses 3 points, therefore it is expected to integrate 2nd order polynomials exactly.
- However it can integrate cubics exactly. This is due to the vanishing third term in integrating the Newton-Gregory polynomial.

Multiple application of Simpson's 1/3 Rule Rule:



In general we have n+1 points and n intervals.

If the points are equispaced h = (b-a)/n

If there are even number of points the integration can not be done with Simpson's 1/3 rule only.

$$I = \int_a^b f(x)\,dx = \int_{x0}^{x2} f(x)\,dx + \int_{x2}^{x4} f(x)\,dx + \ldots + \int_{x(n-2)}^{xn} f(x)\,dx$$

$$I \approx \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] + \frac{h}{3}[f(x_2)+4f(x_3)+f(x_4)] + \ldots + \frac{h}{3}[f(x_{n-2})+4f(x_{n-1})+f(x_n)]$$

$$I \approx (b-a)\left[\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{i=2,4,6}^{n-1} f(x_i) + f(x_n)}{3n}\right] \qquad E_a = -\frac{(b-a)^5}{180\,n^4}\,\bar{f}^{(4)}(x)$$

Example 37: Calculate $\int_0^{\pi} \sin(x)\,dx$ using

(a) Trapezoidal Rule with n=2, n=4 and n=6.

(b) Simpson's 1/3 Rule with n=2, n=4 and n=6.

(a) For n=2, h=π/2,

$$I \approx \frac{h}{2}\left[f(x_0) + 2\,f(x_1) + f(x_2)\right] = \frac{\pi/2}{2}\left[\sin(0) + 2\sin(\pi/2) + \sin(\pi)\right] = \frac{\pi}{2} = 1.570796$$

$$E_a = -\frac{(b-a)^3}{12\,n^2}\,\bar{f}''(x) = -\frac{(\pi-0)^3}{12\,(2)^2}\,\frac{\int_0^{\pi} -\sin(x)\,dx}{\pi - 0} = 0.411234$$

Note that $E_t = 0.429204$

(b) For n=4, h=π/4,

$$I \approx \frac{h}{3}\left[f(x_0) + 4\,f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)\right]$$

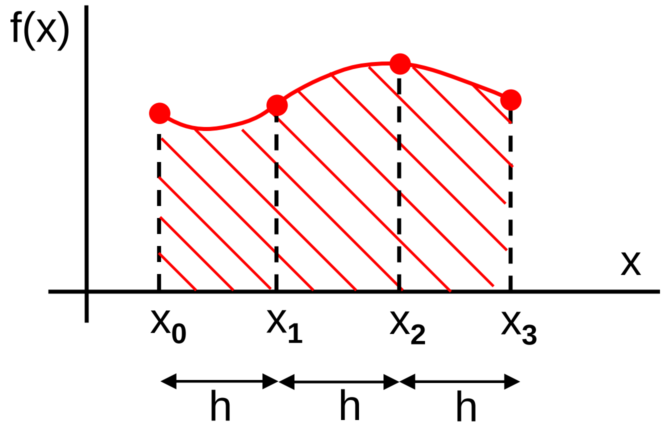
$$= \frac{\pi/4}{3}\left[\sin(0) + 4\sin(\pi/4) + 2\sin(\pi/2) + 4\sin(3\pi/4) + \sin(\pi)\right] = 2.004560$$

$$E_a = -\frac{(b-a)^5}{180\,n^4}\,\bar{f}^{(4)}(x) = -\frac{(\pi-0)^5}{180\,(4)^4}\,\frac{\int_0^{\pi} \sin(x)\,dx}{\pi - 0} = 0.004228$$

Note that $E_t = 0.004560$

Exercise 38: Complete the solution of this example.

Simpson's 3/8 Rule:



$$I \approx \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

$$I \approx (b-a)\left[\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}\right]$$

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi)$$

Exercise 39: Derive this formula by integrating the proper Newton-Gregory polynomial.

Exercise 40: Derive the formula for the multiple application of Simpson's 3/8 Rule.

- Note that 3/8 Rule uses 4 points and it is third order accurate (can integrate cubic polynomials exactly).
- 1/3 Rule does this with 3 points and it is preferred.
- 3/8 rule is useful if there are even number of points.
- 1/3 and 3/8 can be used together, but mixing them with the Trapezoidal Rule is not suggested. Because the accuracy of the Trapezoidal rule is only first order.

Exercise 41: Perform an efficient third order accurate calculation for the previous example with n=7. Use an efficient proper combiation of 1/3 and 3/8 Rules.

Richardson Extrapolation for Integration

Similar to the discussion we made for differentiation,

I: Exact integral (usually not known)

$I = I_1 + E_1$ where I_1: Estimated integral using $h=h_1$. E_1: Error of the estimation I_1.

$I = I_2 + E_2$ where I_2: Estimated integral using $h=h_2$. E_2: Error of the estimation I_2.

If multiple application of the Trapezoidal Rule is used to get the estimates I_1 and I_2, than

$E_1 = O(h_1^2)$, $E_2 = O(h_2^2)$

Using these, I_1 and I_2 can be combined to get a better estimate such as

$$\mathbf{I} \approx \mathbf{I_2} + \frac{\mathbf{I_2} - \mathbf{I_1}}{(\mathbf{h_1}/\mathbf{h_2})^2 - 1}$$

This new estimate is $O(h^4)$ accurate.

A special case of $h_2 = h_1/2$ results in

$$\mathbf{I} \approx \frac{4}{3}\mathbf{I_2} - \frac{1}{3}\mathbf{I_1}$$

Romberg Integration

- Apply multiple Richardson Extrapolation one after the other.
- If we use Trapezoidal Rule and successively halve the step size

$I_{1,1}$ is the integral obtained by h. Usually we start with a single segment, i.e, $h = b - a$

$I_{2,1}$ is the integral obtained by h/2.

$I_{3,1}$ is the integral obtained by h/4.

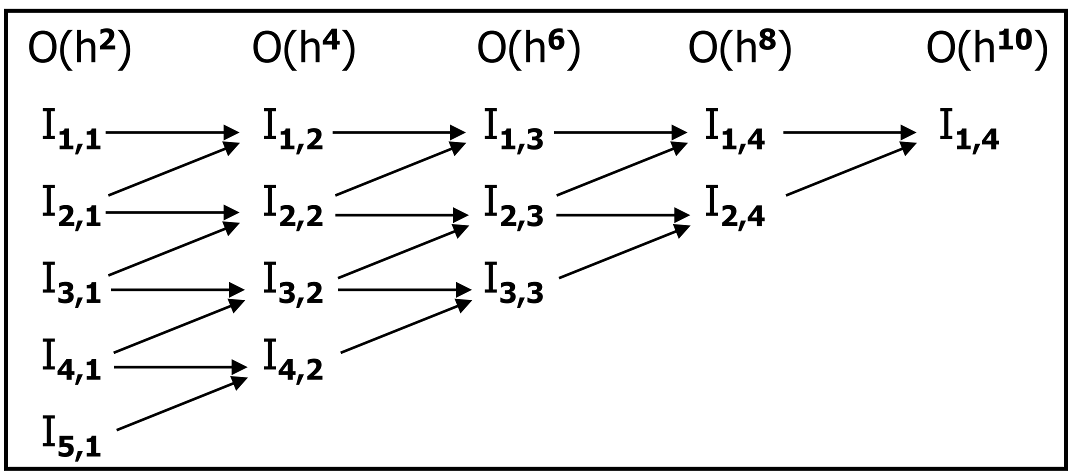
etc.

Combine $I_{1,1}$ and $I_{2,1}$ to get $I_{1,2}$ $\quad I_{1,2} = 4/3\ I_{2,1} - 1/3\ I_{1,1}$

Combine $I_{2,1}$ and $I_{3,1}$ to get $I_{2,2}$ $\quad I_{2,2} = 16/15\ I_{3,1} - 1/15\ I_{2,1}$

Combine $I_{1,2}$ and $I_{2,2}$ to get $I_{1,3}$ $\quad I_{1,3} = 64/63\ I_{2,1} - 1/63\ I_{1,1}$

etc.



$$I_{j,k} \approx \frac{4^{k-1}\, I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

Valid if Trapezoidal Rule with successive halving of the step size is used to get the first column.

$$|\varepsilon_a| = \left| \frac{I_{1,k} - I_{1,k-1}}{I_{1,k}} \right| * 100\%$$

Example 38: Perform 4 levels of Romberg Integration to integrate sin(x) over the interval [0,π].

Use Trapezoidal Rule.

$h=\pi$, $I_{1,1} = \pi/2\, [\sin(0) + \sin(\pi)] = 0.0$

$h=\pi/2$, $I_{1,2} = (\pi/2)/2\, [\sin(0) + 2\sin(\pi/2) + \sin(\pi)] = 1.57079633$

$h=\pi/4$, $I_{1,3} = (\pi/4)/2\, [\sin(0) + 2\sin(\pi/4) + 2\sin(\pi/2) + 2\sin(3\pi/4) + \sin(\pi)] = 1.89611890$

$h=\pi/8$, $I_{1,4} = 1.97423160$

k=1	k=2	k=3	k=4
0.00000000	2.09439511	1.99857073	2.00000555
1.57079633	2.00455976	1.99998313	
1.89611890	2.00026917		
1.97423160			

Sample error calculation

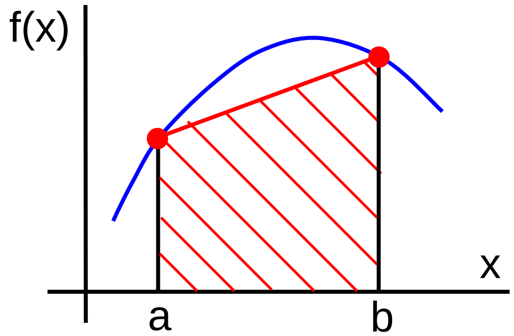
$$\varepsilon_a = \left| \frac{2.00000555 - 1.99857073}{2.00000555} \right| 100 = 0.07\%$$

Exercise 42: The true error of the final result is about $6x10^{-6}$. We can estimate the number of segments to be used to achieve this accuracy with the Trapezoidal Rule.

$$|E_a| = \left| -\frac{(b-a)^3}{12\,n^2}\,\bar{f}''(x) \right| = \frac{(\pi-0)^3}{12\,n^2}\,\frac{\int_0^{\pi} \sin(x)\,dx}{\pi - 0} = 6x10^{-6} \quad \rightarrow \quad n = 370$$

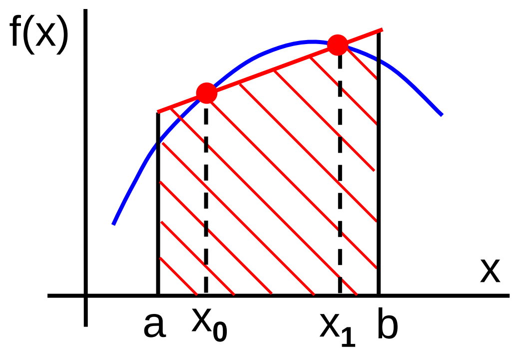
Gauss-Quadrature Integration

• Trapezoidal rule uses two points to perform the integration. These two points are the end points of the interval.



$$I \approx (b-a)\,\frac{f(a)+f(b)}{2}$$

• What if we use some other points?



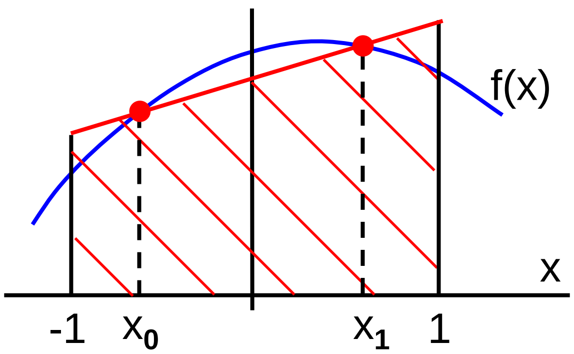
$$I \approx c_0\, f(x_0) + c_1\, f(x_1)$$

• Gauss-Quadrature uses special points in the interval [a,b] to achieve higher accuracy than Newton-Cotes formulas. But it is not suitable for integrating tabulated data, it can be used if the function is known.

• The special points (x_0, x_1) and the weights (c_0, c_1) can be determined using a technique called Method of Undetermined Coefficients.

Derivation of the Two Point Gauss-Quadrature Formula Using the Method of Undetermined Coefficients

Consider the calculation of the integral of f(x) over the interval [-1,1]



$$I \approx c_0 f(x_0) + c_1 f(x_1)$$

- We have 4 unknowns. We need 4 equations to find them.
- We will get these equations by assuming that this formula calculates constant, linear, parabolic and cubic functions exactly (Note that Trapezoidal Rule also uses two points and can only calculate constant and linear functions exactly).

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1\, dx = 2$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x\, dx = 0$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^2\, dx = 2/3$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^3\, dx = 0$$

$$c_0 = 1$$
$$c_1 = 1$$
$$x_0 = -1/\sqrt{3}$$
$$x_1 = 1/\sqrt{3}$$

$$\longrightarrow \quad I \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

• Note that this formula integrates over the domain $x_d \in [-1,1]$. This is done to simplify the mathematics and to get a general formula that can be applied to any domain with a change of variable.

• To apply this formula to a domain of $x \in [a,b]$ we need to change the variable as

$$\int_a^b f(x)\,dx \quad \rightarrow \quad \int_{-1}^{1} f(x_d)\,dx_d \qquad \text{using} \qquad x = \frac{(b+a)+(b-a)\,x_d}{2} \quad , \quad dx = \frac{b-a}{2}\,dx_d$$

Example 39: Integrate sin(x) over $[0,\pi]$ using two-point Gauss Quadrature.

$$x = \pi/2 + (\pi/2)x_d \quad , \quad dx = \pi/2\,dx_d \qquad \rightarrow \qquad \int_0^{\pi} \sin(x)\,dx \; = \; \int_{-1}^{1} \sin\left(\frac{\pi}{2}+\frac{\pi}{2}x_d\right)\frac{\pi}{2}\,dx_d$$

Therefore the function we need to use in the Gauss-Quadrature formula is

$$f(x_d) = \frac{\pi}{2}\sin\left(\frac{\pi}{2}+\frac{\pi}{2}x_d\right)$$

$$I \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = \frac{\pi}{2}\sin\left(\frac{\pi}{2}-\frac{\pi}{2\sqrt{3}}\right) + \frac{\pi}{2}\sin\left(\frac{\pi}{2}+\frac{\pi}{2\sqrt{3}}\right) = 1.9358196$$

For this calculation $|E_t| = 0.064$. To achieve this accuracy with the Trapezoidal Rule we approximately need 5 segments.

$$|E_a| = \left| -\frac{(b-a)^3}{12\,n^2}\,\overline{f''}(x) \right| = \frac{(\pi-0)^3}{12\,n^2}\,\frac{\int_0^{\pi}\sin(x)\,dx}{\pi-0} = 0.064 \quad \rightarrow \quad n = 5$$

Higher Order Gauss-Quadrature Formulas

- The general version of Gauss-Quadrature uses n points.

$$I \approx c_0 f(x_0) + c_1 f(x_1) + \ldots + c_{n-1} f(x_{n-1})$$

- We can use the method of undetermined coefficients to get 2n equations to solve for 2n unknowns.
- Table 22.1 shows the weighting factors and integration points upto n=6.

Exercise 43: Derive the 3-point Gauss-Quadrature formula.

Exercise 44: Use this formula to integrate sin(x) over $[0,\pi]$. Approximately how many segments are necessary to get the same accuracy with the Trapezoidal Rule, Simpson's 1/3 Rule and Simpson's 3/8 Rule?