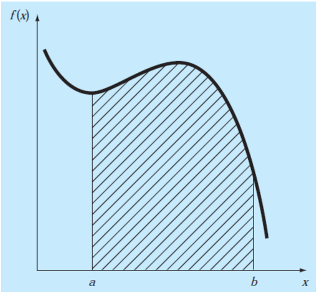
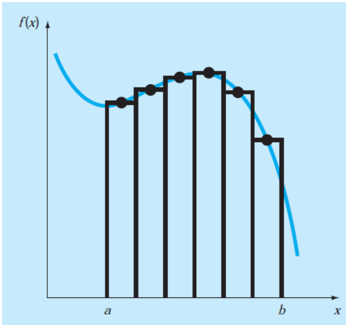
Lecture 13: Numerical Integration





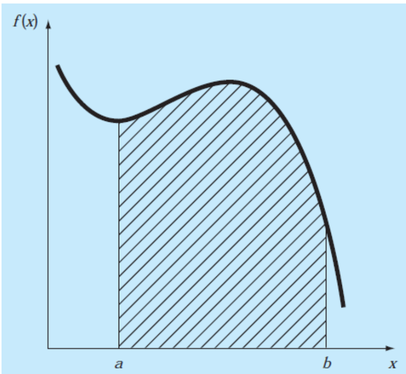
Integration

- The inverse process to differentiation in calculus is integration.
- According to the dictionary definition, to integrate means "to bring together, as parts, into a whole; to unite; to indicate the total amount . . . ."
- Mathematically, integration is represented by

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

- The function *f*(*x*) is referred to as the integrand.

Integration

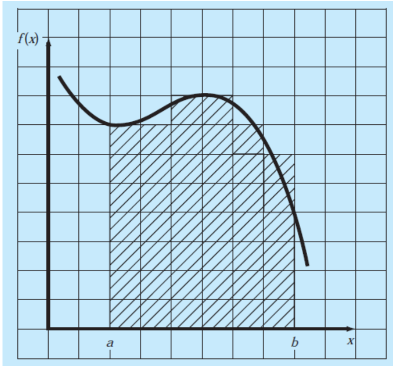


Integration

- The function to be differentiated or integrated will typically be in one of the following three forms:
  1. A simple continuous function such as a polynomial, an exponential, or a trigonometric function.
  2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
  3. A tabulated function where values of x and *f*(*x*) are given at a number of discrete points, as is often the case with experimental or field data.

Non-computer Methods

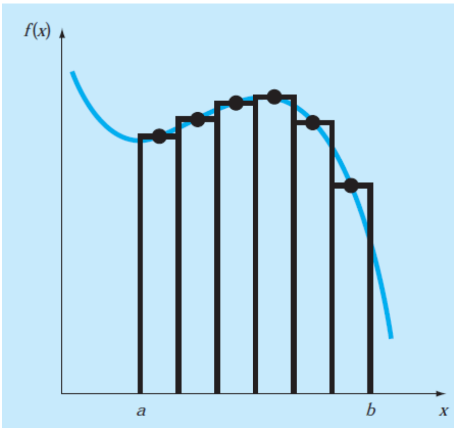
- A simple intuitive approach is to plot the function on a grid and count the number of boxes that approximate the area.
- This number multiplied by the area of each box provides a rough estimate of the total area under the curve.
- This estimate can be refined, at the expense of additional effort, by using a finer grid.



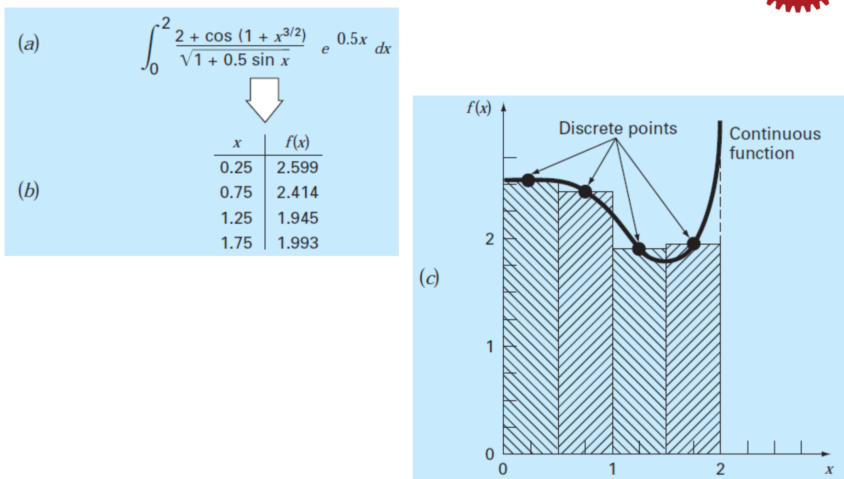
Non-computer Methods

- Another commonsense approach is to divide the area into vertical segments, or strips, with a height equal to the function value at the midpoint of each strip.
- The area of the rectangles can then be calculated and summed to estimate the total area.
- In this approach, it is assumed that the value at the midpoint provides a valid approximation of the average height of the function for each strip.
- As with the grid method, refined estimates are possible by using more (and thinner) strips to approximate the integral.

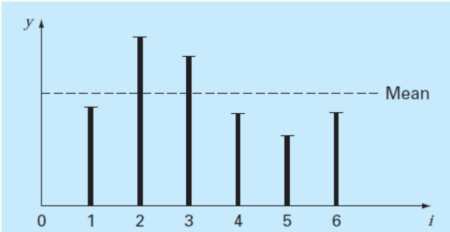
Non-computer Methods



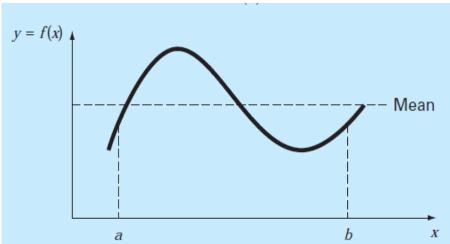
Non-computer Methods



Mean for Data



$$\text{Mean} = \frac{\sum_{i=1}^{n} y_i}{n}$$



$$\text{Mean} = \frac{\int_a^b f(x)\,dx}{b-a}$$

Newton-Cotes Integration Formulas

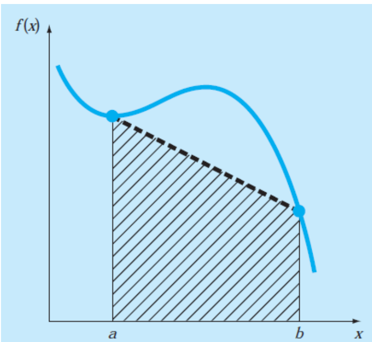
- The Newton-Cotes formulas are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

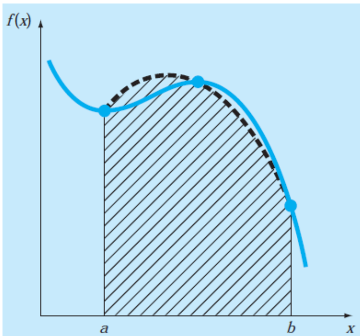
$$I = \int_a^b f(x)\,dx \cong \int_a^b f_n(x)\,dx$$

- where $f_n(x)$ = a polynomial of the form

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

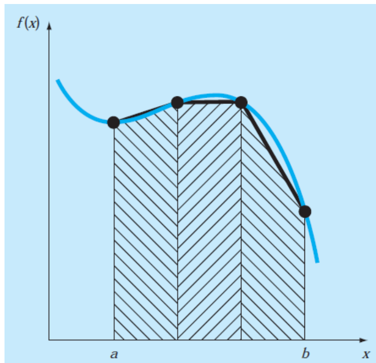
Newton-Cotes Integration Formulas





Newton-Cotes Integration Formulas

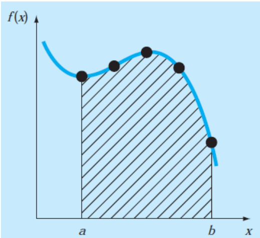
- The integral can also be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length.

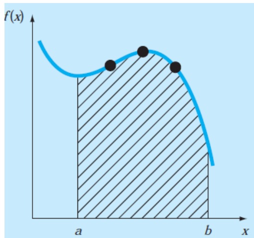


"Strip method" employs a series of zero-order polynomials (that is, constants) to approximate the integral.

Newton-Cotes Integration Formulas

- Closed and open forms of the Newton-Cotes formulas are available.
- The closed forms are those where the data points at the beginning and end of the limits of integration are known.
- The open forms have integration limits that extend beyond the range of the data.





The Trapezoidal Rule

- The trapezoidal rule is the first of the Newton-Cotes closed integration formulas.
- It corresponds to the case where the polynomial is first-order:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_1(x)\,dx$$

- Recall that a straight line can be represented as

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

The Trapezoidal Rule

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

- The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b:

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

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

The trapezoidal rule

Derivation of Trapezoidal Rule

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + f(a) - \frac{a\,f(b) - a\,f(a)}{b - a}$$

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(a) - af(b) + af(a)}{b - a}$$

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(b)}{b - a}$$

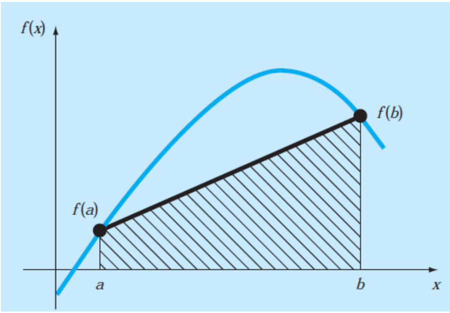
$$I = \frac{f(b) - f(a)}{b - a}\frac{x^2}{2} + \frac{bf(a) - af(b)}{b - a}x\Big|_a^b$$

$$I = \frac{f(b) - f(a)}{b - a}\frac{(b^2 - a^2)}{2} + \frac{bf(a) - af(b)}{b - a}(b - a)$$

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

The Trapezoidal Rule

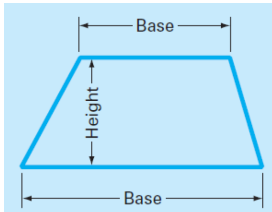
- Geometrically, the trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting $f(a)$ and $f(b)$.

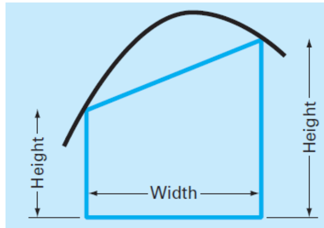


The Trapezoidal Rule

- The formula for computing the area of a trapezoid is the height times the average of the bases.
- In our case, the concept is the same but the trapezoid is on its side.
- Therefore, the integral estimate can be represented as

$$I \cong \text{width} \times \text{average height}$$





The Trapezoidal Rule

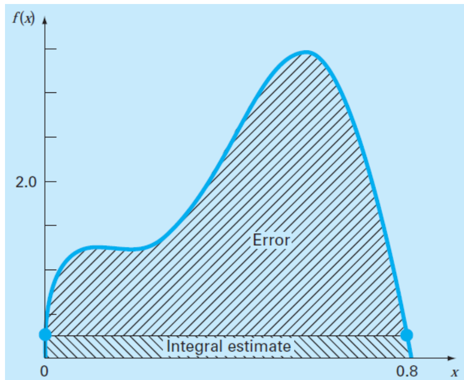
$$I \cong \text{width} \times \text{average height}$$

$$I \cong (b - a) \times \text{average height}$$

- where, for the trapezoidal rule, the average height is the average of the function values at the end points, or $[f(a) + f(b)]/2$.
- All the Newton-Cotes closed formulas can be expressed in the general format of the equation above.
- In fact, they differ only with respect to the formulation of the average height.

Error of the Trapezoidal Rule

- When we employ the integral under a straight-line segment to approximate the integral under a curve, we obviously can incur an error that may be substantial.



Error of the Trapezoidal Rule

- An estimate for the local truncation error of a single application of the trapezoidal rule is

$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

Derivation and Error Estimate of Trapezoidal Rule

- An alternative derivation of the trapezoidal rule is possible by integrating the forward Newton-Gregory interpolating polynomial.

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

$$\alpha = (x-a)/h,$$

$$dx = h\, d\alpha$$

$h = b - a$ (for the one-segment trapezoidal rule)

Derivation and Error Estimate of Trapezoidal Rule

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

- If it is assumed that, for small h, the term $f'(\xi)$ is approximately constant.

$$I = h\left[\alpha f(a) + \frac{\alpha^2}{2}\Delta f(a) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right) f''(\xi)h^2 \right]_0^1$$

$$I = h\left[f(a) + \frac{\Delta f(a)}{2} \right] - \frac{1}{12} f''(\xi)h^3$$

$$\Delta f(a) = f(b) - f(a),$$

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

Example 1

Single Application of the Trapezoidal Rule

Problem Statement. Use Eq. (21.3) to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall from Sec. PT6.2 that the exact value of the integral can be determined analytically to be 1.640533.

$$f(0) = 0.2$$

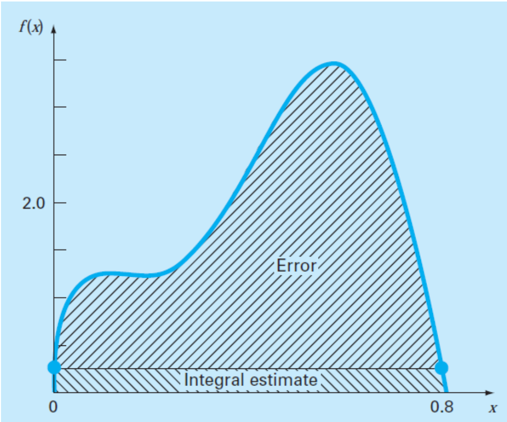
$$f(0.8) = 0.232$$

$$I \cong 0.8\frac{0.2 + 0.232}{2} = 0.1728$$

$$E_t = 1.640533 - 0.1728 = 1.467733$$

$$\varepsilon_t = 89.5\%$$

Example 1



Example 1

$$f''(x) = -400 + 4050x - 10{,}800x^2 + 8000x^3$$

$$\text{Mean} = \frac{\int_a^b f(x)\,dx}{b-a}$$

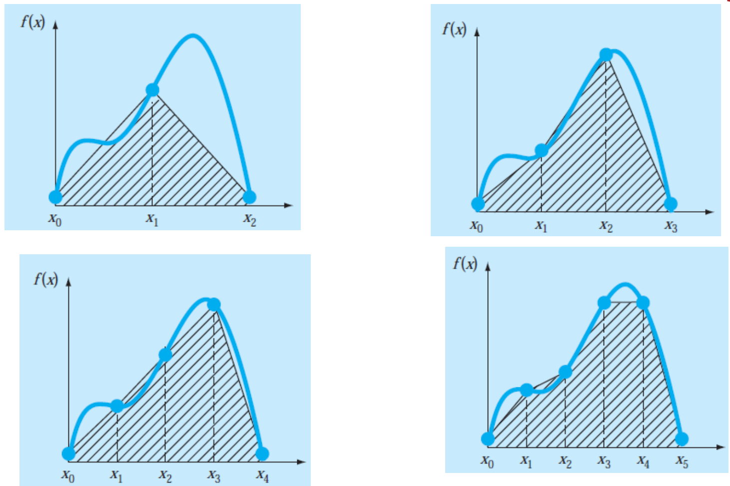
$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4050x - 10{,}800x^2 + 8000x^3)\,dx}{0.8 - 0} = -60$$

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

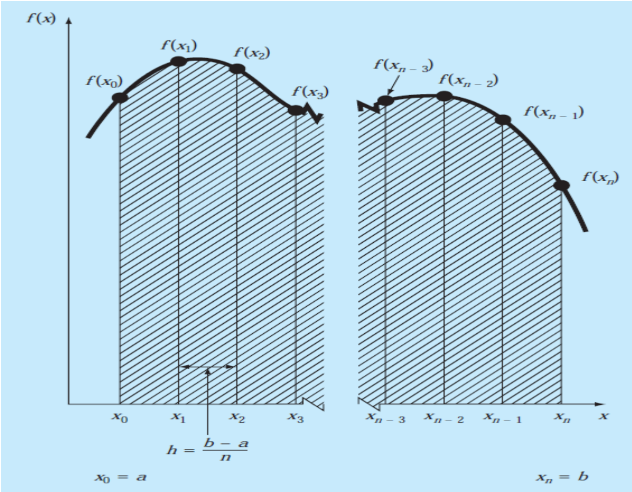
Multiple-Application Trapezoidal Rule

- One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from *a* to *b* into a number of segments and apply the method to each segment.
- The areas of individual segments can then be added to yield the integral for the entire interval.
- The resulting equations are called multiple-application, or composite, integration formulas.

Multiple-Application Trapezoidal Rule



Multiple-Application Trapezoidal Rule



Multiple-Application Trapezoidal Rule

- There are n +1 equally spaced base points (x_0, x_1, x_2, . . . , x_n).
- Consequently, there are n segments of equal width:

$$h = \frac{b-a}{n}$$

$$I = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

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

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

Multiple-Application Trapezoidal Rule

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

$$h = \frac{b-a}{n}$$

$$I = \underbrace{(b-a)}_{\text{Width}}\ \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}}$$

- Because the summation of the coefficients of $f(x)$ in the numerator divided by $2n$ is equal to 1, the average height represents a weighted average of the function values.
- The interior points are given twice the weight of the two end points $f(x_0)$ and $f(x_n)$.

Multiple-Application Trapezoidal Rule

- An error for the multiple-application trapezoidal rule can be obtained by summing the individual errors for each segment to give

$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i=1}^{n} f''(\xi_i)$$

- where $f''(\xi_i)$ is the second derivative at a point ξ_i located in segment i.

Multiple-Application Trapezoidal Rule

$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i=1}^{n} f''(\xi_i)$$

- This result can be simplified by estimating the mean or average value of the second derivative for the entire interval as

$$\bar{f}'' \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

Therefore, $\Sigma f''(\xi_i) \cong n\bar{f}''$

$$E_a = -\frac{(b-a)^3}{12n^2}\bar{f}''$$

If the number of segments is doubled, the truncation error will be quartered

Example 2

Multiple-Application Trapezoidal Rule

Problem Statement. Use the two-segment trapezoidal rule to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Employ Eq. (21.13) to estimate the error. Recall that the correct value for the integral is 1.640533.

Solution. $n = 2$ $(h = 0.4)$:

$f(0) = 0.2$ $\quad f(0.4) = 2.456$ $\quad f(0.8) = 0.232$

$$I = 0.8\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

$$E_t = 1.640533 - 1.0688 = 0.57173 \qquad \varepsilon_t = 34.9\%$$

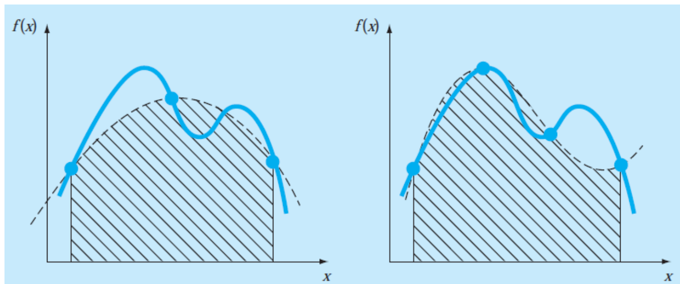
$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

Example 2

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

Simpson's Rules

- Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points.



Simpson's 1/3 Rule

- Simpson's 1/3 rule results when a second-order interpolating polynomial is used as follows:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_2(x)\,dx$$

- If a and b are designated as x_0 and x_2 and $f_2(x)$ is represented by a second-order Lagrange polynomial, the integral becomes

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

Simpson's 1/3 Rule

- After integration and algebraic manipulation,

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

- where, for this case, $h = (b - a)/2$.
- This equation is known as Simpson's 1/3 rule.
- It is the second Newton-Cotes closed integration formula.
- The label "1/3" stems from the fact that h is divided by 3 in the equation above.

Simpson's 1/3 Rule

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4 f(x_1) + f(x_2)}{6}}_{\text{Average height}}$$

- where $a = x_0$, $b = x_2$, and x_1 = the point midway between a and b, which is given by $(b + a)/2$.
- It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi)$$

$h = (b-a)/2$

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Simpson's 1/3 Rule

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \qquad E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

- Simpson's 1/3 rule is more accurate than the trapezoidal rule.
- However, comparison between the equations indicates that it is more accurate than expected.
- Rather than being proportional to the third derivative, the error is proportional to the fourth derivative.
- This is because, the coefficient of the third-order term goes to zero during the integration of the interpolating polynomial.
- Consequently, Simpson's 1/3 rule is third-order accurate even though it is based on only three points.
- In other words, it yields exact results for cubic polynomials even though it is derived from a parabola!

Derivation and Error Estimate of Simpson's 1/3 Rule

$$I = \int_{x_0}^{x_2} \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha-1) + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha-1)(\alpha-2) + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha-1)(\alpha-2)(\alpha-3)h^4 \right] dx$$

$$I = h\int_{0}^{2} \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha-1) + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha-1)(\alpha-2) + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha-1)(\alpha-2)(\alpha-3)h^4 \right] d\alpha$$

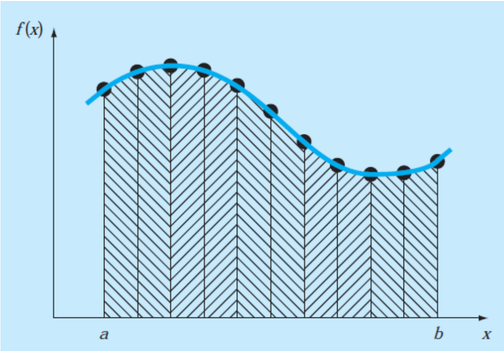
Derivation and Error Estimate of Simpson's 1/3 Rule

$$I = h\left[\alpha f(x_0) + \frac{\alpha^2}{2}\Delta f(x_0) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right)\Delta^2 f(x_0) + \left(\frac{\alpha^4}{24} - \frac{\alpha^3}{6} + \frac{\alpha^2}{6}\right)\Delta^3 f(x_0) + \left(\frac{\alpha^5}{120} - \frac{\alpha^4}{16} + \frac{11\alpha^3}{72} - \frac{\alpha^2}{8}\right) f^{(4)}(\xi)h^4 \right]_0^2$$

$$I = h\left[2 f(x_0) + 2\Delta f(x_0) + \frac{\Delta^2 f(x_0)}{3} + (0)\Delta^3 f(x_0) - \frac{1}{90} f^{(4)}(\xi)h^4 \right]$$

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

The Multiple-Application Simpson's 1/3 Rule



Note: the method can be employed only if the number of segments is even.

The Multiple-Application Simpson's 1/3 Rule

$$h = \frac{b-a}{n}$$

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

$$I \cong 2h\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$

The Multiple-Application Simpson's 1/3 Rule

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$

- The odd points represent the middle term for each application and hence carry the weight of 4.
- The even points are common to adjacent applications and hence are counted twice.
- An error estimate for the multiple-application Simpson's rule

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)}$$

The Multiple-Application Simpson's 1/3 Rule

- Simpson's 1/3 Rule is limited to cases where the values are equispaced.
- Further, it is limited to situations where there are an even number of segments and an odd number of points.
- Consequently, as discussed in the next slide, an odd-segment–even-point formula known as Simpson's 3/8 rule is used in conjunction with the 1/3 rule to permit evaluation of both even and odd numbers of segments.

Simpson's 3/8 Rule

- A third-order Lagrange polynomial can be fit to four points and integrated:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_3(x)\,dx$$

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

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}}_{\text{Average height}}$$

$$E_t = -\frac{(b-a)^5}{6480} f^{(4)}(\xi)$$

Simpson's Rule

- Simpson's 1/3 rule is usually the method of preference because it attains third-order accuracy with three points rather than the four points required for the 3/8 version.
- However, the 3/8 rule has utility when the number of segments is odd.
- For instance, if you desire an estimate for five segments.
- One option would be to use a multiple application version of the trapezoidal rule.
- This may not be advisable, however, because of the large truncation error associated with this method.

Simpson's Rule

- An alternative would be to apply Simpson's 1/3 rule to the first two segments and Simpson's 3/8 rule to the last three.
- In this way, we could obtain an estimate with third-order accuracy across the entire interval.