Numerical Methods
(MTH4002)
Lecture 06: Numerical Integration

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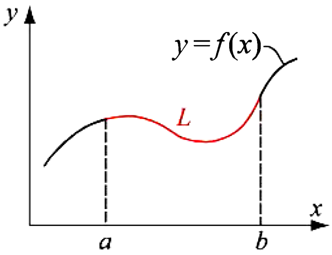
Introduction

- Integration is frequently encountered when solving problems and calculating quantities in engineering and science.
- One of the simplest examples for the application of integration is the calculation of the length of a curve.



- When a curve in the x-y plane is given by the equation $y = f(x)$, the length L of the curve between the points $x = a$ and $x = b$ is given by:

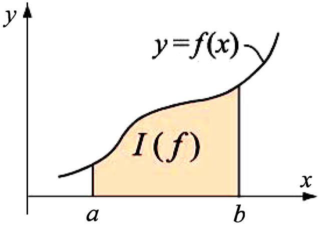
$$L = \int_a^b \sqrt{1 + [f'(x)]^2} dx$$

Background

- The general form of a definite integral (also called an antiderivative) is:

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

where $f(x)$, called the integrand, is a function of the independent variable x, and a and b are the limits of the integration (definite integration).



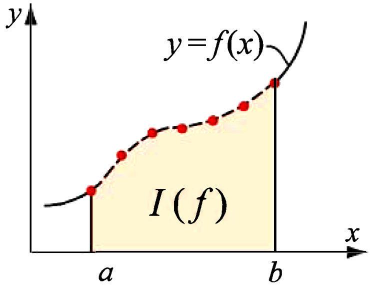
- The value of the integral $I(f)$ is a number when a and b are numbers.
- Graphically, the value of the integral corresponds to the shaded area under the curve of $f(x)$ between a and b.

Need for numerical integration

- The integrand can be an analytical function or a set of discrete points (tabulated data).
- When the integrand is a mathematical expression for which the antiderivative can be found easily, the value of the definite integral can be determined analytically.
- Numerical integration is needed when analytical integration is difficult or not possible, and when the integrand is given as a set of discrete points.

Numerical Integration Approach

- If the integrand $f(x)$ is an analytical function, the numerical integration is done by using a finite number of points at which the integrand is evaluated.



- One strategy is to use only the end points of the interval, $(a, f(a))$ and $(b, f(b))$.
- This, however, might not give an accurate enough result, especially if the interval is wide and/or the integrand varies significantly within the interval.
- Higher accuracy can be achieved by using a composite method where the interval $[a, b]$ is divided into smaller subintervals.

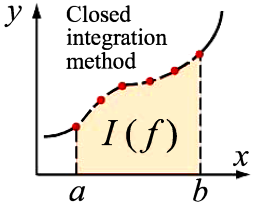
Numerical Integration Approach

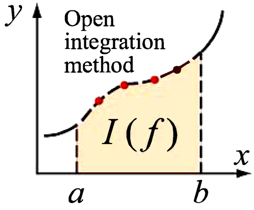
- The integral over each subinterval is calculated, and the results are added together to give the value of the whole integral.
- In all cases, the numerical integration is carried out by using a set of discrete points for the integrand.
- When the integrand is an analytical function, the location of the points within the interval $[a, b]$ can be defined by the user or is defined by the integration method.
- When the integrand is a given set of tabulated points (like data measured in an experiment), the location of the points is fixed and cannot be changed.

Numerical Integration Approach

- Various methods have been developed for carrying out numerical integration.
- In each of these methods, a formula is derived for calculating an approximate value of the integral from discrete values of the integrand.
- The methods can be divided into two groups
  - open methods and
  - closed methods.

Numerical Integration Approach





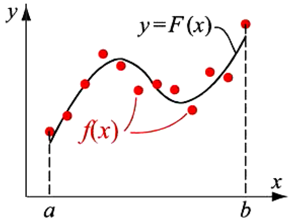
- In numerical methods, a formula is derived for calculating an approximate value of the integral from discrete values of the integrand.
- In closed integration methods, the endpoints of the interval (and the integrand) are used in the formula that estimates the value of the integral.
  - Trapezoidal method
  - Simpson's method
- In open integration methods do not include the end points in the formula.
  - Midpoint method
  - Gauss quadrature

An another approach for integration

- There are various methods for calculating the value of an integral from the set of discrete points of the integrand. Most commonly, it is done by using Newton-Cotes integration formulas.
- When the original integrand is an analytical function, the Newton-Cotes formula replaces it with a simpler function.
- When the original integrand is in the form of data points, the Newton-Cotes formula interpolates the integrand between the given points.
- Most commonly, as with the trapezoidal method and Simpson's methods, the Newton-Cotes integration formulas are polynomials of different degrees.

An another approach for integration

- The approach for integration is to curve-fit the points with a function $F(x)$ that best fits the points (the function $f(x)$ is must be specified as discrete points).
- In other words, $f(x) \approx F(x)$, where $F(x)$ is a polynomial or a simple function whose antiderivative can be found easily. Then, the integral is evaluated by direct analytical methods from calculus.



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

- This procedure requires numerical curve fitting methods for finding $F(x)$, but may not require a numerical method to evaluate the integral if $F(x)$ is an integrable function.

Rectangle and midpoint methods

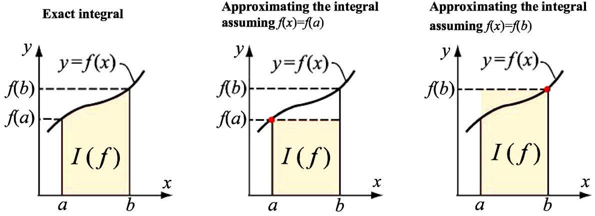
- Rectangle method

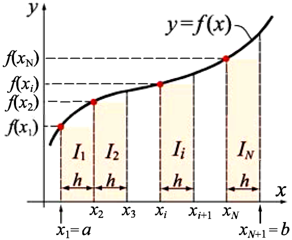
$$I(f) = \int_a^b f(a)dx = f(a)(b-a)$$

or $$I(f) = \int_a^b f(b)dx = f(b)(b-a)$$

- Composite rectangle method

$$I(f) = \int_a^b f(x)dx \approx h\sum_{i=1}^{N} f(x_i)$$





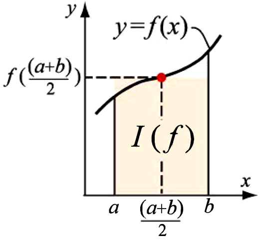
Rectangle and midpoint methods

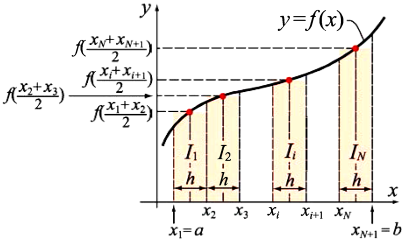
- Midpoint method

$$I(f) = \int_a^b f(x)dx \approx \int_a^b f\left(\frac{a+b}{2}\right) dx = f\left(\frac{a+b}{2}\right)(b-a)$$

- Composite midpoint method

$$I(f) = \int_a^b f(x)dx \approx h \sum_{i=1}^{N} f\left(\frac{x_i + x_{i+1}}{2}\right)$$

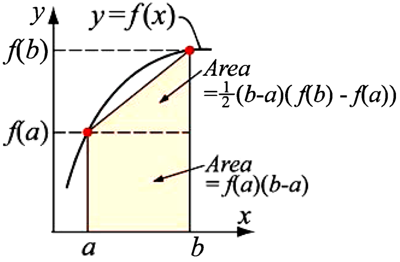




Trapezoidal method

- A refinement over the simple rectangle and midpoint methods is to use a linear function to approximate the integrand over the interval of integration.
- Newton's form of interpolating polynomials with two points $x = a$ and $x = b$, yields:

$$f(x) \approx f(a) + (x-a)f[a,b] = f(a) + (x-a)\frac{[f(b)-f(a)]}{b-a}$$

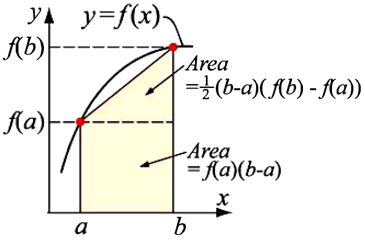


so we can write

$$\begin{aligned} I(f) &\approx \int_a^b \left(f(a) + (x-a)\frac{[f(b)-f(a)]}{b-a} \right) dx \\ &= f(a)(b-a) + \frac{1}{2}[f(b)-f(a)](b-a) \\ &= \frac{[f(a)+f(b)]}{2}(b-a) \end{aligned}$$

Trapezoidal method

- Simplifying the result gives an approximate formula popularly known as the trapezoidal rule or trapezoidal method.



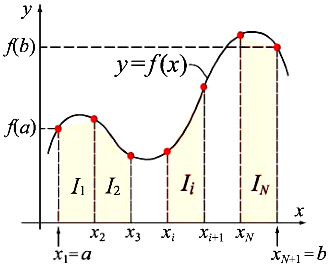
$$I(f) \approx \frac{[f(a) + f(b)]}{2}(b-a)$$

- As with the rectangle and midpoint methods, the trapezoidal method can be easily extended to yield any desired level of accuracy by subdividing the interval $[a, b]$ into subintervals.

Composite Trapezoidal

- The integral over the interval $[a, b]$ can be evaluated more accurately by dividing the interval into subintervals, evaluating the integral for each subintervals (with the trapezoidal method), and adding the results. (subintervals have identical width h)

$$I(f) = \int_a^b f(x)dx \approx \frac{1}{2}\sum_{i=1}^{N}\left[f\left(x_i\right) + f\left(x_{i+1}\right)\right]\left(x_{i+1} - x_i\right)$$



$$I(f) \approx \frac{h}{2}\sum_{i=1}^{N}\left[f\left(x_{i+1}\right) + f\left(x_i\right)\right]$$

$$I(f) \approx \frac{h}{2}\left[f(a) + 2f\left(x_2\right) + 2f\left(x_3\right) + \ldots + 2f\left(x_N\right) + f(b)\right]$$

$$\boxed{I(f) \approx \frac{h}{2}[f(a) + f(b)] + h\sum_{i=2}^{N} f\left(x_i\right)}$$

Example

Question: Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite trapezoidal rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$.

Simpson's methods

- The trapezoidal method described in the last section relies on approximating the integrand by a straight line. A better approximation can possibly be obtained by approximating the integrand with a nonlinear function that can be easily integrated.
- One class of such methods, called Simpson's rules or Simpson's methods, uses
  - quadratic (Simpson's 1/3 method), and
  - cubic (Simpson's 3/8 method)

  polynomials to approximate the integrand.

Simpson's $1/3$ Method

- In this method, a quadratic (second-order) polynomial is used to approximate the integrand.
- The coefficients of a quadratic polynomial can be determined from three points.
- For an integral over the domain $[a, b]$, the three points used are the two endpoints $x_1 = a$, $x_3 = b$, and the midpoint $x_2 = (a + b)/2$.
- The polynomial can be written in the form:

$$p(x) = \alpha + \beta\,(x - x_1) + \gamma\,(x - x_1)\,(x - x_2)$$

where α, β, and γ are unknown constants evaluated from the condition that the polynomial passes through the points, $p(x_1) = f(x_1)$, $p(x_2) = f(x_2)$, and $p(x_3) = f(x_3)$.

Simpson's $1/3$ Method

- These conditions yields

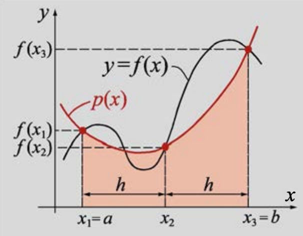
$$\alpha = f\left(x_1\right)$$
$$\beta = \left[f\left(x_2\right) - f\left(x_1\right)\right] / \left(x_2 - x_1\right)$$
$$\gamma = \frac{f\left(x_3\right) - 2f\left(x_2\right) + f\left(x_1\right)}{2(h)^2}$$

where $h = (b-a)/2$

- Substituting the constants back and integrating $p(x)$ over the interval $[a, b]$ gives

$$I = \int_{x_1}^{x_3} f(x)dx \approx \int_{x_1}^{x_3} p(x)dx = \frac{h}{3}\left[f\left(x_1\right) + 4f\left(x_2\right) + f\left(x_3\right)\right]$$
$$= \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Simpson's $1/3$ Method

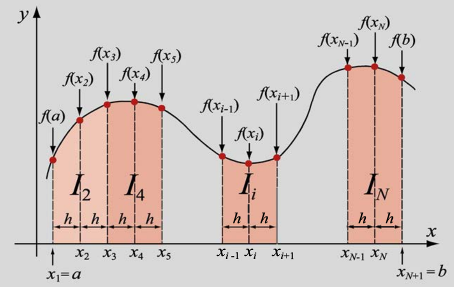


$$I = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

- The name $1/3$ in the method comes from the fact that there is a factor of $1/3$ multiplying the expression in the brackets.
- As with the rectangular and trapezoidal methods, a more accurate evaluation of the integral can be done with a composite Simpson's $1/3$ method.

Composite Simpson's $1/3$ method

- The whole interval is divided into small subintervals. Simpson's $1/3$ method is used to calculate the value of the integral in each subinterval, and the values are added together.



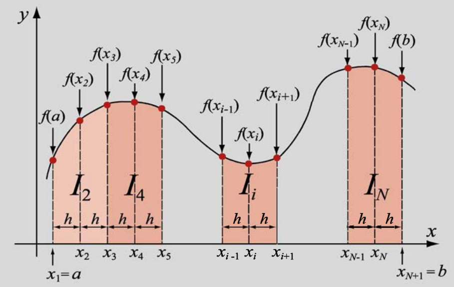
$$I_i(f) = \int_{x_{i-1}}^{x_{i+1}} f(x)dx \approx \frac{h}{3}\left[f\left(x_{i-1}\right) + 4f\left(x_i\right) + f\left(x_{i+1}\right)\right]$$

where $h = x_{i+1} - x_i = x_i - x_{i-1} = \frac{b-a}{N}$

$$I(f) \approx \frac{h}{3}\left[f(a) + 4f\left(x_2\right) + f\left(x_3\right) + f\left(x_3\right) + 4f\left(x_4\right) + f\left(x_5\right) + f\left(x_5\right) + 4f\left(x_6\right) + f\left(x_7\right) + \ldots + f\left(x_{N-1}\right) + 4f\left(x_N\right) + f(b)\right]$$

Composite Simpson's $1/3$ method

$$I(f) \approx \frac{h}{3}\left[f(a)+4f\left(x_2\right)+f\left(x_3\right)+f\left(x_3\right)+4f\left(x_4\right)+f\left(x_5\right)+f\left(x_5\right)+4f\left(x_6\right) + f\left(x_7\right)+\ldots+f\left(x_{N-1}\right)+4f\left(x_N\right)+f(b)\right]$$



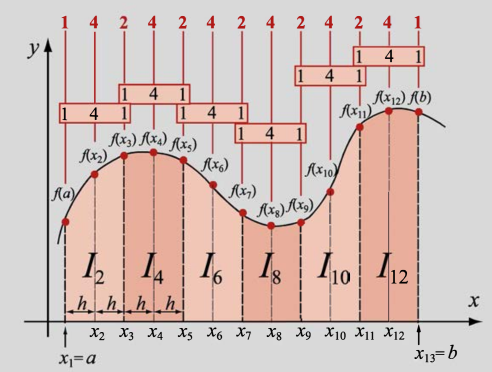
$$I(f) \approx \frac{h}{3}\left[f(a)+4\sum_{i=2,4,6}^{N} f\left(x_i\right)+2\sum_{j=3,5,7}^{N-1} f\left(x_j\right)+f(b)\right]$$

Composite Simpson's $1/3$ method

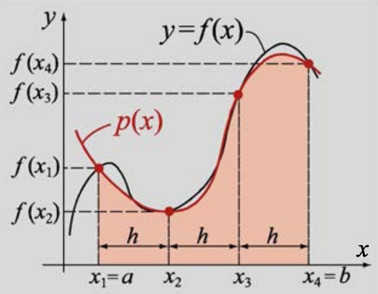
- It is important to point out that previous equation can be used only if two conditions are satisfied:
  - The subintervals must be equally spaced.
  - The number of subintervals within $[a, b]$ must be an even number.
- Simpson's $1/3$ formula is a weighted addition of the value of the function at the points that define the subintervals. The weight is 4 at all the points x; with an even index. These are the middle points of each set of two adjacent subintervals.
- The weight is 2 at all the points x; with an odd index (except the first and last points). These points are at the interface between adjacent pairs of subintervals.

Composite Simpson's $1/3$ method

- Each point is used once as the right endpoint of a pair of subinterval and once as the left endpoint of the next pair of subintervals. The endpoints are used only once.



Simpson's 3/8 Method



- In this method a cubic (third-order) polynomial is used to approximate the integrand.
- A third-order polynomial can be determined from four points.
- For an integral over the domain $[a, b]$, the four points used are the two endpoints $x_1 = a$ and $x_4 = b$, and two points x_2 and x_3 that divide the interval into three equal sections.
- The polynomial can be written in the form:

$$p(x) = c_3x^3 + c_2x^2 + c_1x + c_0$$

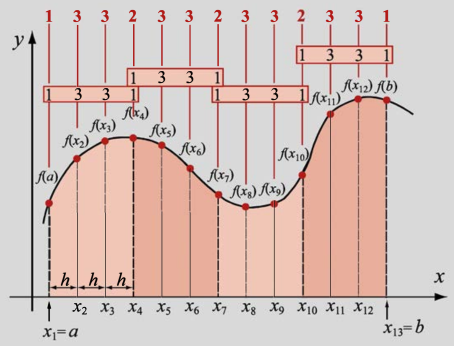
Simpson's $3/8$ Method

- where c_3, c_2, c_1, and c_0 are constants evaluated from the conditions that the polynomial passes through the points, $p(x_1) = f(x_1)$, $p(x_2) = f(x_2)$, $p(x_3) = f(x_3)$, and $p(x_4) = f(x_4)$.
- Once the constants are determined, the polynomial can be easily integrated to give:

$$I = \int_a^b f(x)dx \approx \int_a^b p(x)dx = \frac{3}{8}h\left[f(a) + 3f\left(x_2\right) + 3f\left(x_3\right) + f(b)\right]$$

- The name $3/8$ method comes from the $3/8$ factor in the expression

Simpson's 3/8 Method



- In the composite Simpson's $3/8$ method, the whole interval $[a, b]$ is divided into N subintervals.
- In general, the subintervals can have arbitrary width. The derivation here, however, is limited to the case where the subintervals have an equal width h, where $h = (b - a)/N$.

$$I(f) \approx \frac{3h}{8}\left[f(a) + 3\sum_{i=2,5,8}^{N-1}\left[f\left(x_i\right) + f\left(x_{i+1}\right)\right] + 2\sum_{j=4,7,10}^{N-2} f\left(x_j\right) + f(b)\right]$$

Simpson's $3/8$ Method

- Simpson's $3/8$ method can be used if the following two conditions are met:
  - The subintervals are equally spaced.
  - The number of subintervals within $[a, b]$ must be divisible by 3.
- Since Simpson's $1/3$ method is only valid for an even number of subintervals and Simpson's $3/8$ method is only valid for a number of subintervals that is divisible by 3, a combination of both can be used for integration when there are any odd number of intervals.

Example

Question: Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$.

References

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Thank you!