Numerical Methods in Engineering - LW6

Athanasios A. Markou

PhD, University Lecturer
Aalto University
School of Engineering
Department of Civil Engineering

February 14, 2024

Numerical Integration

Introduction

Introduction

- 'Numerical integration' is also known as 'quadrature'.
- Numerical integration is much **more accurate** than numerical differentiation.
- The quadrature approximates the definite integral:

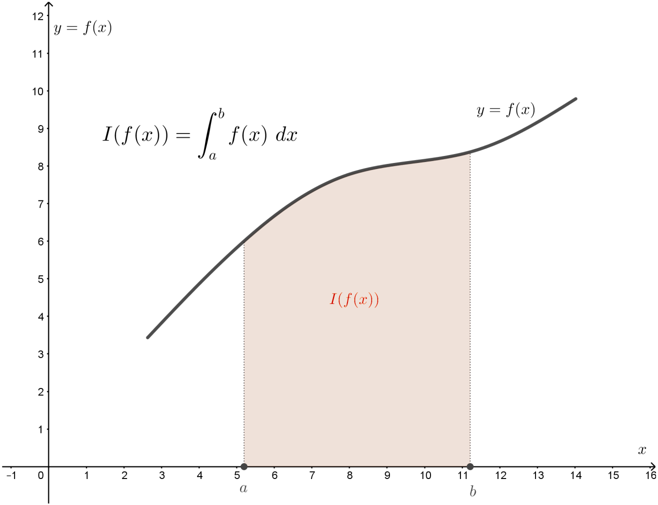
  $$\int_a^b f(x)dx$$

  (where $f(x)$ is called the integrand) by the sum:

  $$I = \sum_{i=1}^{n} A_i f(x_i)$$

  where A_i are the weights depending on the specific method and x_i is the nodal abscissas.
- All quadrature rules are derived from **polynomial interpolation** of the integrand and they work best if they are approximated by a polynomial.

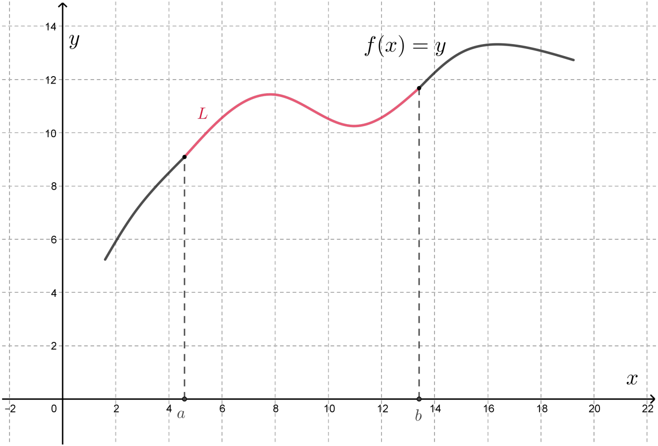
Numerical Integration



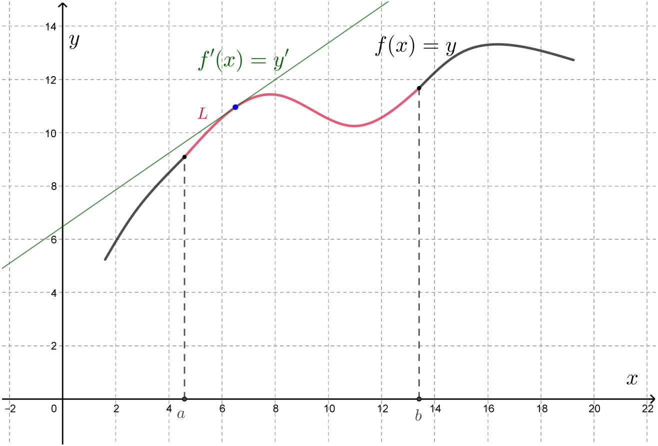
Introduction

- Numerical integration is commonly used for solving problems and calculating quantities, [1].
- Integration can be used to:
  1. calculate quantities
  2. solving differential equations
- The integrand can be either an analytical function or discrete points.
- When integrand is a mathematical expression, an analytical solution can be found for most cases.
- In the case of discrete points, numerical integration is needed.

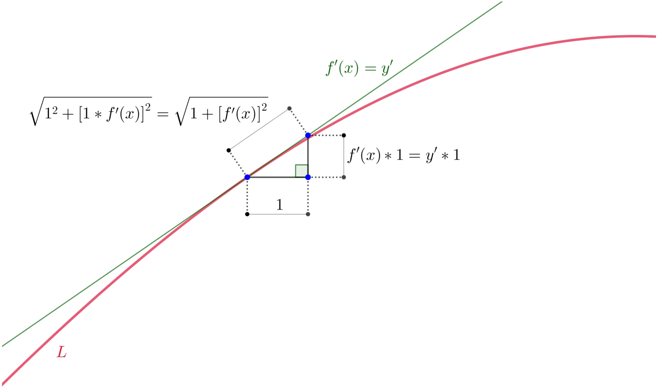
Numerical Integration



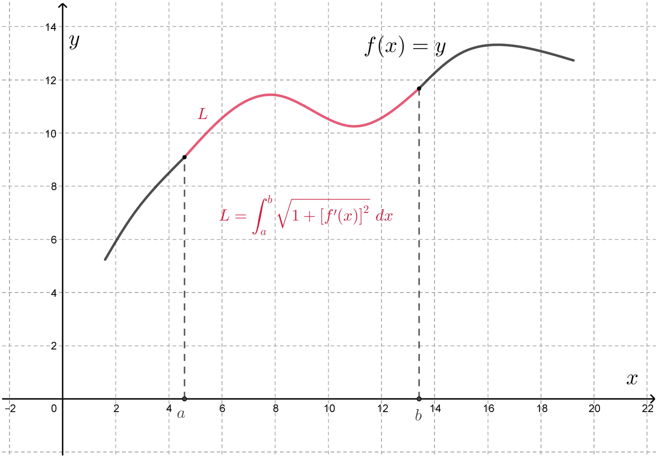
Numerical Integration



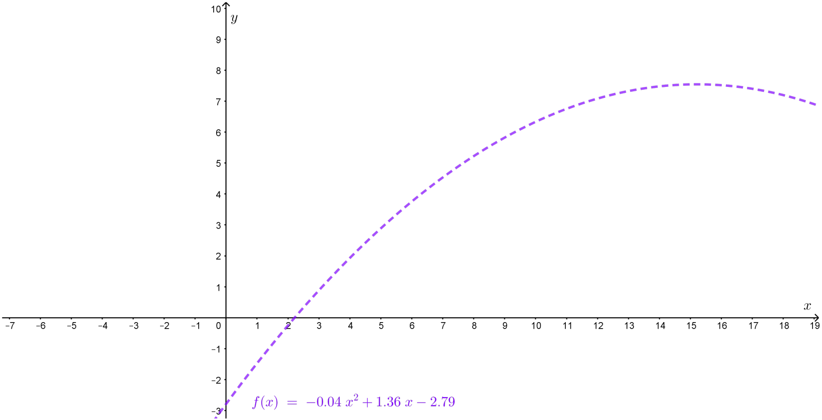
Numerical Integration



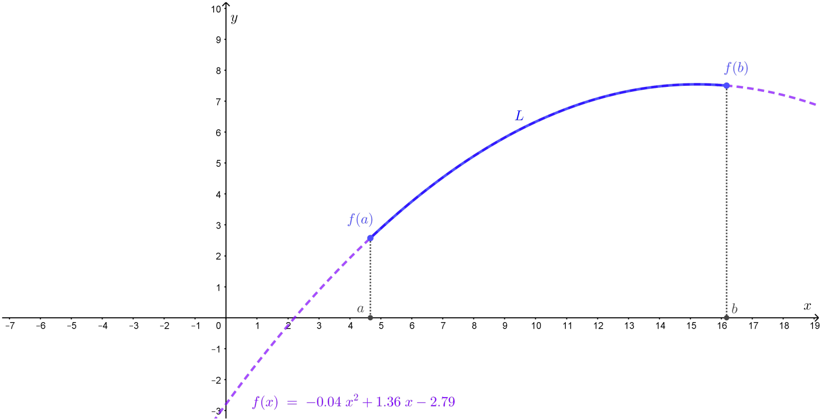
Numerical Integration



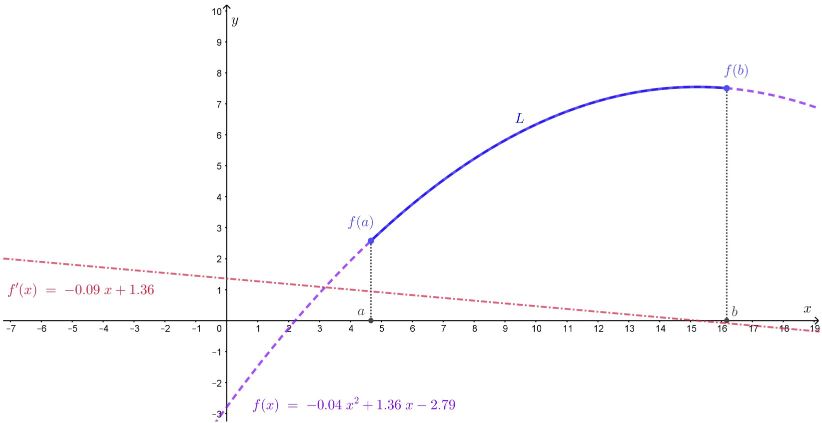
Numerical Integration - Example



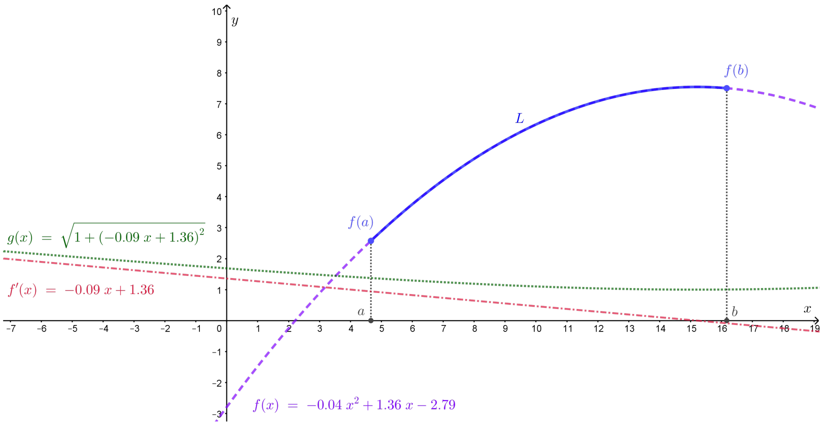
Numerical Integration - Example



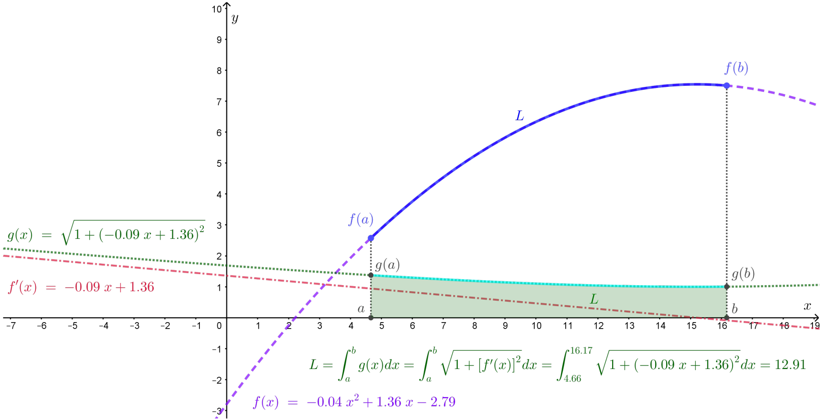
Numerical Integration - Example



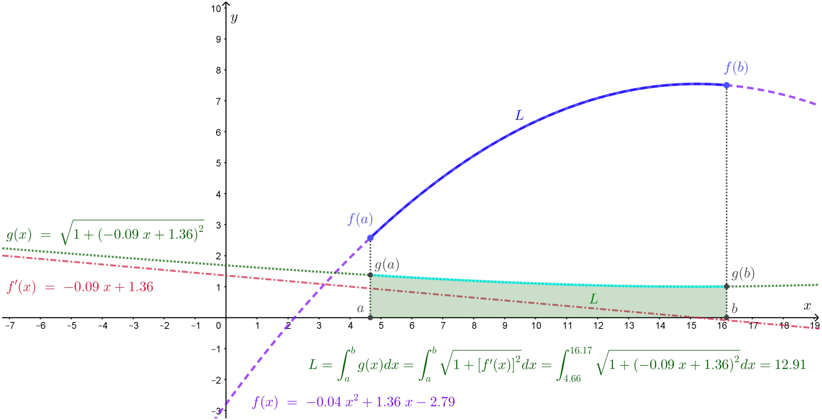
Numerical Integration - Example



Numerical Integration - Example

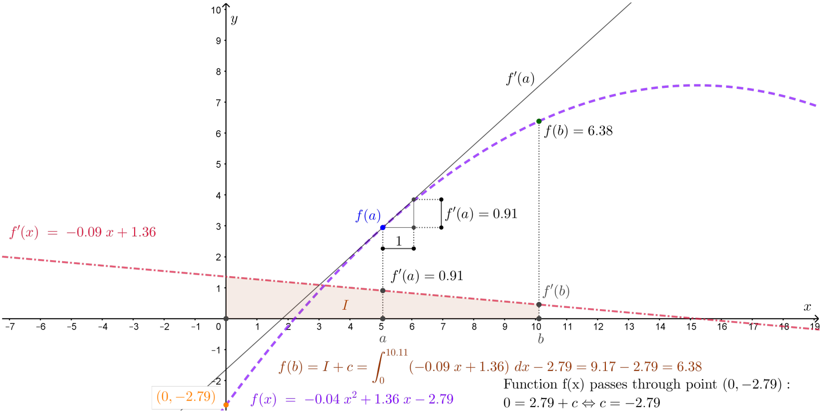


Numerical Integration - Example



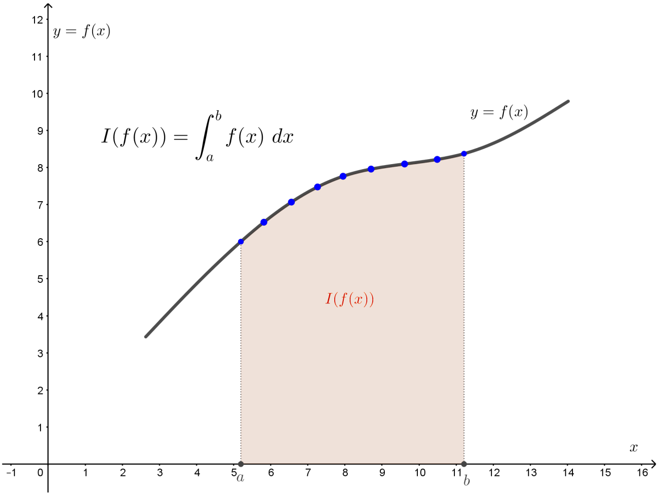
We have just transformed the measurement of length, to measurement of area.

Integration - Differentiation



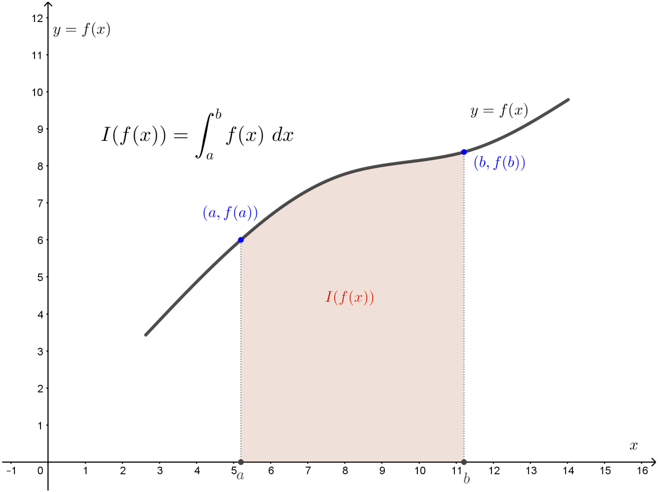
Numerical Integration - Approaches

If the integrand is an analytic function, the numerical integrand can be done by using finite number at which the integrand is evaluated.



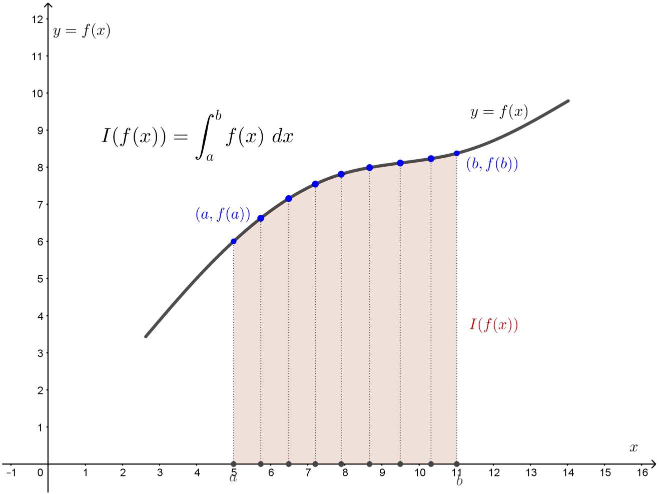
Numerical Integration - Approaches

One approach is to use only the endpoints of the interval $(a, f(a))$ and $(b, f(b))$, but not give accurate results.



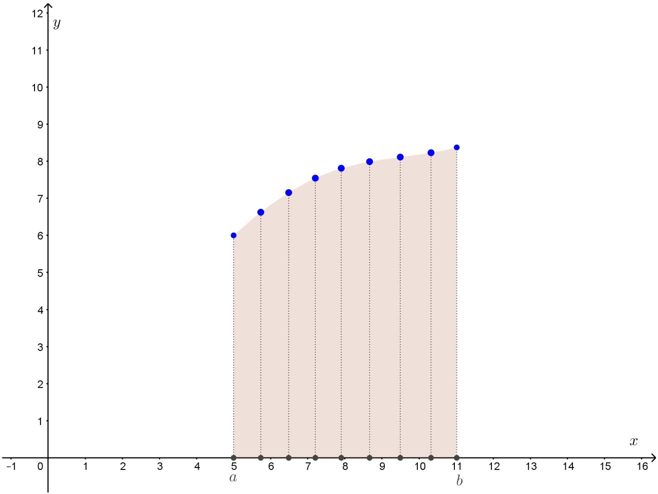
Numerical Integration - Approaches

To achieve higher accuracy the interval $[a, b]$ is divided into smaller subintervals. The interval for each subintervall is calculated and the results are added to give the value of the whole integral



Numerical Integration - Approaches

If the integrand is given as a set of discrete points, then the numerical integration is done in these points.



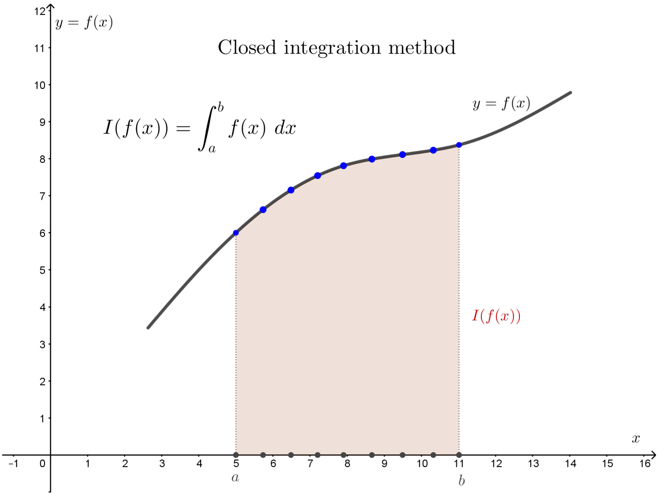
Numerical Integration - Approaches

The groups of methods for deriving numerical integration are the following.

1. Open
2. Closed

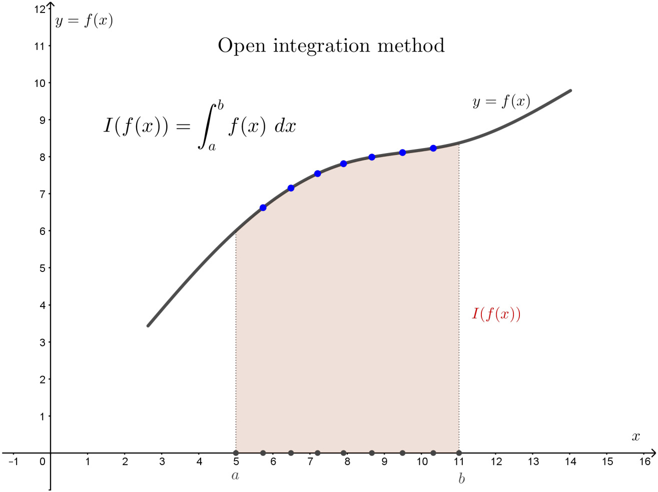
Numerical Integration - Approaches

In closed integration methods, the endpoints of the interval (and the integrand) are used in the estimation of the value of the integral.



Numerical Integration - Approaches

In open integration methods, the interval extends out of the range of the endpoints.



Numerical Integration - Approaches

Closed methods:

1. Trapezoidal
2. Simpson's

Open methods:

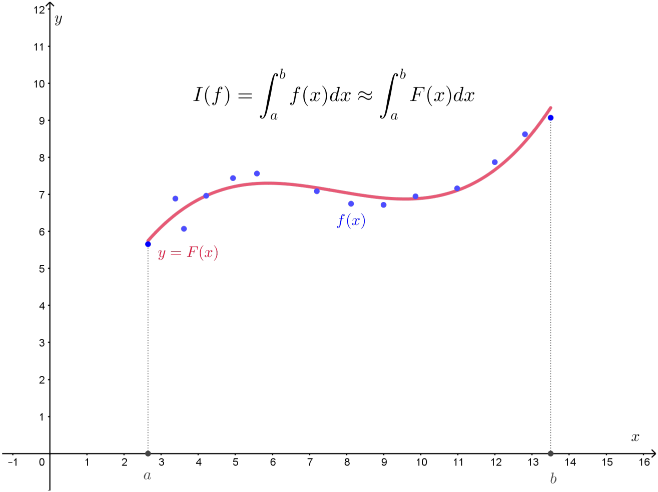
1. Midpoint
2. Gauss

Numerical Integration - Newton-Cotes integration formulas

- When using Newton-Cotes integration formulas, the value of the integrand between discrete points is estimated using a function that can easily be integrated (the value is obtained by integration), [1]
- When the original integrand is an analytical function, then the Newton-Cotes formula replaces it with a simpler function
- When the original integrand is given as data points, the Newton-Cotes formula interpolates between the points (Trapezoidal, Simpson where the interpolation is done by polynomials with different degrees)
- Another option when there are data points is to use curve fitting with a function $F(x)$ that fits best the points.

Numerical Integration - Approaches

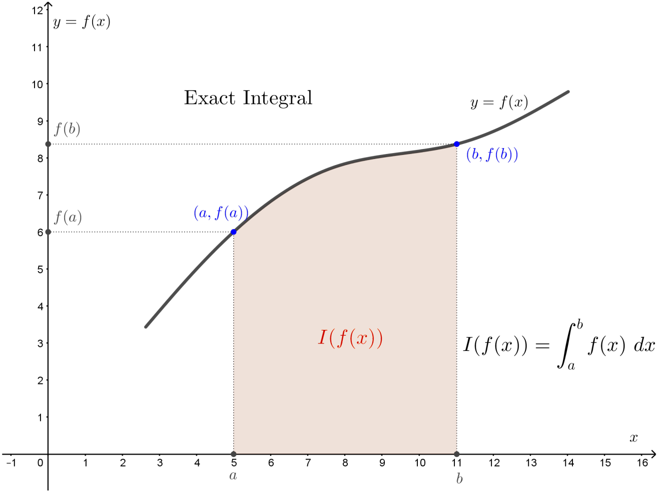
A polynomial or simpler function $F(x)$ is fitted to the data and the integral is calculated analytically. (Numerical method is used for curve fitting, but not for solving the integral)



Numerical Integration - Rectangle and midpoint methods

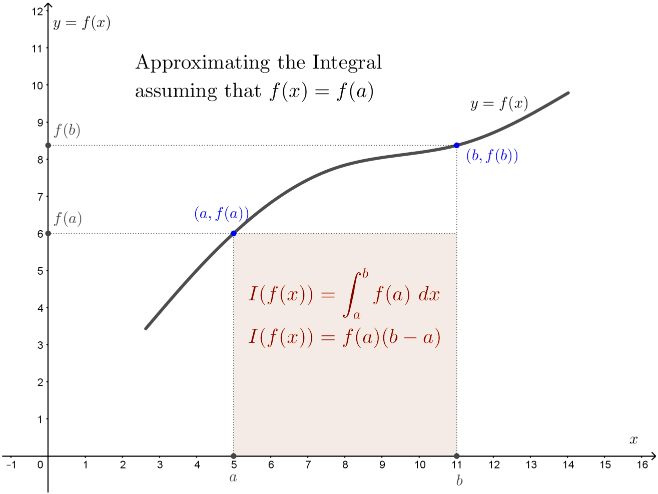
Numerical Integration - Rectangle method

The simplest approximation for the integral $\int_a^b f(x)dx$ is to assume $f(x)$ as constant (at either one of the endpoints) over the interval $x \in [a, b]$



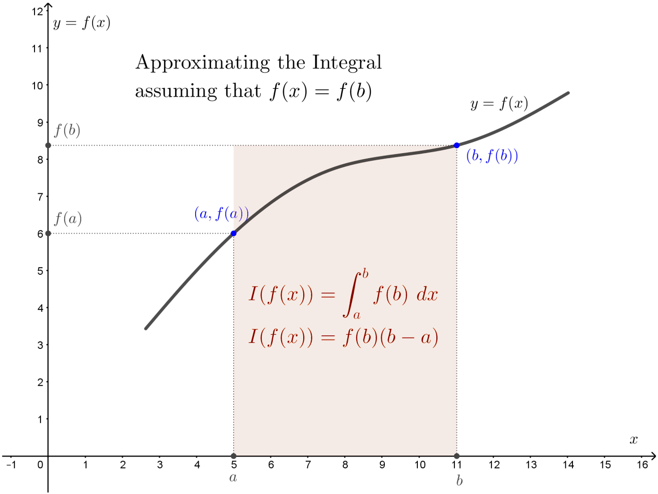
Numerical Integration - Rectangle method

The actual integral is approximated by an area of a rectangle. The value of the integral is underestimated when $f(x) = f(a)$. The error can be large.



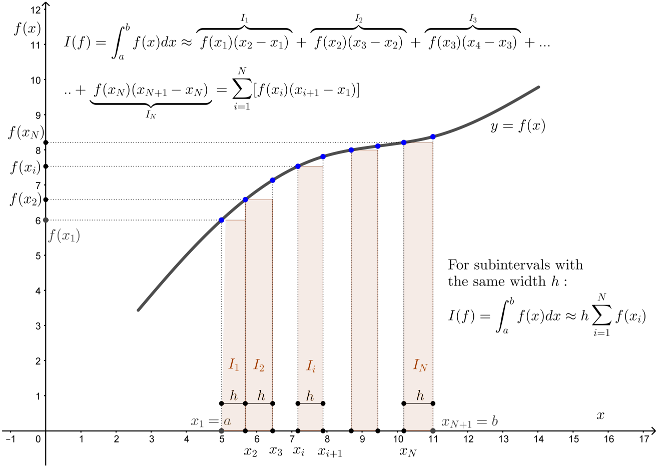
Numerical Integration - Rectangle method

The actual integral is approximated by an area of a rectangle. The value of the integral is overestimated when $f(x) = f(b)$. The error can be large.



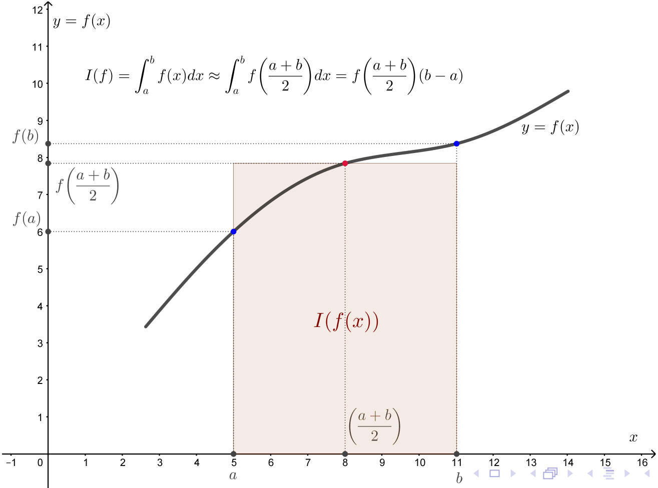
Numerical Integration - Composite Rectangle method

The error can be reduced by using the composite rectangle method, where the domain $[a, b]$ is divided into N intervals.



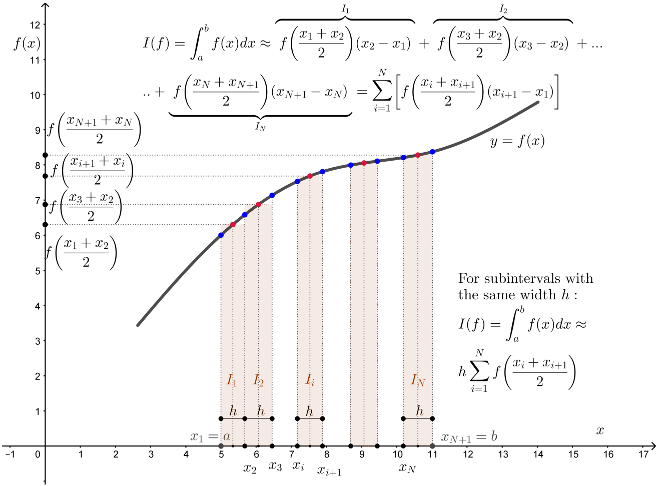
Numerical Integration - Midpoint method

A more accurate method compared to the rectangle method, is the midpoint method. Instead of approximating the integrand by the values of the function at $x = a$ or $x = b$, the value of the integrand at the middle of the interval is obtained.



Numerical Integration - Composite Midpoint method

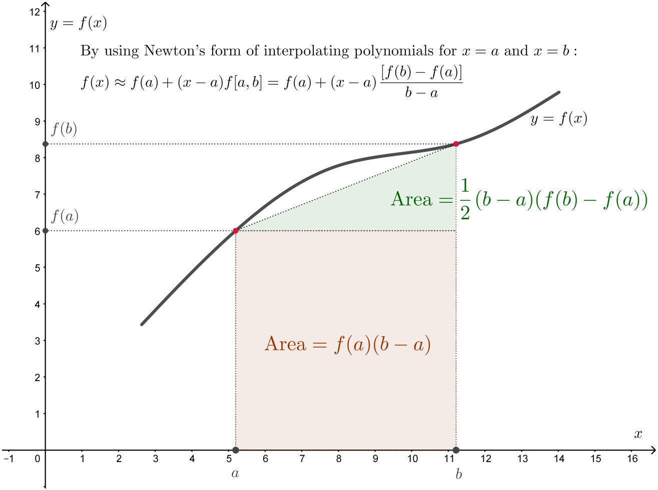
The composite midpoint method divides the domain $[a, b]$ into N subintervals.



Numerical Integration - Trapezoid method

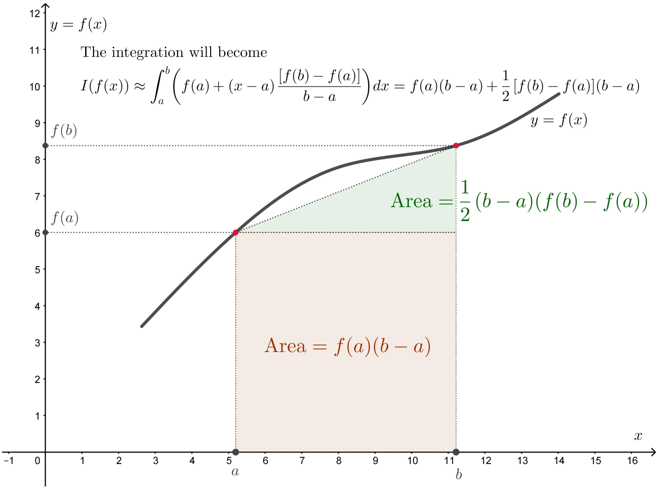
Numerical Integration - Trapezoid method

A refinement of the simple rectangle and midpoint methods is to use a linear function to approximate the integrand over the interval of integration. Using Newton's form of interpolating polynomials:



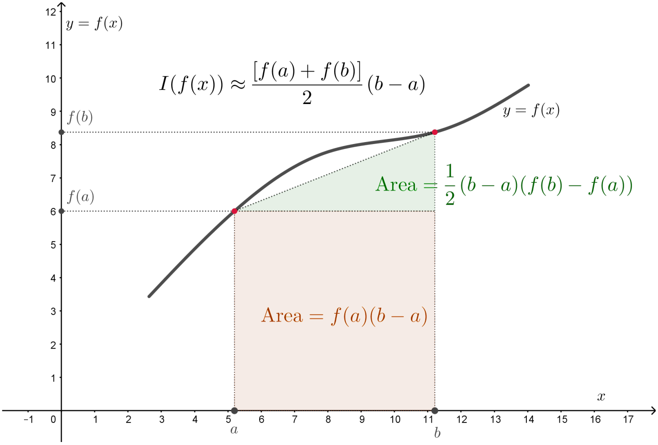
Numerical Integration - Trapezoid method

Substituting into the integral:



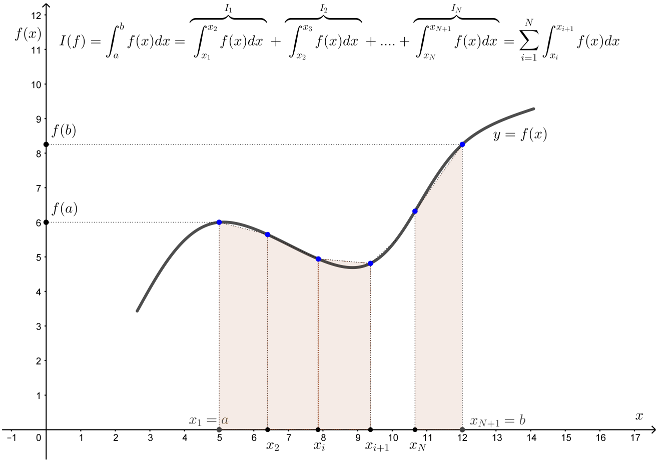
Numerical Integration - Trapezoid method

The final form:



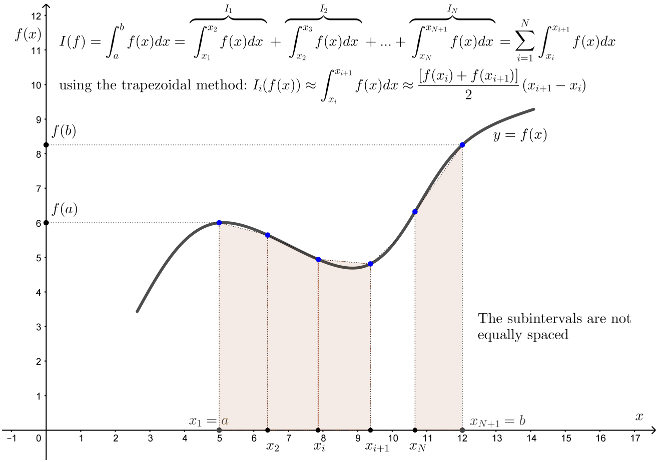
Numerical Integration - Composite Trapezoid method

As with the previous methods (rectangle, midpoint) the accuracy can be increased by using subintervals:



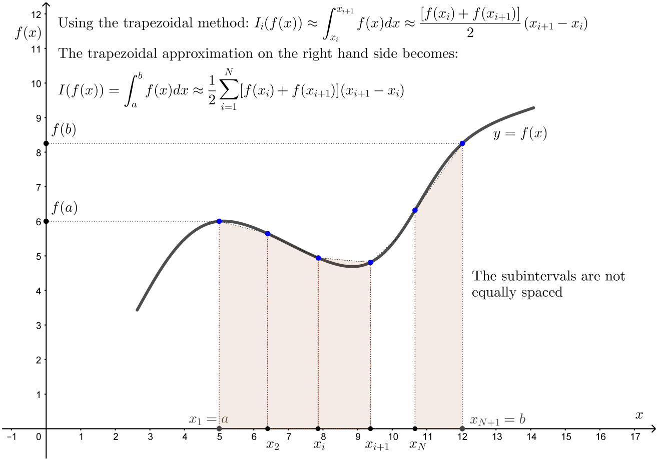
Numerical Integration - Composite Trapezoid method

The interval $[a, b]$ is divided into N subintervals with the first point being $x_1 = a$ and the last one $x_{N+1} = b$. The integral can be written:



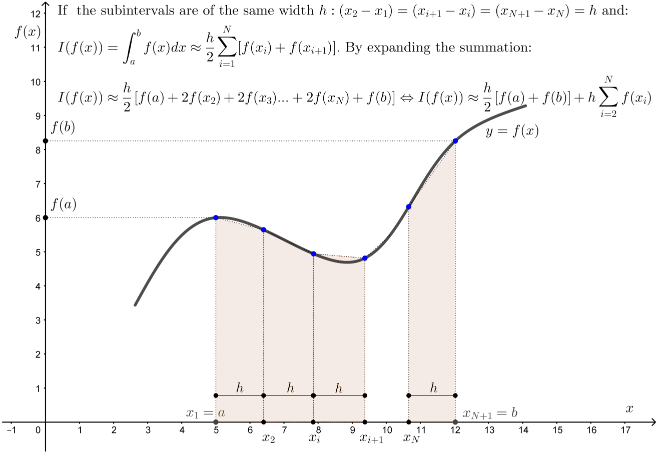
Numerical Integration - Composite Trapezoid method

Using the trapezoidal method to each subinterval $[x_i, x_{i+1}]$:



Numerical Integration - Composite Trapezoid method

For the case of N equally spaced subintervals:



Examples

Comparison - Example

The function is given in the following tabulated form. Compute $\int_0^1 f(x)dx$ with $h = 0.25$ and with $h = 0.5$, using:
(a) The composite rectangle method.
(b) The composite midpoint method. Use linear interpolation to determine at the midpoints.
(c) The composite trapezoidal method

x	0	0.25	0.5	0.75	1.0
f(x)	0.9162	0.8109	0.6931	0.5596	0.4055

Comparison - Example: Solution

x	0	0.25	0.5	0.75	1.0
f(x)	0.9162	0.8109	0.6931	0.5596	0.4055

(a) Rectangle method: $I(f(x)) = h\sum_{i=1}^{N} f(x_i)$, where $h = 0.25$ and $N = 4$:

$$I(f(x)) = 0.25(0.9162 + 0.8109 + 0.6931 + 0.5596) = 0.7450$$

Rectangle method: $I(f(x)) = h\sum_{i=1}^{N} f(x_i)$, where $h = 0.5$ and $N = 4$:

$$I(f(x)) = 0.5(0.9162 + 0.6931) = 0.8467$$

(b) Midpoint method: $I(f(x)) = h\sum_{i=1}^{N} f(\frac{x_i + x_{i+1}}{2})$, where $h = 0.25$ and $N = 4$:

$$I(f(x)) = 0.25\left(\frac{0.9162 + 0.8109}{2} + \frac{0.8109 + 0.6931}{2} + \frac{0.6931 + 0.5596}{2} + \frac{0.5596 + 0.4055}{2}\right)$$
$$= 0.6811$$

Comparison - Example: Solution

x	0	0.25	0.5	0.75	1.0
f(x)	0.9162	0.8109	0.6931	0.5596	0.4055

(b) Midpoint method: $I(f(x)) = h\sum_{i=1}^{N} f(\frac{x_i + x_{i+1}}{2})$, where $h = 0.5$ and $N = 4$:

$$I(f(x)) = 0.25\,(0.8109 + 0.5596) = 0.6853$$

(c) Trapezoid method: $I(f(x)) = \frac{h}{2}(f(a) + f(b)) + h\sum_{i=2}^{N-1} f(x_i)$, where $h = 0.25$ and $N = 4$:

$$\begin{aligned} I(f(x)) = 0.25/2\,(0.9162 + 0.4055) + 0.25\,(0.8109 + 0.6931 + 0.5596) \\ = 0.6811 \end{aligned}$$

Trapezoid method: $I(f(x)) = \frac{h}{2}(f(a) + f(b)) + h\sum_{i=2}^{N-1} f(x_i)$, where $h = 0.5$ and $N = 4$:

$$I(f(x)) = 0.5/2\,(0.9162 + 0.4055) + 0.5\,(0.6931) = 0.6770$$

Composite Trapezoid method - Example

An airplane of mass $m = 97000kg$ lands at a speed of $93m/s$ and applies its thrust reversers (braking system) at t = 0. The force F that is applied to the airplane, as it decelerates, is given by $F = -5v^2 - 570000$, where v is the airplane's velocity. Using Newton's second law of motion and flow dynamics, the relationship between the velocity and the position x of the airplane can be written as:

$$mv\frac{dv}{dx} = -5v^2 - 570000$$

where x is the distance measured from the location of the jet at $t = 0$. Determine how far the airplane travels before its speed is reduced to $40m/s$ by using the composite trapezoidal method to evaluate the integral resulting from the governing differential equation. Create a user-defined function in MatLab `trapezoidal1(Fun,a,b,N)`, where `Fun` is an anonymous function, `a` and `b` are the lower and upper bounds respectively, and `N` is the number of subintervals, which will return the result of the integral `I`.

Composite Trapezoid method - Example: Solution

Solving for dx:

$$\int_0^x dx = -\int_{93}^{40} \frac{97000 v dv}{-5v^2 - 570000} = \int_{40}^{93} \frac{97000 v dv}{5v^2 + 570000}$$

The analytical solution gives $x = 574.1494$.
For $N = 10$: $x = 574.0854$.
For $N = 100$: $x = 574.1488$.
For $N = 1000$: $x = 574.1494$.

Numerical Integration - Recursive Composite Trapezoid method

- I_k is the integral evaluated with the composite trapezoidal rule using 2^{k-1} subintervals. If k is increased by 1, the number of subintervals is doubled.
- For $H = b - a$, the equation $I(f(x)) \approx \frac{h}{2}[f(a) + 2f(x_2) + 2f(x_3)... + 2f(x_N) + f(b)]$ will yield for k=1,2,3, [2]:

$$I_1(f(x)) = [f(a) + f(b)]\frac{H}{2}; \quad k = 1$$

$$I_2(f(x)) = \left[f(a) + 2f\left(a + \frac{H}{2}\right) + f(b)\right]\frac{H}{4} = \frac{1}{2}I_1 + f\left(a + \frac{H}{2}\right)\frac{H}{2}; \quad k = 2$$

- Generally, for $k > 1$, [2]:

$$I_k = \frac{1}{2}I_{k-1} + \frac{H}{2^{k-1}}\sum_{i=1}^{2^{k-2}} f\left[a + \frac{(2i-1)H}{2^{k-1}}\right]; \quad k = 2, 3, ...$$

Trapezoid method - Refinement - Control the accuracy

- The trapezoidal method for equal spacing $h \equiv \Delta x$, integrating from x_a to x_b can be written as:

$$I = \int_{x_a}^{x_b} f(x)dx = \frac{\Delta x}{2}\left(f(x_0) + f(x_n)\right)$$
$$+\Delta x\left(f(x_1) + f(x_2) + ... + f(x_{n-1})\right)$$

  where n is the number of the points (not N the intervals), and the first term in the right hand side is the trapezoid by using only the endpoints.

- As a first step, we start with the first term on the right hand side to estimate I.
- In the next steps we refine our estimate until:
  1. successive estimates show no improvement
  2. the interval Δx has become very small

Trapezoid method - Refinement - Control the accuracy

- For every refinement r, the spacing is Δx_r and is equal to $\Delta x_{r-1}/2$.
- In every refinement the number of new control points k is given by $k = 2^{r-1}$ and the location of the points is:

$$x_{2m-1} = (x_a + (2m-1)\Delta x_r)\,; \quad m = 1, 2, ..., k$$

- when we calculate the new estimate in terms of the old estimate we get:

$$I_r = \frac{I_{r-1}}{2} + \Delta x_r (f(x_1) + f(x_3) + ... + f(x_{2m-1}))$$

Trapezoid method - Refinement - Control the accuracy

- Refinement $r = 0$,
  $\Delta x_0 = (x_a - x_b)$,
  $I_0 = \Delta x_0 (f(x_a) + f(x_b))/2$
- Refinement $r = 1$,
  $\Delta x_1 = \Delta x_0/2$,
  $k = 2^{r-1} = 2^{1-1} = 1$,
  $m = 1$,
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_1 = (x_a + \Delta x_1)$,
  $I_1 = I_0/2 + \Delta x_1 (f(x_1))$
- Refinement $r = 2$,
  $\Delta x_2 = \Delta x_1/2$,
  $k = 2^{r-1} = 2^{2-1} = 2$,
  $m = 1, 2$,
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_1 = (x_a + \Delta x_2),\ m = 1$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_3 = (x_a + 3\Delta x_2),\ m = 2$
  $I_2 = I_1/2 + \Delta x_2 (f(x_1) + f(x_3))$

Trapezoid method - Refinement - Control the accuracy

- Stop criteria:
  $\Delta x_r < \epsilon_\Delta$ or
  $\Delta I_r = I_r - I_{r-1} < \epsilon_I$
- The refinement function works best for cases of the values of the integrand $f(x)$ are all non-negative or all non-positive.
- The function will not work for example in the case of $f(x) = e^{-x} \sin x$ with limits $x_a = 0$ and $x_b = 2\pi$, because $f(x)$ is zero at x_a, x_b and $(x_a + x_b)/2$ and therefore I_0 and I_1 will both be zero.
- Solution is to split the integral in two parts from 0 to π and from π to 2π.

Example

Example: Trapezoid method - Refinement

Derive the I_3, I_4 for the third and fourth step of refinement, $r = 3, r = 4$, by hand.

Trapezoid method - Refinement - Example: Solution

- Refinement $r = 3$,
  $\Delta x_3 = \Delta x_2/2$,
  $k = 2^{r-1} = 2^{3-1} = 4$,
  $m = 1, 2, 3, 4$,
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_1 = (x_a + \Delta x_3),\ m = 1$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_3 = (x_a + 3\Delta x_3),\ m = 2$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_5 = (x_a + 5\Delta x_3),\ m = 3$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_7 = (x_a + 7\Delta x_3),\ m = 4$
  $I_3 = I_2/2 + \Delta x_3(f(x_1) + f(x_3) + f(x_5) + f(x_7))$

Trapezoid method - Refinement - Example: Solution

- Refinement $r = 4$,
  $\Delta x_4 = \Delta x_3/2$,
  $k = 2^{4-1} = 2^{4-1} = 8$,
  $m = 1, 2, 3, 4, 5, 6, 7, 8$,
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_1 = (x_a + \Delta x_4),\ m = 1$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_3 = (x_a + 3\Delta x_4),\ m = 2$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_5 = (x_a + 5\Delta x_4),\ m = 3$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_7 = (x_a + 7\Delta x_4),\ m = 4$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_9 = (x_a + 9\Delta x_4),\ m = 5$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_{11} = (x_a + 11\Delta x_4),\ m = 6$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_{13} = (x_a + 13\Delta x_4),\ m = 7$
  $x_{2m-1} = (x_a + (2m-1)\Delta x_r) = x_{15} = (x_a + 15\Delta x_4),\ m = 8$
  $I_4 = I_3/2 + \Delta x_4(f(x_1) + f(x_3) + f(x_5) + f(x_7) + f(x_9) + f(x_{11}) + f(x_{13}) + f(x_{15}))$

Numerical Integration - Simpson's methods

Numerical Integration - Simpson's methods

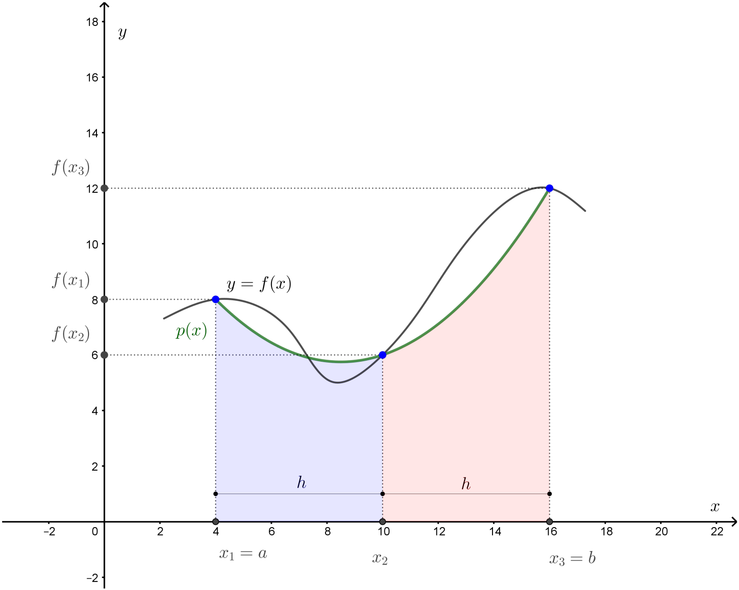
Numerical Integration - Simpson's methods

- 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 using a nonlinear function to approximate the integrand
- Simpson's methods, uses quadratic (Simpson's $1/3$ method) and cubic (Simpson's $3/8$ method) polynomials to approximate the integrand.

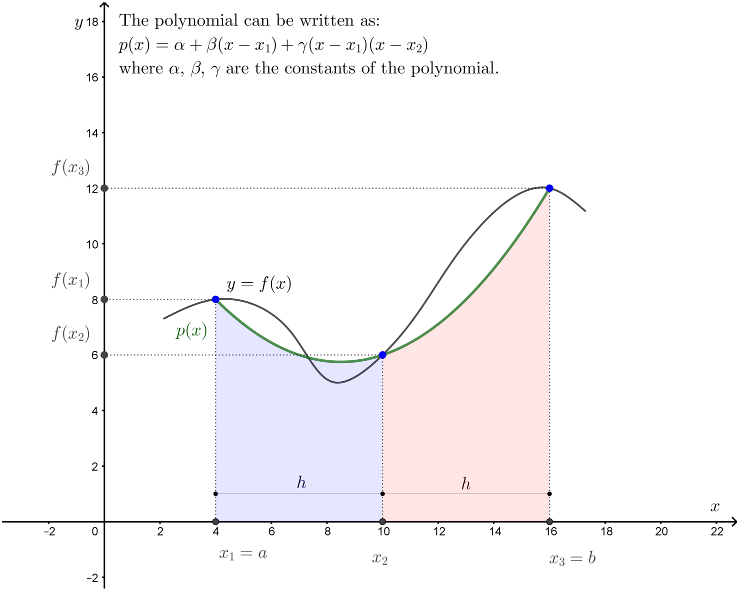
Numerical Integration - Simpson's 1/3 method

- A quadratic (2nd order) polynomial is used to approximate the integrand
- Three points are enough to determine the coefficients
- For a domain $[a, b]$ the three points used are $x_1 = a$, $x_3 = b$ and the midpoint $x_2 = (a + b)/2$

Numerical Integration - Simpson 1/3 method



Numerical Integration - Simpson 1/3 method



Numerical Integration - Simpson 1/3 method

The polynomial can be written as:

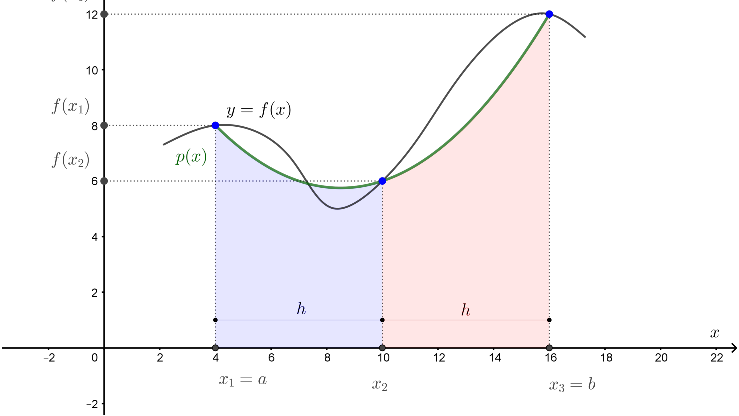
$p(x) = \alpha + \beta(x - x_1) + \gamma(x - x_1)(x - x_2)$

where α, β, γ are the constants of the polynomial.

Considering that the polynomial passes though:

$p(x_1) = f(x_1),\ p(x_2) = f(x_2),\ p(x_3) = f(x_3)$

$$\alpha = f(x_1); \quad \beta = \frac{f(x_2) - f(x_1)}{x_2 - x_1}; \quad \gamma = \frac{f(x_3) - 2f(x_2) + f(x_1)}{2h^2}; \quad h = \frac{b-a}{2}$$



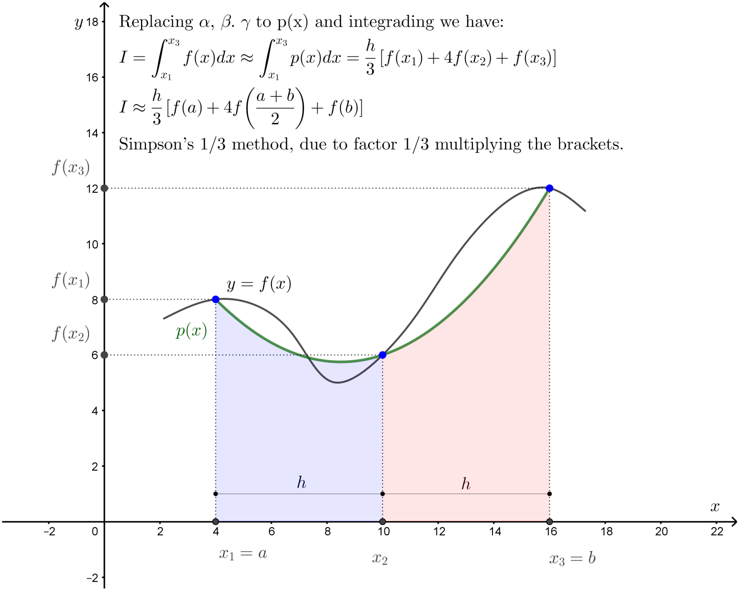
Numerical Integration - Simpson 1/3 method

Replacing α, β. γ to p(x) and integrading we have:

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

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

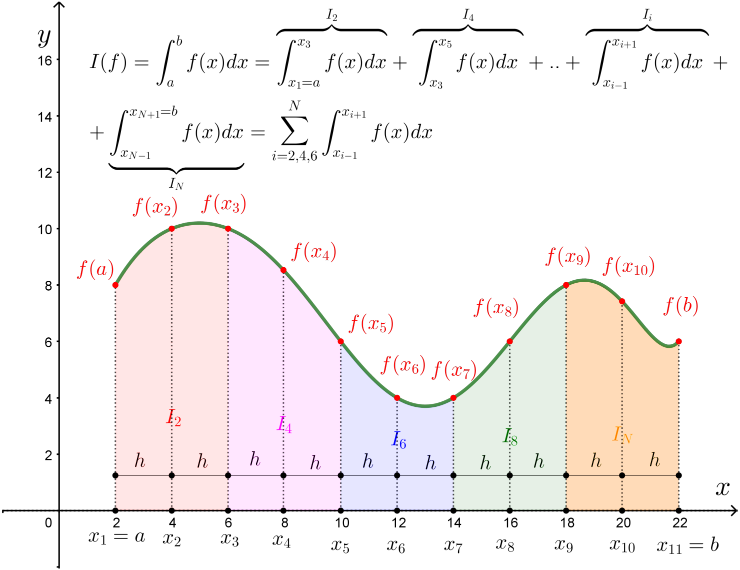
Simpson's 1/3 method, due to factor 1/3 multiplying the brackets.



Numerical Integration - Composite Simpson 1/3 method

- As with the previous methods a more accurate method can be derived by using the composite Simpson's method 1/3. The interval is divided into N subintervals.
- The intervals can have variable width.
- Here we will present the case with constant width of subintervals equal to $h = \frac{b-a}{N}$.
- Due to the fact that the 1/3 method needs 3 points, two adjacent intervals will be used (first and second together, third and fourth together and so on).
- The interval $[a, b]$ is divided into even number of subintervals.

Numerical Integration - Composite Simpson 1/3 method



$$I(f) = \int_a^b f(x)dx = \overbrace{\int_{x_1=a}^{x_3} f(x)dx}^{I_2} + \overbrace{\int_{x_3}^{x_5} f(x)dx}^{I_4} + .. + \overbrace{\int_{x_{i-1}}^{x_{i+1}} f(x)dx}^{I_i} +$$

$$+ \underbrace{\int_{x_{N-1}}^{x_{N+1}=b} f(x)dx}_{I_N} = \sum_{i=2,4,6}^{N} \int_{x_{i-1}}^{x_{i+1}} f(x)dx$$

Numerical Integration - Composite Simpson 1/3 method

- By using the equation $I_i(f) \approx \frac{h}{3}[f(x_{i-1}) + 4f(x_i) + f(x_{i+1})]$ where $h = x_{i+1} - x_i = x_i - x_{i-1}$:

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

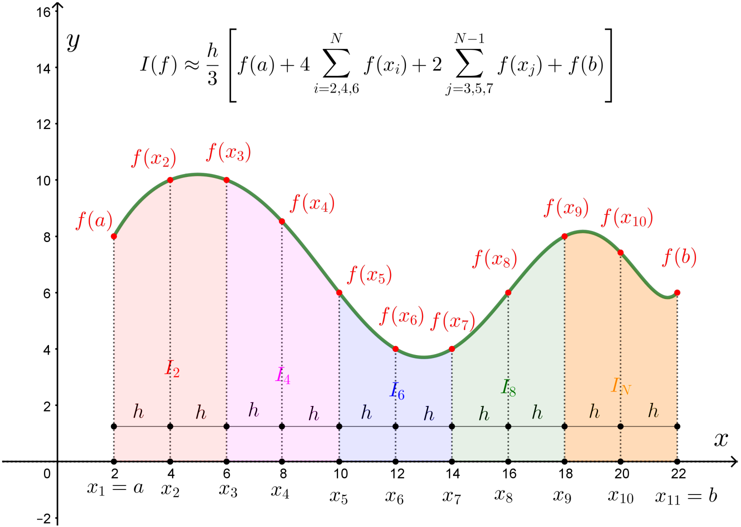
- Finally by collecting similar terms on the right hand side we derive:

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

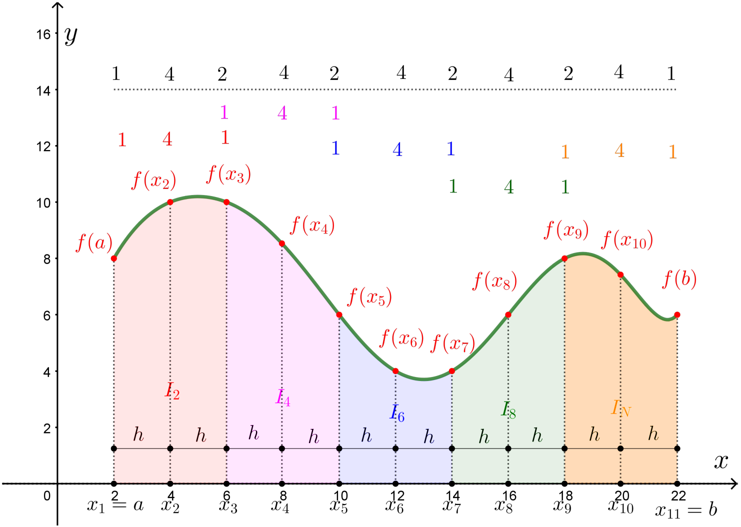
  where $h = (b-a)/N$

- The method can be used when:
  1. The subintervals are equally spaced
  2. The number of subintervals within $[a, b]$ must be even

Numerical Integration - Composite Simpson 1/3 method



Numerical Integration - Composite Simpson 1/3 method



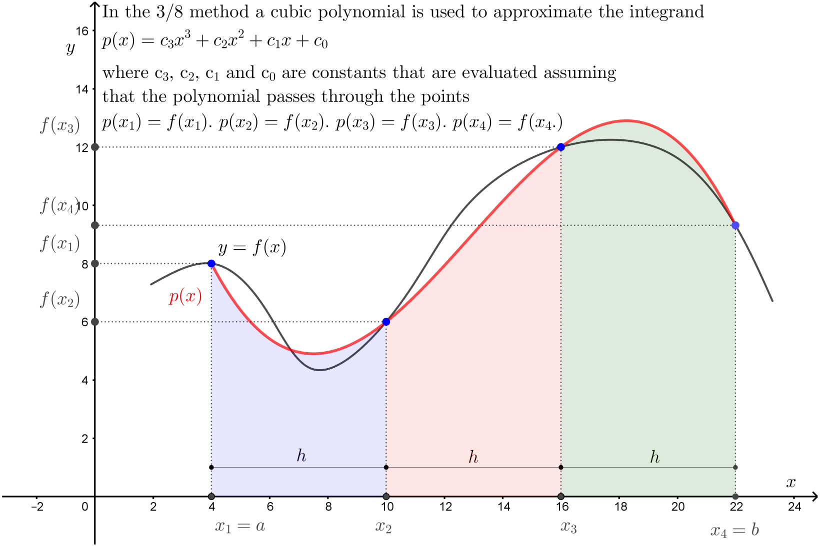
Numerical Integration - Simpson 3/8 method

In the 3/8 method a cubic polynomial is used to approximate the integrand

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

where c_3, c_2, c_1 and c_0 are constants that are evaluated assuming that the polynomial passes through the points

$p(x_1) = f(x_1).\ p(x_2) = f(x_2).\ p(x_3) = f(x_3).\ p(x_4) = f(x_4.)$

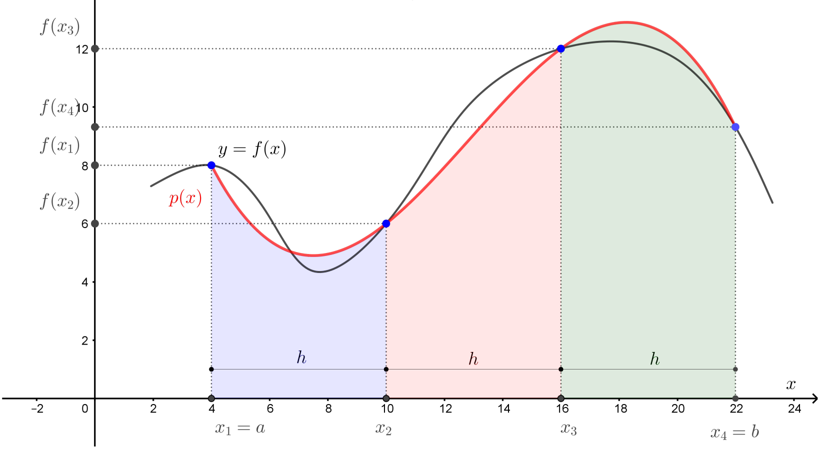


Numerical Integration - Simpson 3/8 method

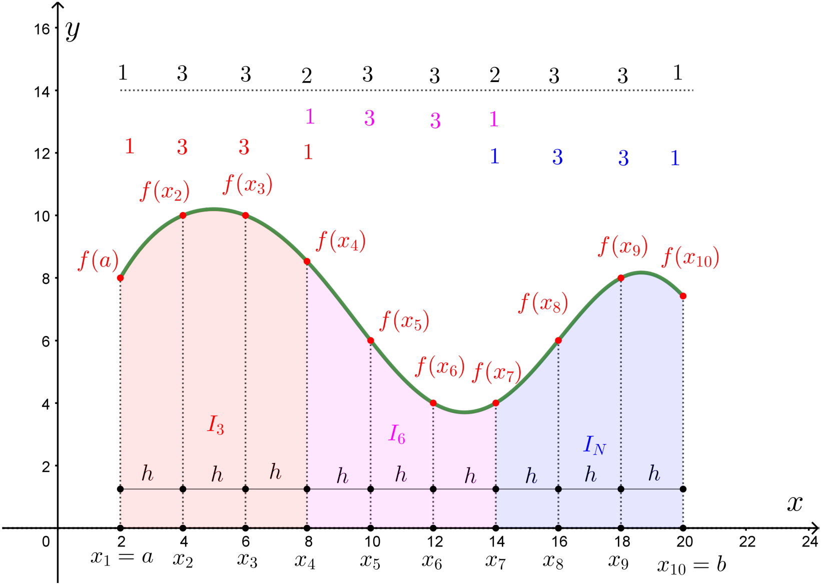
The polynomial will take the following form:

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

The name of the method comes from 3/8 factor



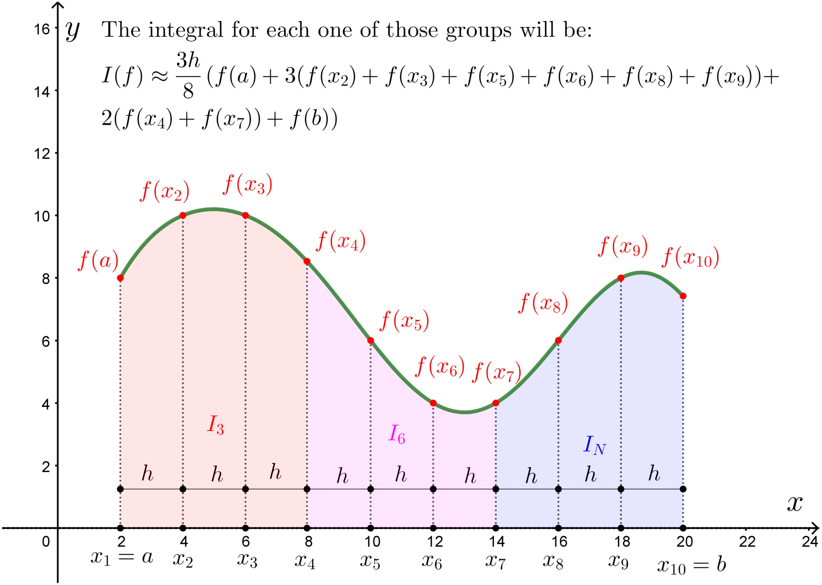
Numerical Integration - Composite Simpson 3/8 method



Numerical Integration - Composite Simpson 3/8 method

The integral for each one of those groups will be:

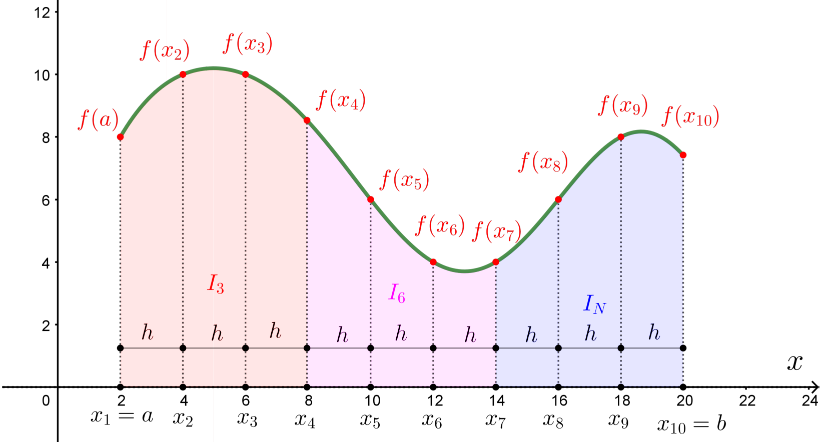
$$I(f) \approx \frac{3h}{8}(f(a) + 3(f(x_2) + f(x_3) + f(x_5) + f(x_6) + f(x_8) + f(x_9)) + 2(f(x_4) + f(x_7)) + f(b))$$



Numerical Integration - Composite Simpson 3/8 method

Finally, the for the general case of domain [a,b] divided into N subinter

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



Numerical Integration - Composite Simpson 3/8 method

- The subintervals can have arbitrary width.
- The derivation here is limited in the case of equal spacing.
- The subintervals have spacing $h = (b - a)/N$.
- Four points are needed, and therefore 3 intervals are required.
- The whole interval should be divided into a number of subintervals that is divisible by 3, [1].
- A combination of both 1/3 and 3/8 methods can be used for odd number of intervals. For the first 3 (or the last 3) intervals the 3/8 method is used and 1/3 method is used for the remaining subintervals. It works because both methods have the same order of error.

Numerical Integration - Error Analysis

Numerical Integration - Romberg integration

- For the composite trapezoid method, the error is, [2]:

$$E = c_1 h^2 + c_2 h^4 + c_3 h^6 + \ldots$$

- For the composite Simpson's rule, the error is, [2]:

$$E = \frac{(b-a)h^4}{180} f''''(\xi)$$

Numerical Integration - Romberg integration

Numerical Integration - Romberg integration

- Romberg integration is using Richardson extrapolation to the limit.
- By using the trapezoid rule for error is $E = c_1 h^2 + c_2 h^4 + \ldots$, [2] with $h = \frac{b-a}{2^{i-1}}$ is the width of each interval.
- We start the integration with one panel $R_{1,1} = I_1$ (one interval) and $R_{2,1} = I_2$ (two intervals).
- The error is eliminated by using Richardson extrapolation (see material of week 5). The leading error is $c_1 h^2$, so $p = 2$ and from $I = \frac{2^p A_2 - A_1}{2^p - 1}$ we get:

$$R_{2,2} = \frac{2^2 R_{2,1} - R_{1,1}}{2^2 - 1} = \frac{4}{3} R_{2,1} - \frac{1}{3} R_{1,1}$$

- The next term is $R_{3,1} = I_3$ (four intervals) and again using Richardson extrapolation:

$$R_{3,2} = \frac{2^2 R_{3,1} - R_{2,1}}{2^2 - 1} = \frac{4}{3} R_{3,1} - \frac{1}{3} R_{2,1}$$

Numerical Integration - Romberg integration

- We can represent the terms in a matrix form:

$$\begin{bmatrix} R_{1,1} & \\ R_{2,1} & R_{2,2} \\ R_{3,1} & R_{3,2} \end{bmatrix}$$

- The leading error in the second column is $c_2 h^4$. By using Richardson extrapolation for $p = 4$:

$$R_{2,2} = \frac{2^4 R_{3,2} - R_{2,2}}{2^4 - 1} = \frac{16}{15} R_{3,2} - \frac{1}{15} R_{2,2}$$

- The result has an error of order $O(h^6)$. In a matrix form:

$$\begin{bmatrix} R_{1,1} & & \\ R_{2,1} & R_{2,2} & \\ R_{3,1} & R_{3,2} & R_{3,3} \end{bmatrix}$$

Numerical Integration - Romberg integration

- After another round we get:

$$\begin{bmatrix} R_{1,1} & & & \\ R_{2,1} & R_{2,2} & & \\ R_{3,1} & R_{3,2} & R_{3,3} & \\ R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} \end{bmatrix}$$

  where the error in $R_{4,4}$ is $O(h^8)$.

- Generally, we can say for this scheme:

$$R_{i,j} = \frac{4^{j-1} R_{i,j-1} - R_{i-1,j-1}}{4^{j-1} - 1}; \quad i > 1; \quad j = 2, 3, .., i$$

Numerical Integration - Romberg integration, [2]

$$\begin{tikzcd}
\boxed{R_{i-1,j-1}} \arrow[dr] & & \\
& \alpha \arrow[dr] & \\
\boxed{R_{i,j-1}} \arrow[r] & \beta \arrow[r] & \boxed{R_{i,j}}
\end{tikzcd}$$

j	2	3	4	5	6
α	$-1/3$	$-1/15$	$-1/63$	$-1/255$	$-1/1023$
β	$4/3$	$16/15$	$64/63$	$256/255$	$1024/1023$

Numerical Integration - Romberg integration - Example, [2]

Use Romberg integration to evaluate $\int_0^{\pi} \sin(x)$.

Numerical Integration - Romberg integration - Example, [2]

Use Romberg integration to evaluate $\int_0^\pi \sin(x)$.
Solution

$$R_{1,1} = I_1 = \frac{\pi}{2}\left(f(0) + f(\pi)\right) = 0$$

$$R_{2,1} = I_2 = \frac{1}{2}I_1 + \frac{\pi}{2}\left(f(\pi/2)\right) = 1.5708$$

$$R_{3,1} = I_3 = \frac{1}{2}I_2 + \frac{\pi}{4}\left(f(\pi/4) + f(3\pi/4)\right) = 1.8961$$

$$R_{4,1} = I_4 = \frac{1}{2}I_3 + \frac{\pi}{8}\left(f(\pi/8) + f(3\pi/8) + f(5\pi/8) + f(7\pi/8)\right) = 1.9742$$

Using the extrapolation:

$$\begin{bmatrix} R_{1,1} & & & \\ R_{2,1} & R_{2,2} & & \\ R_{3,1} & R_{3,2} & R_{3,3} & \\ R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} \end{bmatrix} = \begin{bmatrix} 0 & & & \\ 1.5708 & 2.0944 & & \\ 1.8961 & 2.0046 & 1.9986 & \\ 1.9742 & 2.0003 & 2.0000 & 2.0000 \end{bmatrix}$$

Numerical Integration - Gauss quadrature

Numerical Integration - Gauss method

- In all previous methods, the integral of $f(x)$ over interval $[a, b]$ has been approximated by using a polynomial that can easilty be integraded.
- The polynomial and $f(x)$ have the same value at one (rectangular, midpoint methods), two (trapezoid), or more (Simpson's methods) points.
- The integral is approximated from values of $f(x)$ at the common points.
- When two or more points are involved, a weighted addition of the values of $f(x)$ is used.
- The location of these points is predetermined
- All methods shown were using equally spaced points (presented here).

Numerical Integration - Gauss method

Integration Method	Values of the function used in evaluating the integral in $[a, b]$
Rectangle	$f(a)$ or $f(b)$ (Either one at endpoints)
Midpoint	$f((a+b)/2)$ (Middle point)
Trapezoidal	$f(a)$ and $f(b)$ (Both points)
Simpson 1/3	$f(a)$,$f(b)$ and $f(\frac{1}{2}(a+b))$ (Endpoints and middle point)
Simpson 3/8	$f(a)$, $f(b)$, $f(a+\frac{1}{3}(a+b))$ and $f(a+\frac{2}{3}(a+b))$[1]

[1] (Endpoints and two points that divide the interval into three equal width subintervals)

Numerical Integration - Gauss method

- The Gauss integration is also using weighted addition of values of $f(x)$ at different points (Gauss points).
- Gauss points are not equally spaced.
- Gauss points do not include endpoints.
- The location of the points and the weights of $f(x)$ are determined SIMULTANEOUSLY so that the error is minimized.
- General form of Gauss quadrature:

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

where the coefficients C_i are the weights and the x_i are the Gauss points within $[a, b]$.

Numerical Integration - Gauss method

- General form of Gauss quadrature:

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

  where the coefficients C_i are the weights and the x_i are the Gauss points within $[a, b]$.

- For example for $n = 2$ and $n = 3$:

$$\int_a^b f(x)dx \approx C_1 f(x_1) + C_2 f(x_2)$$

$$\int_a^b f(x)dx \approx C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3)$$

  the value of the coefficients C_i and the location of points x_i depend on the values n, a and b and they are determined so that the right hand side is equal to the left for specific functions $f(x)$.

Numerical Integration - Gauss method

- For the domain $[-1, 1]$ the form of Gauss quadrature can be:

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

  the coefficients C_i and the location of the Gauss points x_i are determined by enforcing the above equation to be exact for the cases when $f(x) = 1, x, x^2, x^3, ..$

- The number of cases that need to be considered depends on the value n. For $n = 2$:

$$\int_{-1}^{1} f(x)dx = C_1 f(x_1) + C_2 f(x_2)$$

Numerical Integration - Gauss method

- The number of cases that need to be considered depends on the value n. For $n = 2$:

$$\int_{-1}^{1} f(x)dx = C_1 f(x_1) + C_2 f(x_2)$$

- The values C_1, C_2, x_1, x_2 are defined by forcing the integral to be exact for the following cases:

$$f(x) = 1 \quad \int_{-1}^{1} 1dx = 2 = C_1 + C_2$$

$$f(x) = x \quad \int_{-1}^{1} xdx = 0 = C_1 x_1 + C_2 x_2$$

$$f(x) = x^2 \quad \int_{-1}^{1} x^2 dx = \frac{2}{3} = C_1 x_1^2 + C_2 x_2^2$$

$$f(x) = x^3 \quad \int_{-1}^{1} x^3 dx = 0 = C_1 x_1^3 + C_2 x_2^3$$

Numerical Integration - Gauss method

- The equations provide a set of four equations with four unknowns.
- The equations are nonlinear and multiple solutions might exist.
- One solution can be obtained by imposing some constraint.
- Assume that points x_1 and x_2 should be symmetrically located about $x = 0$ ($x_1 = -x_2$)
- From this follows, considering the equation $\int_{-1}^{1} x dx = 0 = C_1 x_1 + C_2 x_2$, that $C_1 = C_2$. Now solving the equations:

$$C_1 = 1, C_2 = 1, x_1 = -\frac{1}{\sqrt{3}}, x_2 = \frac{1}{\sqrt{3}}$$

- Now going back to the equation $\int_{-1}^{1} f(x) dx = C_1 f(x_1) + C_2 f(x_2)$ for $n = 2$:

$$\int_{-1}^{1} f(x) dx = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

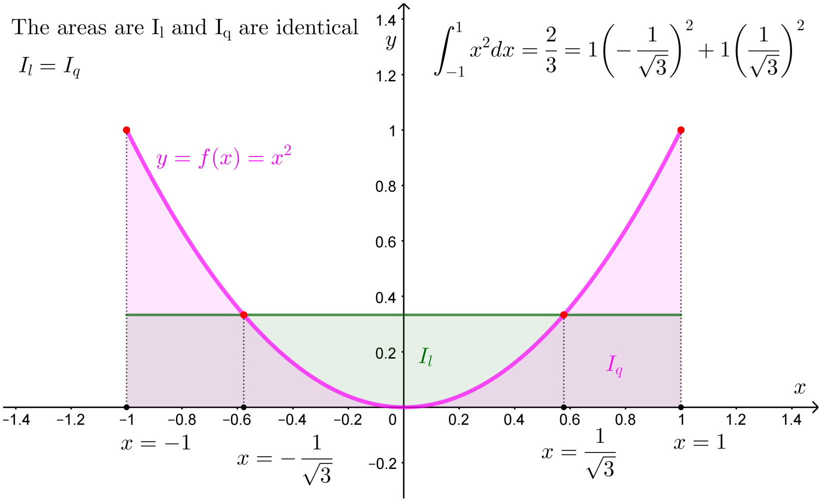
Numerical Integration - Gauss method

- The right hand side gives the exact value of the integral on the left side of the equation when $f(x) = 1$, $f(x) = x$, $f(x) = x^2$ or $f(x) = x^3$. In this case:

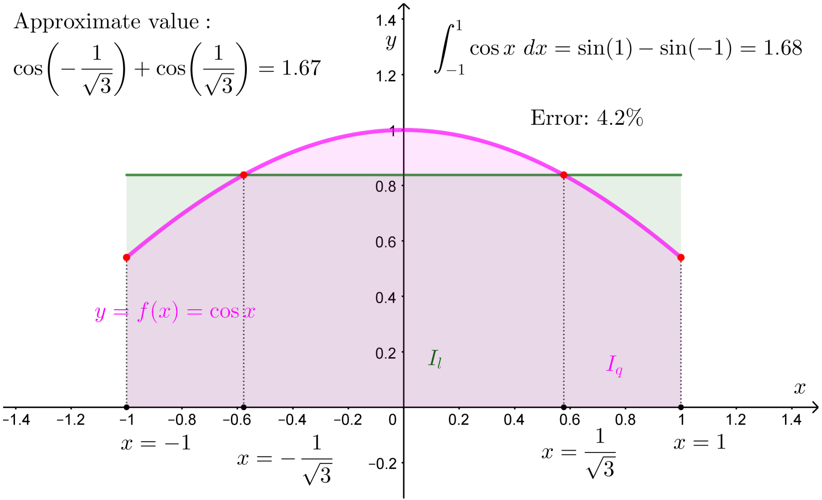
$$\int_{-1}^{1} x^2 dx = \frac{2}{3} = 1\left(-\frac{1}{\sqrt{3}}\right)^2 + 1\left(\frac{1}{\sqrt{3}}\right)^2$$

- The value of the integral $\int_{-1}^{1} x^2 dx$ is the area under the curve $f(x) = x^2$

Numerical Integration - Gauss method



Numerical Integration - Gauss method



Numerical Integration - Gauss method

- The accuracy of Gauss quadrature can be improved by using higher value for the Gauss points n. For example for $n = 3$:

$$\int_{-1}^{1} f(x)dx = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3)$$

and the six constants can be calculated by forcing the function to be exact when :

$$f(x) = 1,\ f(x) = x,\ f(x) = x^2,\ f(x) = x^3,\ f(x) = x^4,\ f(x) = x^5$$

Numerical Integration - Gauss method

n (Number of points)	Coefficients C_i (weights)	Gauss points x_i
2	$C_1 = 1$ $C_2 = 1$	$x_1 = -0.57735027$ $x_2 = 0.57735027$
3	$C_1 = 0.5555556$ $C_2 = 0.8888889$ $C_3 = 0.5555556$	$x_1 = -0.77459667$ $x_2 = 0$ $x_3 = 0.77459667$
4	$C_1 = 0.3478548$ $C_2 = 0.6521452$ $C_3 = 0.6521452$ $C_4 = 0.3478548$	$x_1 = -0.86113631$ $x_2 = -0.33998104$ $x_3 = 0.33998104$ $x_4 = 0.86113631$
5	$C_1 = 0.2369269$ $C_2 = 0.4786287$ $C_3 = 0.5688889$ $C_4 = 0.4786287$ $C_5 = 0.2369269$	$x_1 = -0.90617985$ $x_2 = -0.53846931$ $x_3 = 0$ $x_4 = 0.53846931$ $x_5 = 0.90617985$
6	$C_1 = 0.1713245$ $C_2 = 0.3607616$ $C_3 = 0.4679139$ $C_4 = 0.4679139$ $C_5 = 0.3607616$ $C_6 = 0.1713245$	$x_1 = -0.93246951$ $x_2 = -0.66120938$ $x_3 = -0.23861919$ $x_4 = 0.23861919$ $x_5 = 0.66120938$ $x_6 = 0.93246951$

Numerical Integration - Gauss method

- What we have seen so far is valid only for the interval $[-1, 1]$
- The interval in general can be $[a, b]$
- The Gauss points determined by using interval $[-1, 1]$ can still be used by using a transformation
- We need to transform the integral $\int_a^b f(x)dx$ to $\int_{-1}^1 f(t)dt$, by changing variables:

$$x = \frac{1}{2}[t(b-a) + a + b]; \quad dx = \frac{1}{2}(b-a)dt$$

And the integration becomes:

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

Example

Gauss integration - Example

Evaluate $\int_0^3 e^{-x^2}$ using four-point Gauss quadrature.

Gauss integration - Example: Solution

Evaluate $\int_0^3 e^{-x^2}\,dx$ using Gauss quadrature with four-points.

Solution

1^{st} step: The limits of integration are $[0,3]$, and we can transform it to the form $\int_{-1}^{1} f(t)\,dt$. Here $a=0$ and $b=3$. We use the transformation:

$x = \frac{1}{2}[t(b-a)+a+b]$ $\rightsquigarrow$ for $t=-1 \rightsquigarrow x=a$

$t=1 \rightsquigarrow x=b$

$x = \frac{1}{2}[t(3-0)+0+3] \Rightarrow$

$x = \frac{3}{2}(t+1) \rightsquigarrow \frac{dx}{dt} = \frac{3}{2} \rightsquigarrow dx = \frac{3}{2}dt$

Using the values $x=\frac{3}{2}(t+1)$; $dx=\frac{3}{2}dt$

$$I = \int_0^3 e^{-x^2}dx = \int_{-1}^{1} f(t)\,dt = \int_{-1}^{1} \frac{3}{2}\, e^{-\left[\frac{3}{2}(t+1)\right]^2} dt$$

2^{nd} Step: Use four-point Gauss quadrature to solve integral.

$$I = \int_{-1}^{1} f(t)\,dt \approx C_1 f(t_1) + C_2 f(t_2) + C_3 f(t_3) + C_4 f(t_4)$$

$C_1 = 0{,}3478548$ $\quad x_1 = -0{,}86113631$ $\quad$ see Table in slides

$C_2 = 0{,}6521452$ $\quad x_2 = -0{,}33998104$

$C_3 = 0{,}6521452$ $\quad x_3 = 0{,}33998104$

$C_4 = 0{,}3478548$ $\quad x_4 = 0{,}86113631$

$0{,}3478548 \cdot f(-0{,}86113681) + 0{,}6521402\, f(-0{,}33998104) +$
$0{,}6521452 \cdot f(0{,}33998104) + 0{,}3478548\, f(0{,}86115651) =$

$f(t) = \frac{3}{2} e^{-\left[\frac{3}{2}(t+1)\right]^2}$:

$$I = 0{,}3478548\,\frac{3}{2}\,e^{-\left[\frac{3}{2}(-0{,}86113631+1)\right]^2} + 0{,}6521452\,\frac{3}{2}\,e^{-\left[\frac{3}{2}(-0{,}33998104+1)\right]^2}$$
$$+ 0{,}6521452\,\frac{3}{2}\,e^{-\left[\frac{3}{2}(0{,}33998104+1)\right]^2} + 0{,}3478548\,\frac{3}{2}\,e^{-\left[\frac{3}{2}(0{,}86113631+1)\right]^2}$$

$= 0{,}8841309$

The exact solution, when solved analytically is $0{,}8862073$. The error is about 1%

Numerical Integration - MatLab build-in functions

Numerical Integration - MatLab build-in functions

- MatLab has several built-in functions for implementing integration.
- The functions `quad`, `quadl`, `trapz` and `integral`.
- The function `I=quad(function,a,b)`, where the function can be uses as a string expression or as a function handle and should as a function of x.
- The function `quad` does not handle singularities.
- The function `quadl` is using the adaptive method developed by Lobatto.
- MatLab suggests to use `integral` instead of `quad` and `quadl`.
- The `integral` is based on a vectorized adaptive method developed by Shampine, [3].

Numerical Integration - MatLab build-in functions

- The function `integral2` and `integral3` calculate double and triple integrals.
- The function `q=trapz(x,y)` is used for integrating discrete points by using the trapezoidal method, where x and y are vectors with the x and y coordinates with the same length.

Example

References

Amos Gilat and Vish Subramaniam.
Numerical Methods for Engineers and Scientists, An Introduction with Applications Using MATLAB.
Wiley, Danvers, Massachusetts, 2014.

Jan Kiusalaas.
Numerical Methods in Engineering with MATLAB.
Cambridge University Press, Cambridge, United Kingdom, 2016.

L.F. Shampine.
Vectorized adaptive quadrature in matlab.
Journal of Computational and Applied Mathematics, 211(2):131–140, 2008.