



Numerical integration

Problem formulation

Let $y = f(x)$ be a function, defined and Riemann-integrable in the interval $[a, b]$. Considering a given table of values $y_i = f(x_i)$ of the function in the points (nodes) $x_0, x_1, x_2, \dots, x_n \in [a, b]$, find the approximate value of the integral $I = \int_a^b f(x) dx$.

Newton-Cotes quadrature formulas

If n is a natural number and $h = \frac{b-a}{n}$ is a step, with the help of which the interval of iteration is divided into n equal sub-intervals, which means that $x_0 = a$, $x_{i+1} = x_i + h$, $i = 0, 1, \dots, n-1$, then the most frequently used sum quadrature formulas of Newton-Cotes are given in the table below. Here $M_k = \max_{x \in [a, b]} |f^{(k)}(x)|$, under condition that there exists a continuous k -th derivative of $y = f(x)$.

Name	Quadrature formula for numerical integration	Error evaluation $ R(f, x) $
Left rectangle formula	$I_1 \approx h \sum_{i=0}^{n-1} f(x_i)$	$\frac{(b-a)^2}{2n} M_1$, i.e. $\frac{(b-a)M_1}{2} h$
Right rectangle formula	$I_2 \approx h \sum_{i=1}^n f(x_i)$	$\frac{(b-a)^2}{2n} M_1$, i.e. $\frac{(b-a)M_1}{2} h$
Mid-rectangle formula	$I_3 \approx h \sum_{i=0}^{n-1} f(x_i + \frac{h}{2})$	$\frac{(b-a)^3}{24n^2} M_2$, i.e. $\frac{(b-a)M_2}{24} h^2$
Trapezoid formula	$I_T \approx \frac{h}{2} \left(f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right)$	$\frac{(b-a)^3}{12n^2} M_2$, i.e. $\frac{(b-a)M_2}{12} h^2$
Simpson's formula	$n = 2m,$ $I_S \approx \frac{h}{3} \left(f(a) + 4 \sum_{i=1}^m f(x_{2i-1}) + 2 \sum_{i=1}^{m-1} f(x_{2i}) + f(b) \right)$	$\frac{(b-a)^5}{180n^4} M_4$, i.e. $\frac{(b-a)M_4}{180} h^4$

Example 1. The values for the function $y = f(x) = \ln(x^2)$ in the interval $[2,3]$ are given in the first two columns of table 1. Calculate the approximate values of the integral $I = \int_2^3 f(x) dx$, using all the quadrature formulas from the table above.

Solution:

In this case we have a step of $h = 0,1$ and the number of sub-intervals is $n = 10$.

Table 1

i	x_i	y_i
0	2,0	1,38629
1	2,1	1,48387
2	2,2	1,57691
3	2,3	1,66582
4	2,4	1,75094
5	2,5	1,83258
6	2,6	1,91102
7	2,7	1,98650
8	2,8	2,05924
9	2,9	2,12942
10	3,0	2,19722

Table 2

i	$x_i + \frac{h}{2}$	$y_{i+\frac{1}{2}}$
0	2,05	1,43568
1	2,15	1,53094
2	2,25	1,62186
3	2,35	1,70883
4	2,45	1,79218
5	2,55	1,87219
6	2,65	1,94912
7	2,75	2,02320
8	2,85	2,09464
9	2,95	2,16361

a) Using the left rectangle formula we have to add together the values from y_0 to y_9 and to multiply the resulting number by h . We get

$$I_1 \approx h \sum_{i=0}^{n-1} f(x_i) = h \sum_{i=0}^9 y_i = 0,1 \cdot (17,7826) = 1,77826.$$

b) Using the right rectangle formula we find the sum from y_1 to y_{10} and the resulting number we multiply by h . We get

$$I_2 \approx h \sum_{i=1}^n f(x_i) = h \sum_{i=1}^{10} y_i = 0,1 \cdot 18,5935 = 1,85935.$$

c) In the case of the mid-rectangle formula using table 2 we calculate:

$$I_3 \approx h \sum_{i=0}^{n-1} f\left(x_i + \frac{h}{2}\right) = h \sum_{i=0}^9 y_{i+\frac{1}{2}} = 0,1 \cdot 18,1923 = 1,81923.$$

d) Respectively for trapezoids we have

$$I_T \approx \frac{h}{2} \left(f(a) + 2 \sum_{i=1}^{n-1} f(x_i) + f(b) \right) = \frac{h}{2} \left(y_0 + 2 \sum_{i=1}^9 y_i + y_{10} \right)$$

$$= 0,05 (y_0 + 2(y_1 + y_2 + \dots + y_9) + y_{10}) = 0,05 (1,38629 + 2 \cdot (16,39631) + 2,19722) = 0,05 \cdot (36,37615) = 1,818807;$$

e) Using Simpson's summation formula:

$$\begin{aligned}
I_S &\approx \frac{h}{3} \left(f(a) + 4 \sum_{i=1}^m f(x_{2i-1}) + 2 \sum_{i=1}^m f(x_{2i}) - f(b) \right) \\
&= \frac{0,1}{3} (y_0 + 4(y_1 + y_3 + \dots + y_9) + 2(y_2 + y_4 + \dots + y_8) + y_{10}) \\
&= \frac{0,1}{3} (1,38629 + 4 \cdot (9,09820) + 2 \cdot (7,29812) + 2,19722) = \frac{0,1}{3} \cdot (54,57254) = 1,819085.
\end{aligned}$$

Example 2. Evaluate the error of numerical integration for I_1 , I_T , I_S from example 1.

Solution:

We find one by one the derivatives of $f(x) = \ln(x^2)$:

$$f'(x) = \frac{2}{x}, \quad f''(x) = \frac{-2}{x^2}, \quad f'''(x) = \frac{4}{x^3}, \quad f^{(4)}(x) = \frac{-12}{x^4}.$$

$$\text{Then } M_1 = \max_{2 \leq x \leq 3} |f'(x)| = f'(2) = 1, \quad M_2 = \max_{2 \leq x \leq 3} |f''(x)| = |f''(2)| = \frac{1}{2},$$

$$M_4 = \max_{2 \leq x \leq 3} |f^{(4)}(x)| = |f^{(4)}(2)| = \frac{3}{4}.$$

By substituting in the error formula of the left rectangle method we get:

$$|R_1(f, h)| \leq \frac{M_1(b-a)h}{2} = \frac{0,1}{2} = 0,05 \quad \text{i.e. the first-second digit of the result is correct.}$$

Consequently after rounding off up to the second digit we have $I_1 \approx 1,78$.

$$\text{For the trapezoid formula we calculate: } |R_T(f, h)| \leq \frac{M_2(b-a)h^2}{12} = \frac{0,01}{24} \leq 0,005 \quad \text{or two-three}$$

digits after the decimal comma. Then $I_T \approx 1,819$.

For Simpson's quadrature formula:

$$|R_S(f, h)| \leq \frac{M_4(b-a)h^4}{180}, \quad \text{i.e. all digits are correct and } I_S = \int_2^3 \ln(x^2) dx \approx 1,819085.$$

Note. The formula of the function is not usually given or finding the derivative is difficult or there might not even exist derivatives for a given row. Then simpler formulas are used which give a small error. Accuracy in such cases is achieved by reducing the step h .

Example 3. Determine the step of numerical integration h so that the approximation of calculation of the integral $\int_{-1}^3 \sqrt{1+x^2} dx$ using the trapezoid method guarantees accuracy of the result $\varepsilon = 0,000001$.

Solution:

Here $a = -1$, $b = 3$. For the derivatives we have: $f'(x) = \frac{x}{\sqrt{1+x^2}}$, $f''(x) = \frac{1}{(1+x^2)\sqrt{1+x^2}}$.

It is obvious that $0 \leq f''(x) \leq 1$ for every x , and consequently $M_2 \leq 1$. By substituting in the error formula for the trapezoid method we find that:

$$|R_T(f, h)| \leq \frac{M_2(b-a)h^2}{12} = \frac{(3-(-1))h^2}{12} = \frac{h^2}{3}.$$

To guarantee the sought accuracy we introduce the condition $\frac{h^2}{3} \leq \varepsilon$, or $h \leq \sqrt{3\varepsilon} = \sqrt{0,000003} \approx 0,00173$. It is convenient to use the step $h = 0,001$ and accordingly to divide the interval $[-1, 3]$ by $n = 4000$ equal sub-intervals. To carry out the calculations it is obvious that a computer is needed as well as a mediating accuracy of 10^{-8} .

Author: Snezhana Gocheva-Ilieva, snow@uni-plovdiv.bg