On Newton-Cotes formulas

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Abstract

Integration is one of the important aspects of numerical analysis, with its application ranging from mathematical finance to engineering. In this report, we look at numerical methods of approximating the definite integral $I = \int_a^b f(x)dx$ for a continuous function f on an interval $[a, b]$. These methods are called Newton-Cotes formulas.

1 Integration

Let $f : \mathbb{R} \to \mathbb{R}$ be a real-valued function. Assume that a is the lower limit and b is the upper limit of the interval $\mathcal{I} = [a, b]$. The definite integral I is given by:

$$I = \int_a^b f(x)dx. \tag{1}$$

By the *fundamental theorem of calculus*, I can be evaluated as follows:

$$I = \int_a^b f(x)dx = F(b) - F(a), \tag{2}$$

where F is the antiderivative of a function f such that $F'(x) = f(x)$.

If function F can be obtained, then we are good to go; however, in practice, it is hard to find such a function. Hence, numerical methods are employed. For example, if $f(x) = x^2$ then $F(x) = \frac{x^3}{3}$. But for a function like $f(x) = e^{x^2} \cos(e^{\sin x + x^2}) - x^3$, it is not easy to obtain F.

2 Newton-Cotes formulas

The aim of Newton-Cotes is to approximate the integral I. To do that, we start by partitioning the interval $\mathcal{I}$. There are various ways to do that; in this report, we stick with uniform partition.

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2.1 The Weights

We assume a is the first point in the interval and b is the last point. This is obvious, isn't it? Assume that there are $n + 1$ points to be partitioned.

We compute the step size as:

$$\Delta x = \frac{b - a}{n}. \tag{3}$$

Now, for $i = 0, ..., n$ then $x_i \in \mathcal{I}$ is computed as:

$$x_i = a + i\Delta x, \tag{4}$$

which can then be written as:

$$x_{i+1} = x_i + \Delta x. \tag{5}$$

The lower limit $a = x_0$ and the upper limit $b = x_n$.

There are two types of formulas: closed formulas and open formulas. In this report, we only consider closed formulas in which the steps are as given above.

The integral is then approximated as follows:

$$I \approx \sum_{i=0}^{n} w_i f(x_i), \tag{6}$$

where w are weights. This formulation is also called the quadrature rule.

We derive the weights for Newton-Cotes via polynomial interpolation. We assume that function f can be approximated by some polynomial function p such that:

$$p(x) = \sum_{i=0}^{n} f(x_i) L_{n,i}(x), \tag{7}$$

where L is some n polynomial interpolation function expressed in the form of Lagrange. The Lagrangian function is written as:

$$\begin{aligned} L_{n,i}(x) &= \frac{(x - x_0)(x - x_1)...(x - x_n)}{(x_i - x_0)(x_i - x_1)...(x_i - x_n)}, && (8) \\ &= \prod_{0 \leq k \leq n, k \neq i} \frac{x - x_k}{x_i - x_k}. && (9) \end{aligned}$$

So we have:

$$\begin{aligned} I &\approx \int_a^b f(x)dx, && (10) \\ &\approx \int_a^b p(x)dx, && (11) \\ &\approx \int_a^b \left(\sum_{i=0}^{n} f(x_i) L_{n,i}(x) \right) dx, && (12) \\ &\approx \sum_{i=0}^{n} \left(\int_a^b L_{n,i}(x)dx \right) f(x_i). && (13) \end{aligned}$$

Now, the weights are determined by $w_i = \int_a^b L_{n,i}(x)dx$.

The standard integration formulas, like the trapezoidal rule and Simpson's rule, can be derived from the Newton-Cotes approach.

Next, we present the standard trapezoidal rule and Simpson's rule.

2.2 Trapezoidal rule

We set $n = 1$ so that we have $n + 1$ (2) points, and then we compute the weights. The step size $\Delta x = \frac{b-a}{2}$ and $x_0 = a, x_1 = b$.

We want to compute the following weights:

$$\begin{aligned} w_0 &= \int_a^b L_{1,0} dx, && (14) \\ &= \int_a^b \frac{x - x_1}{x_0 - x_1} dx, && (15) \\ w_1 &= \int_a^b L_{1,1} dx, && (16) \\ &= \int_a^b \frac{x - x_0}{x_1 - x_0} dx. && (17) \end{aligned}$$

We consider the following transformation from interval $[a, b]$ to $[0, 2]$:

$$t = \frac{x - a}{\Delta x} = \frac{x - a}{b - a}. \tag{18}$$

Now, we have the following transformed variables in the interval $[0, 2]$:

$$\begin{aligned} \frac{x - x_1}{x_0 - x_1} &= \frac{(a + t\Delta x) - b}{a - b}, && (19) \\ &= 1 + \frac{t\Delta x}{-\Delta x}, && (20) \\ &= 1 - t, && (21) \\ \frac{x - x_0}{x_1 - x_0} &= \frac{(a + t\Delta x) - a}{b - a}, && (22) \\ &= \frac{t\Delta x}{\Delta x}, && (23) \\ &= t. && (24) \end{aligned}$$

The differential dx is transformed as $dx = \Delta x dt$.

We compute the weights as follows:

$$
\begin{aligned}
w_0 &= \int_a^b \frac{x - x_1}{x_0 - x_1} dx, && (25)\\
&= \int_0^1 (1-t)\Delta x dt, && (26)\\
&= \frac{\Delta x}{2}, && (27)\\
w_1 &= \int_a^b \frac{x - x_0}{x_1 - x_0} dx, && (28)\\
&= \int_0^1 t\Delta x dt, && (29)\\
&= \frac{\Delta x}{2}. && (30)
\end{aligned}
$$

The trapezoidal rule is thus written as:

$$
\begin{aligned}
\int_a^b f(x)dx &\approx w_0 f(x_0) + w_1 f(x_1), && (31)\\
&= \frac{\Delta x}{2}(f(x_0) + f(x_1)), && (32)\\
&= \frac{b-a}{2}(f(a) + f(b)). && (33)
\end{aligned}
$$

The generalized trapezoidal rule divides the interval $[a, b]$ into n subintervals of equal width $\Delta x = \frac{b-a}{n}$ and approximates the integral as:

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{2}\left(f(a) + 2\sum_{i=1}^{n-1} f(a + i\Delta x) + f(b)\right).$$

This is also called the composite trapezoidal rule.

2.3 Simpson's rule

We set $n = 2$ so that we have $n + 1$ (3) points, and then we compute the weights. The step size $\Delta x = \frac{b-a}{2}$ and $x_0 = a, x_1 = a + \Delta x = \frac{a+b}{2}, x_2 = b$.

The weights are expressed as follows:

$$
\begin{aligned}
w_0 &= \int_a^b L_{2,0} dx, && (34)\\
&= \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx, && (35)\\
w_1 &= \int_a^b L_{2,1} dx, && (36)\\
&= \int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_0-x_2)} dx, && (37)\\
w_2 &= \int_a^b L_{2,2} dx, && (38)\\
&= \int_a^b \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx. && (39)
\end{aligned}
$$

To solve this, we can apply a linear transformation of any type. Similarly, consider the following transformation from interval $[a, b]$ to $[0, 2]$:

$$
t = \frac{x-a}{\Delta x} = \frac{x-a}{(b-a)/2}. \tag{40}
$$

Now, with some algebra, we have the transformed variables:

$$
\begin{aligned}
\frac{x-x_1}{x_0-x_1} &= \frac{t\cdot\Delta x - \Delta x}{-\Delta x} = 1-t, && (41)\\
\frac{x-x_2}{x_0-x_2} &= \frac{t\cdot\Delta x + (a-b)}{a-b} = 1-\frac{t}{2} && (42)\\
\frac{x-x_0}{x-x_2} &= \frac{(a+t\cdot\Delta x)-a}{(a+t\cdot\Delta x)-b} = \frac{t}{t-2}, && (43)\\
\frac{x-x_0}{x_1-x_0} &= \frac{(a+t\cdot\Delta x)-a}{(a+\Delta x)-a} = t, && (44)\\
\frac{x-x_1}{x_2-x_1} &= \frac{(a+t\cdot\Delta x)-(a+\Delta x)}{b-(a+\Delta x)} = t-1, && (45)\\
\frac{x-x_2}{x_1-x_2} &= \frac{(a+t\cdot\Delta x)-b}{(a+\Delta x)-b} = 2-t, && (46)\\
\frac{x-x_0}{x_2-x_0} &= \frac{(a+t\cdot\Delta x)-a}{b-a} = \frac{t}{2}, && (47)\\
\frac{x-x_1}{x_2-x_0} &= \frac{(a+t\cdot\Delta x)-(a+\Delta x)}{b-a} = \frac{t-1}{2}. && (48)
\end{aligned}
$$

The transformed dx is $dx = \Delta x dt$. We arrive at the following weights:

$$
\begin{aligned}
w_0 &= \int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx, && (49)\\
&= \int_0^2 \frac{(1-t)(2-t)}{2} \Delta x dt, && (50)\\
&= \frac{\Delta x}{2} \int_0^2 (1-t)(2-t) dt, && (51)\\
&= \frac{\Delta x}{2} \int_0^2 (t^2-3t+2) dt, && (52)\\
&= \frac{\Delta x}{2} \frac{2}{3}, && (53)\\
&= \frac{\Delta x}{3}, && (54)\\
w_1 &= \int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_0-x_2)} dx, && (55)\\
&= \int_0^2 \frac{t(t-2)}{-1} \Delta x dt, && (56)\\
&= -\Delta x \int_0^2 t(2-t) dt, && (57)\\
&= -\Delta x \int_0^2 (2t-t^2) dt, && (58)\\
&= -\Delta x \frac{-4}{3}, && (59)\\
&= \frac{4}{3} \Delta x, && (60)\\
w_2 &= \int_a^b \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx, && (61)\\
&= \int_0^2 \frac{t(t-1)}{2} \Delta x dt, && (62)\\
&= \frac{\Delta x}{2} \int_0^2 (t^2-t) dt, && (63)\\
&= \frac{\Delta x}{2} \frac{2}{3}, && (64)\\
&= \frac{\Delta x}{3}. && (65)
\end{aligned}
$$

The Simpson's rule is thus written as:

$$\int_a^b f(x)dx \approx w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2), \tag{66}$$

$$= \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b), \tag{67}$$

$$= \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right). \tag{68}$$

Similarly, the generalized Simpson's rule divides the interval $[a, b]$ into n subintervals (where n is even) and approximates the integral as:

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{3}\left(f(a) + 4\sum_{\substack{i=1 \\ i \text{ odd}}}^{n-1} f(a + i\Delta x) + 2\sum_{\substack{i=2 \\ i \text{ even}}}^{n-2} f(a + i\Delta x) + f(b)\right).$$

This is also called the composite Simpson's rule.

Other formulas can be obtained when $n \geq 3$.

3 Results

For analysis, we look at the generalized version of the trapezoidal rule and Simpson's rule. We consider the following functions on an interval $[0, 2]$:

$$f_1(x) = e^{-x}\sin(10x), \tag{69}$$

$$f_2(x) = \frac{1}{\sqrt{1+x^4}}, \tag{70}$$

$$f_3(x) = \ln(1+x)\cdot\cos(x). \tag{71}$$

We employ Scipy's quad as a reference value.

3.1 Oscillatory with Exponential Decay

The convergence of the trapezoidal rule and Simpson's rule for the function $f(x) = e^{-x} \cdot \sin(10x)$ is shown in Figure 1.

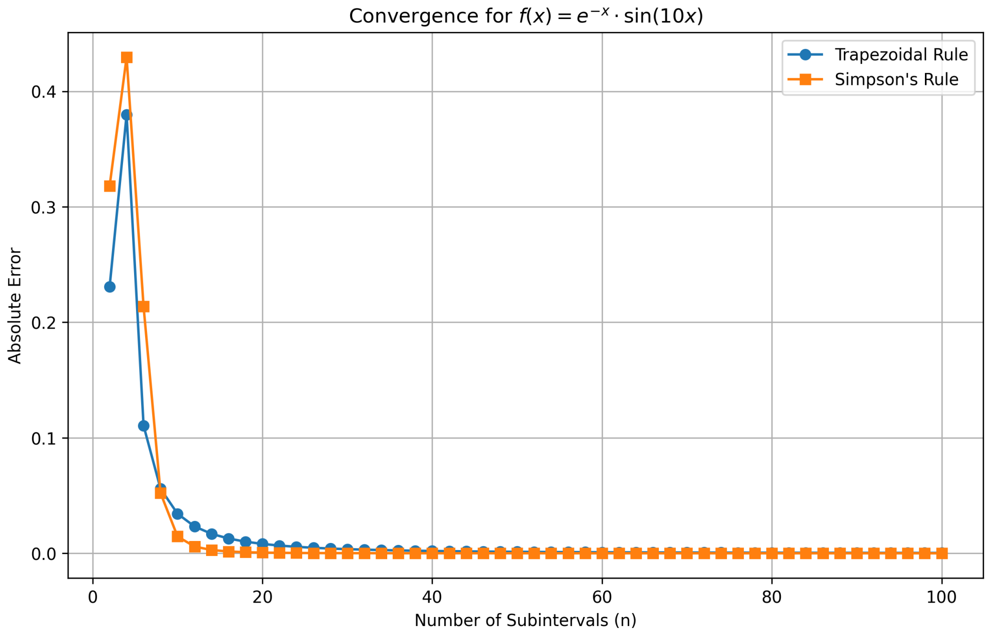

Figure 1: Convergence for $f(x) = e^{-x} \cdot \sin(10x)$.

3.2 Rational with Singularity

The convergence of the trapezoidal rule and Simpson's rule for the function $f(x) = \frac{1}{\sqrt{1+x^4}}$ is shown in Figure 2.

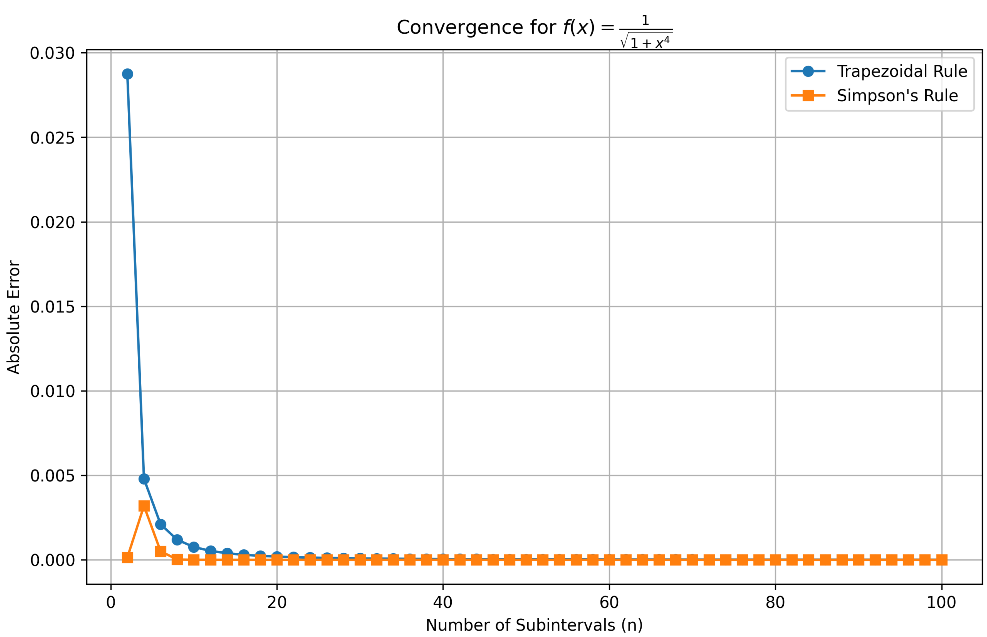

Figure 2: Convergence for $f(x) = \frac{1}{\sqrt{1+x^4}}$.

3.3 Composite Function

The convergence of the trapezoidal rule and Simpson's rule for the function $f(x) = \ln(1 + x) \cdot \cos(x)$ is shown in Figure 3.

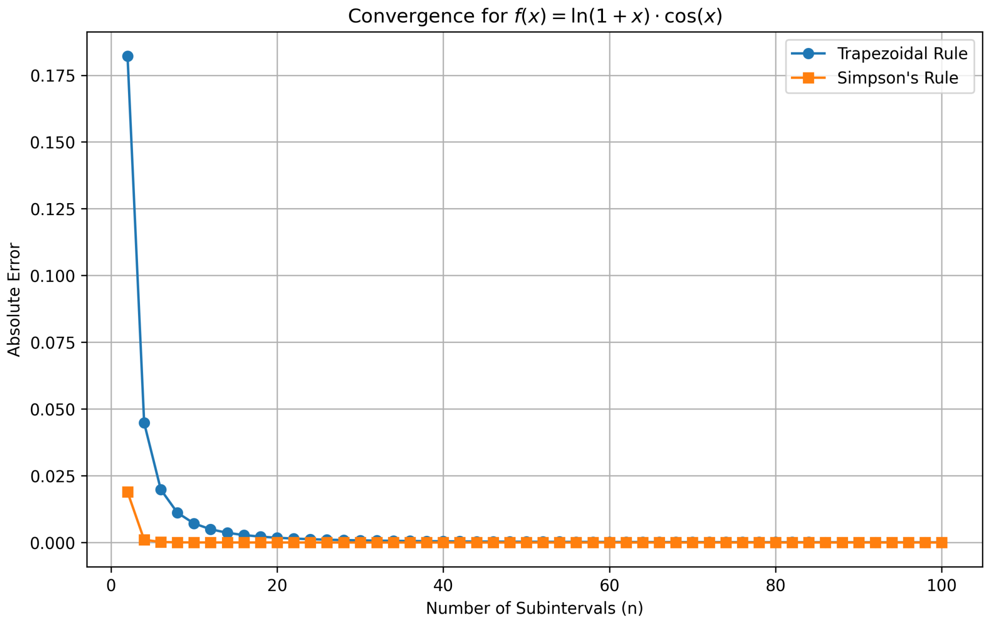

Figure 3: Convergence for $f(x) = \ln(1 + x) \cdot \cos(x)$.

References

[1] Germund Dahlquist and Åke Björck. *Numerical methods*. Courier Corporation, 2003.

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