

Computational Astrophysics

E. Larrañaga

Observatorio Astronómico Nacional
Universidad Nacional de Colombia

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Integration

We want to evaluate numerically the integral

$$Q = \int_a^b f(x) dx , \quad (1)$$

where $f(x)$ may be a well behaved analytical function or a function given as discrete data $f(x_i)$.

Integration based on Piecewise Polynomial Interpolation

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This integration, based on interpolation polynomials, is generally called *Newton-Cotes quadrature formulae*.

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Now, consider that the full interval over which we intend to integrate can be broken down into N sub-intervals $[a_i, b_i]$ that encompass $N + 1$ nodes x_i ($i = 0, \dots, N$) at which we know the integrand $f(x)$.

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The full integral Q can be written as the sum of the sub-integrals Q_i :

$$Q = \sum_{i=0}^{N-1} Q_i = \sum_{i=0}^{N-1} \int_{a_i}^{b_i} f(x) dx . \quad (2)$$

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There are many ways to evaluate these sub-integrals.

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Hence, using its central value we write

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Note that we need to be able to evaluate $f(x)$ at the midpoint (knowing the value or using an interpolating polynomial).

MidPoint Rule

The error in the midpoint quadrature can be estimated using a Taylor expansion about the midpoint $m_i = (a_i + b_i)/2$,

$$f(x) = f(m_i) + f'(m_i)(x - m_i) + \frac{f''(m_i)}{2}(x - m_i)^2 + \frac{f'''(m_i)}{6}(x - m_i)^3 + \dots \quad (4)$$

Integrating this expression from a_i to b_i , the odd-order terms drop out, and what is left is

$$Q_i = \int_{a_i}^{b_i} f(x) dx = f(m_i)(b_i - a_i) + \frac{f''(m_i)}{24}(b_i - a_i)^3 + \dots \quad (5)$$

$$Q_i = \int_{a_i}^{b_i} f(x) dx = f(m_i)(b_i - a_i) + \mathcal{O}(h^3) + \dots \quad (6)$$

where $h = (b_i - a_i) \approx \frac{(b-a)}{N}$.

Trapezoidal Rule

This method approximates $f(x)$ with a linear polynomial on $[a_i, b_i]$,

$$Q_i = \int_{a_i}^{b_i} f(x) dx = \frac{1}{2}(b_i - a_i) [f(b_i) + f(a_i)] . \quad (7)$$

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Using a Taylor expansion it is shown that the trapezoidal rule has a local error that, like the midpoint rule, goes with h^3 .

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$$Q_i = \frac{b_i - a_i}{6} \left[f(a_i) + 4f\left(\frac{a_i + b_i}{2}\right) + f(b_i) \right] + \mathcal{O}([b_i - a_i]^5) . \quad (8)$$

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This method has an error going with h^5

Simpson's Rule (non-equidistant intervals)

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Write

$$f(x) = ax^2 + bx + c \quad \text{for } x \in [x_{i-1}, x_{i+1}] , \quad (9)$$

where,

$$\begin{aligned} a &= \frac{h_{i-1}f(x_{i+1}) - (h_{i-1} + h_i)f(x_i) + h_if(x_{i-1})}{h_{i-1}h_i(h_{i-1} + h_i)} , \\ b &= \frac{h_{i-1}^2f(x_{i+1}) + (h_i^2 - h_{i-1}^2)f(x_i) - h_i^2f(x_{i-1})}{h_{i-1}h_i(h_{i-1} + h_i)} , \\ c &= f(x_i) , \end{aligned} \quad (10)$$

with $h_i = x_{i+1} - x_i$ and $h_{i-1} = x_i - x_{i-1}$.

Simpson's Rule (non-equidistant intervals)

Since the integral

$$\int_{x_{i-1}}^{x_{i+1}} f(x) dx$$

is independent of the origin of the coordinates, we can choose $x_i = 0$, and hence $-h_{i-1} = x_{i-1}$, $h_i = x_{i+1}$ to obtain

$$\int_{x_{i-1}}^{x_{i+1}} f(x) dx = \int_{-h_{i-1}}^{h_i} f(x) dx = \alpha f(x_{i+1}) + \beta f(x_i) + \gamma f(x_{i-1}) , \quad (11)$$

with

$$\begin{aligned} \alpha &= \frac{2h_i^2 + h_i h_{i-1} - h_{i-1}^2}{6h_i} , & \beta &= \frac{(h_i + h_{i-1})^3}{6h_i h_{i-1}} , \\ \gamma &= \frac{-h_i^2 + h_i h_{i-1} + 2h_{i-1}^2}{6h_{i-1}} , \end{aligned} \quad (12)$$

Gaussian Quadrature

Gaussian quadrature is an integration method in which there are chosen two quantities, nodes and weights, to maximize the degree of the resulting integration rule.

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Gaussian quadrature is an integration method in which there are chosen two quantities, nodes and weights, to maximize the degree of the resulting integration rule.

Using $2n$ degrees of freedom, it is possible to integrate polynomials of degree $2n - 1$. The condition is that, for a set of n nodes x_i and n weights w_i at which a function f is known,

$$\int_a^b f(x) dx \approx \sum_{i=1}^n w_i f(x_i) \quad (13)$$

2-point Gaussian Quadrature

In the 2-point Gaussian quadrature we consider 2 nodes x_i and 2 weights w_i on the interval $[a, b]$ to integrate exactly a polynomial of degree 3. Hence

$$\int_a^b f(x) dx = w_1 f(x_1) + w_2 f(x_2). \quad (14)$$

We can find the unknowns w_1 , w_2 , x_1 , and x_2 by demanding that the formula give exact results for integrating a general polynomial of degree 3,

$$\begin{aligned} \int_a^b f(x) dx &= \int_a^b (c_0 + c_1 x + c_2 x^2 + c_3 x^3) dx, \\ &= c_0(b-a) + c_1 \left(\frac{b^2 - a^2}{2} \right) + c_2 \left(\frac{b^3 - a^3}{3} \right) + c_3 \left(\frac{b^4 - a^4}{4} \right). \end{aligned} \quad (15)$$

2-point Gaussian Quadrature

However, we have

$$\begin{aligned}\int_a^b f(x) dx &= w_1 f(x_1) + w_2 f(x_2) \\ &= w_1(c_0 + c_1 x_1 + c_2 x_1^2 + c_3 x_1^3) + w_2(c_0 + c_1 x_2 + c_2 x_2^2 + c_3 x_2^3).\end{aligned}$$

Therefore, comparing these results gives

$$w_1 = \frac{b-a}{2}, \quad w_2 = \frac{b-a}{2}, \quad (16)$$

$$x_1 = \left(\frac{b-a}{2}\right) \left(-\frac{1}{\sqrt{3}}\right) + \left(\frac{b+a}{2}\right), \quad (17)$$

$$x_2 = \left(\frac{b-a}{2}\right) \left(\frac{1}{\sqrt{3}}\right) + \left(\frac{b+a}{2}\right). \quad (18)$$

2-point Gaussian Quadrature

In the special case of the interval $[-1, 1]$:

$$w_1 = w_2 = 1, \quad x_1 = -\frac{1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}}, \quad (19)$$

and

$$\int_{-1}^1 f(x) dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \quad (20)$$

Change of Interval

Using an affine transformation that maps $[a, b] \rightarrow [-1, 1]$ as

$$t = \frac{b-a}{2}x + \frac{a+b}{2}, \quad (21)$$

and a change of variables

$$dt = \frac{b-a}{2}dx, \quad (22)$$

it is possible to change the interval of integration,

$$\int_a^b f(x)dx = \frac{b-a}{2} \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right) dx. \quad (23)$$