Computational Astrophysics

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Outline

Integration

We want to evaluate numerically the integral

$$Q = \int_a^b f(x)dx \ , \tag{1}$$

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 $(i = 0, \cdots, N)$ 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:

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

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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 $m_i = (a_i + b_i)/2$,

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

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

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

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

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

Trapezoidal Rule

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

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

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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

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

where,

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

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

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

with

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

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,

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

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

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

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,

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

2-point Gaussian Quadrature

However, we have

$$\begin{aligned}\int_a^b f(x)dx &= w_1 f(x_1) + w_2 f(x_2) \\ &= w_1(c_0 + c_1x_1 + c_2x_1^2 + c_3x_1^3) + w_2(c_0 + c_1x_2 + c_2x_2^2 + c_3x_2^3).\end{aligned}$$

Therefore, comparing these results gives

$$w_1 = \frac{b-a}{2}\ , \qquad w_2 = \frac{b-a}{2}\ , \tag{16}$$

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

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

2-point Gaussian Quadrature

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

$$w_1 = w_2 = 1 \ , \qquad x_1 = -\frac{1}{\sqrt{3}} \ , \qquad x_2 = \frac{1}{\sqrt{3}} \ , \tag{19}$$

and

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

Change of Interval

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

$$t = \frac{b-a}{2}x + \frac{a+b}{2} \ , \tag{21}$$

and a change of variables

$$dt = \frac{b-a}{2}dx \ , \tag{22}$$

it is possible to change the interval of integration,

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

Cubic Natural Spline Interpolation

Integration of this interpolated second derivative two times and using $f_i = p_i(x_i) = f(x_i)$ gives

$$p_i(x) = \alpha_i(x - x_i)^3 + \beta_i(x - x_{i+1})^3 + \gamma_i(x - x_i) + \eta_i(x - x_{i+1}), \tag{24}$$

where

$$\alpha_i = \frac{p''_{i+1}}{6h_i} \qquad \beta_i = \frac{-p''_i}{6h_i}, \tag{25}$$

$$\gamma_i = \frac{f_{i+1}}{h_i} - \frac{h_i p''_{i+1}}{6} \qquad \eta_i = \frac{h_i p''_i}{6} - \frac{f_i}{h_i}, \tag{26}$$

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

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

Hence, all we need to find the spline is to know all of its second derivatives $p''_i = p''_i(x_i)$.

Cubic Natural Spline Interpolation

Now apply the condition $p'_{i-1}(x_i) = p'_i(x_i)$ to the interpolated polynomial to obtain the equation

$$h_{i-1}p''_{i-1} + 2(h_{i-1} + h_i)p''_i + h_i p''_{i+1} = 6\left(\frac{g_i}{h_i} - \frac{g_{i-1}}{h_{i-1}}\right) \ , \qquad (27)$$

where $g_i = f_{i+1} - f_i$.

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where $g_i = f_{i+1} - f_i$.

This is a linear system with $n-1$ unknowns: p''_i for $i = 1, \cdots, n-1$ (remember that $p''_0 = p''_n = 0$, as set by the natural spline condition.

Cubic Natural Spline Interpolation

Defining $d_i = 2(h_{i-1} + h_i)$ and $b_i = 6\left(\frac{g_i}{h_i} - \frac{g_{i-1}}{h_{i-1}}\right)$, we can write

$$Ap'' = b \quad \text{with } A_{ij} = \begin{cases} d_i & \text{if } i = j\,, \\ h_i & \text{if } i = j - 1\,, \\ h_{i-1} & \text{if } i = j + 1\,, \\ 0 & \text{otherwise.} \end{cases} \tag{28}$$

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The coefficient matrix A_{ij} is real, symmetric, and tri-diagonal. The solution of such a linear system of equations will be presented later in the course.