Quadrature Algorithms

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What is Quadrature?

A method utilized to approximate a definite integral,

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

either numerically or analytically.

Methodology Overview

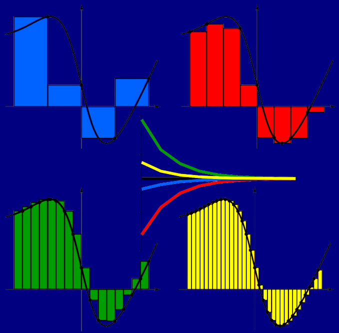
Quadrature methods require the selection followed by the evaluation of abscissa on the integrand $f(x)$, to produce an approximation for the value of the definite integral.

All quadrature methods have the same basic structure: the multiplication of a quadrature weight by the sum of function values at specified points within the domain of integration.

$$\int_a^b f(x)\,dx \approx w_1 f(x_1) + w_2 f(x_2) + \cdots + w_n f(x_n)$$
$$= \sum_{i=1}^{n} f(x_i) w_i$$

where x = quadrature point, n = number of abscissa, w = weight

Rectangle Rule



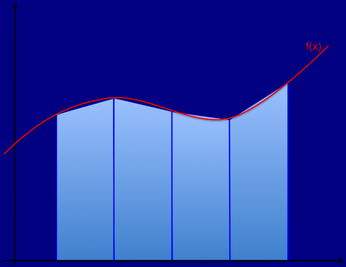
Rectangle rule is the simplest, but least accurate method out of the three.

1. We must first divide the interval $[a, b]$ into n sub-intervals of an equal length, $h = \frac{b-a}{n}$
2. Approximate f in each subinterval by $f(x_j^*)$ where x_j^* is the midpoint of the sub-interval
3. The area of each of the rectangles will be $f(x_1^*)h, f(x_2^*)h, f(x_3^*)h$ and so on until $f(x_n^*)h$

Equation

$$\int_a^b f(x)\,dx \approx f(x_1^*)h + f(x_2^*)h + f(x_3^*)h + \ldots + f(x_m^*)h$$
$$\approx h[f(x_1^*) + f(x_2^*) + f(x_3^*) + \ldots + f(x_m^*)]$$

Trapezoidal Rule



Provides far more accuracy than the classical rectangular rule. Rather than using rectangles to approximate area, we use a series of trapezia.

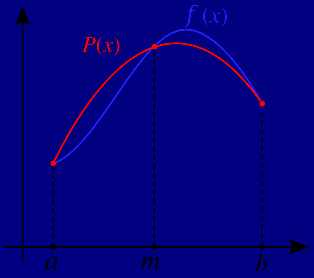
1. We must first divide the interval $[a, b]$ into n sub-intervals of an equal length, $h = \frac{b-a}{n}$
   Any point on the x-axis can be written as $x_r = a + h \cdot r$
2. The area of the trapezium is given by

$$A_r = \frac{f(x_r) + f(x_r + 1)}{2} \cdot h = \frac{f(a + h \cdot r) + f(a + h \cdot (r + 1))}{2} \cdot h$$

Equation

$$\int_a^b f(x)\, dx \approx \sum_{r=0}^{r=n-1} \frac{f(a + h \cdot r) + f(a + h \cdot (r+1))}{2} \cdot h$$

Simpson's Rule



Simpson's rule provides the greatest accuracy out of all three methods.

- The rule is based on the fact that the equation of a quadratic function can be derived using 3 points.

Example

Consider 3 points, (1, 5),(5, 9) and (3, 12). Using $y = ax^2 + bx + c$, we get the equations:
$12 = 9a + 3b + c$
$5 = a + b + c$
$9 = 25a + 5b + c$
Solving this system, yields $y = -1.25x^2 + 8.5x–2.25$

- We obtain Simpson's Rule by finding the area under each parabola and adding up all the areas.

Proving Simpson's Rule

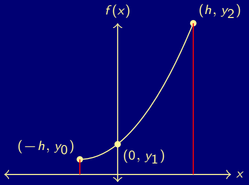
We can denote Simpson's Rule as follows:

$$\int_a^b f(x)\,dx \;\approx\; \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \ldots + 4y_{n-1} + y_n)$$

But how can we prove it?

Proof.

Consider the area under a parabola y with equation $y = ax^2 + bx + c$



If we integrate the area enclosed within the red lines above, we get:

$$\int_{-h}^{h} (ax^2 + bx + c)\,dx \;=\; \left[\frac{ax^3}{3} + \frac{bx^2}{2} + cx\right]_{-h}^{h}$$

$$= (\frac{ah^3}{3} + \frac{bh^2}{2} + ch) - (-\frac{ah^3}{3} + \frac{bh^2}{2} - ch)$$

$$= \frac{2ah^3}{3} + 2ch$$

$$= \frac{h}{3}(2ah^2 + 6c)$$

The parabola passes through $(-h, y_0)$, $(0, y_1)$ and (h, y_2). If we substitute these points into $y = ax^2 + bx + c$, we obtain the equations

$$y_0 = ah^2 - bh + c \qquad (1)$$

$$y_1 = c \qquad (2)$$

$$y_2 = ah^2 + bh + c \qquad (3)$$

Proving Simpson's Rule (Continued)

Proof.

From these equations, we can deduce that:

$$c = y_1$$

and

$$2ah^2 = y_0 - 2y_1 + y_2$$

which is the sum of equation (1) and (3) By substituting these equations into $A = \frac{h}{3}(2ah^2 + 6c)$, we have

$$A = \frac{h}{3}(2ah^2 + 6c)$$
$$= \frac{h}{3}(y_0 - 2y_1 + y_2 + 6y_1)$$
$$= \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Now, we can consider the area of the parabola for the next 3 points:

$$A = \frac{h}{3}(y_2 + 4y_3 + y_4)$$

Adding the 2 areas together, we obtain:

$$A = \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + y_4)$$

If we keep going, we finally arrive at Simpson's rule:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \ldots + 4y_{n-1} + y_n)$$

The Gaussian Method

The Gaussian method of numerical integration involves the selection of optimum quadrature points on a curve at which to evaluate the function. A suitable weight is selected for the points, and this weight is then applied across these points. The sum of these points with their applied weights produces a value for the approximation of the definite integral.

Gaussian quadrature is designed for polynomials of degree $\leq (2n-1)$

Selecting the right abscissae within the interval $[a, b]$ is crucial in providing the most accurate result.

Gauss-Legendre Quadrature

This quadrature has incredibly high accuracy when compared against other quadrature, and its precision is hard to match.

- A Gaussian quadrature over the interval $[-1, 1]$.
- The abscissae for quadrature order n are given by the roots of the Legendre polynomials $P_n(x)$ which occur symmetrically about 0.
- The weighting function is given by $W(x) = 1$

Several questions remain to be answered:

Why a weighting function of 1?
To answer this, we consider a variant of Gauss-Legendre known as the 2 point rule. For the 2 point rule, we need to find the weights w_1 and w_2. To do so, we use the definite integral of 1 and x.

$$\int_{-1}^{1} 1 \, dx = 2 = w_1 + w_2$$

$$\int_{-1}^{1} x \, dx = 0 = w_1 f\left(\frac{1}{\sqrt{3}}\right) + w_2 f\left(-\frac{1}{\sqrt{3}}\right)$$

$$w_1 = w_2 = 1$$

Gauss-Legendre Quadrature (Continued)

How do we calculate the roots of a Legendre polynomial?
Legendre polynomials are derived from what are known as contour integrals, as displayed below:

$$P_n(z) = \frac{1}{2\pi i} \oint (1 - 2tz + t^2)^{-\frac{1}{2}} t^{-n-1} \, dt$$

Here are the first few Legendre polynomials:

$P_0(x)$	1
$P_1(x)$	x
$P_2(x)$	$\frac{1}{2}(3x^2 - 1)$
$P_3(x)$	$\frac{1}{2}(5x^3 - 3x)$
$P_4(x)$	$\frac{1}{8}(35x^4 - 30x^2 + 3)$

A generalised formula for n points can be displayed as:

Formula

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

Lebedev Quadrature

We have, till this point, explored quadrature in a one dimensional plane. But what if we wanted to carry out quadrature on a sphere?

Lebedev evaluates the surface area of a three-dimensional sphere. The weights utilized and the number of and which abscissa are to be chosen for evaluation on the grid are determined by carrying out the integration and evaluation of sphere harmonics to a certain order, all with perfect accuracy.