

DOING PHYSICS WITH MATLAB

MATHEMATICAL ROUTINES

COMPUTATION OF ONE-DIMENSIONAL INTEGRALS

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math_integration_1D.m

Demonstration mscript evaluating the integral of two functions using a number of different methods

simpson1d.m

Function to give the integral of a function using Simpson's 1/3 rule.

NUMERICAL INTEGRATION COMPUTATION OF ONE-DIMENSIONAL INTEGRALS

The function **simpson1d.m** is a very versatile , accurate and easy to implement function that can be used to evaluate a definite integral of a function between a lower bound and an upper bound. It is easier to use than the standard Matlab integration functions such as **quad**. The function **simpson1d.m** is described in detail below.

We want to compute a number expressing the definite integral of the function $f(x)$ between two specific limits a and b

$$I = \int_a^b f(x) dx$$

The evaluation of such integrals is often called *quadrature*.

We will consider the following integrands to test the accuracy of different integration procedures:

$$(1) \quad f(x) = \cos(x)$$

$$(2) \quad f(x) = e^{jx}$$

The integrals are evaluated over a quarter cycle in an attempt to find a minimum number of partitions of the domain that produce accurate results within a reasonable time. For the testing procedures, the following integrals are to be evaluated from $a = 0$ to $b = \pi/2$

$$I = \int_0^{\pi/2} \cos(x) dx \quad \text{and} \quad I = \int_0^{\pi/2} e^{jx} dx$$

These integrals can be evaluated analytically and the exact answers are

$$I = \int_0^{\pi/2} \cos(x) dx = [\sin(x)]_0^{\pi/2} = \sin(\pi/2) - \sin(0) = 1$$

$$I = \int_0^{\pi/2} e^{jx} dx = \left[\frac{1}{j} (e^{jx}) \right]_0^{\pi/2} = \frac{1}{j} (e^{j\pi/2} - 1) = 1 + j$$

The numerical procedures assume that neither the integrand $f(x)$ nor any of its derivatives become infinite at any point over the domain of the integration $[a, b]$, and that the limits of integration a and b are finite. Furthermore, we assume that $f(x)$ can be computed, or its values are known at N points x_c where $c = 1, 2, \dots, N$ that are distributed in some manner over the domain $[a, b]$ with $x_1 = a$ and $x_N = b$.

The qualifier *closed* signifies that the integration involves the values of the integrand at both the end-points. If only one or none of the end points are included, the qualifiers used are *semi-closed* and *open* respectively.

A major problem that arises with non-adaptive methods is that the number N of partitions of the function required to provide a given accuracy is initially unknown. One approach to this problem is to successively double the number of partitions, and compare the results as the number of partitions increase.

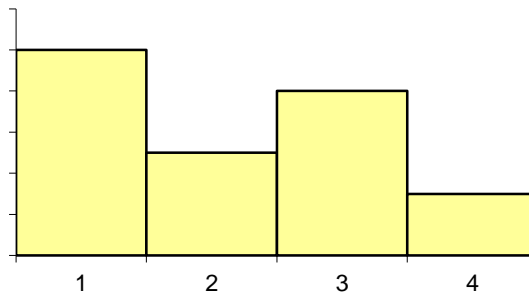
Closed Rectangle Rule

The region from a to b is divided into N rectangles of equal width $\Delta x \equiv h$ where

$$\Delta x = h = \frac{b-a}{N-1}$$

with each rectangle centre occurring at the points $x_1 = a$, $x_2 = x_1 + h$, \dots $x_N = b$.

For example, the plot below shows the domain divided into 4 rectangles, $N = 4$. However, the sub-division of the domain by this means extends from $a - h/2$ to $b + h/2$ and not simply from a to b .



The integral is approximated by the contribution from each rectangle, such that

$$I = \sum_{i=1}^N f(x_i) \Delta x$$

For the case shown in the plot above where $N = 4$, the integral is approximated by

$$I = \{f(x_1) + f(x_2) + f(x_3) + f(x_4)\} h \quad \text{where } h = \frac{b-a}{3}.$$

Open Midpoint Rule

The mid-point rule is the first member of a family of open Newton-Cotes rules corresponding to quadratic, cubic and higher-order interpolating polynomials with evenly spaced points. In the open midpoint rule, the area of each rectangle is added to find the integral. The domain a to b is divided into N partitions, with the width of each partition being $h = (b - a)/N$. The function is evaluated at the midpoint x_i of each rectangle where $x_i = a + (h/2)(2N-1)$. The value of the integral is then given by

$$I = \int_a^b f(x) dx = h \sum_1^N f(x_i)$$

Trapezoidal Rule

The function $f(x)$ is approximated by a straight line segment connecting adjacent points. The area under the curve is then approximated by adding the area of each trapezium. The interval a to b is divided into $N-1$ partitions of width h ($h \equiv \Delta x$) where $h = (b - a)/(N - 1)$. The area of each partition is simply the area of a trapezium which is its base times its mean height. The area of the i^{th} trapezium is

$$h \left(\frac{f_i + f_{i+1}}{2} \right) \quad \text{where } f_i \equiv f(x_i) \text{ and } i = 1, 2, \dots, N-1$$

Summing all the trapezia gives the *composite, closed trapezoidal rule*

$$I = h \left(\frac{f_1 + f_N}{2} + \sum_2^{N-1} f_i \right) = h \left(\sum_1^N f_i - \frac{f_1 + f_N}{2} \right)$$

For evenly distributed spacings, the composite rule is equivalent to the trapezoidal version of the closed *Newton-cotes rule*.

The Matlab function, `trapz` implements a procedure to calculate the integral by the trapezoidal rule. For example, the integration of the function y_1 w.r.t the variable x

```
Integral_1 = trapz(x,y1)      % estimate of the integral
```

Simpson's 1/3 rule

This rule is based on using a quadratic polynomial approximation to the function $f(x)$ over a pair of partitions. $N-1$ is the number of partitions where N must be **odd** and $h = (b - a) / (N-1)$. The integral is expressed below and is known as *composite Simpson's 1/3 rule*.

$$I = \frac{h}{3} \{ (f_1 + f_N + 4(f_2 + f_4 + \dots + f_{N-2}) + 2(f_3 + f_5 + \dots + f_{N-1})) \}$$

Simpson's rule can be written vector form as

$$I = \frac{h}{3} \mathbf{c} \mathbf{f}^T$$

where $\mathbf{c} = [1 \ 4 \ 2 \ 4 \ \dots \ 2 \ 4 \ 1]$ and $\mathbf{f} = [f_1 \ f_2 \ \dots \ f_N]$.

Simpson's rule is an example of a *closed Newton's-Cotes* formula for integration. Other examples can be obtained by fitting higher degree polynomials through the appropriate number of points. In general we fit a polynomial of degree N through $N + 1$ points. The resulting polynomials can then be integrated to provide an integration formula. Because of the lurking oscillations associated with the Gibbs effect, higher-order formulas are not used for practical integration.

simpson1d.m

The function f and the lower bound a and the upper bound b are passed onto the function (in the order f, a, b) and the function returns the value of the integral

```
function integral = simpson1d(f,a,b)

% [1D] integration - Simpson's 1/3 rule
%   f function    a = lower bound    b = upper bound
%   Must have odd number of data points
%   Simpson's coefficients    1 4 2 4 ... 2 4 1

numS = length(f);           % number of data points

sc = 2*ones(numS,1);
sc(2:2:numS-1) = 4;
sc(1) = 1; sc(numS) = 1;

h = (b-a)/(numS-1);

integral = (h/3) * f * sc;
```

EXAMPLES

$$(1) \quad I = \int_0^{\pi/2} \cos(x) dx = 1 \qquad (2) \quad I = \int_0^{\pi/2} e^{jx} dx = 1 + j$$

Method	Estimate	N
Closed Rectangle	(1) 1.0950	9
	(2) 1.0950 + 1.0950i	99
	(1) 1.0080	
	(2) 1.0080 + 1.0080i	
Open-Midpoint	(1) 0.9978	9
	(2) 0.9978 + 0.9978i	99
	(1) 0.9968	
	(2) 0.9733 + 0.9733i	
Trapezoidal	(1) 1.0000	9
	(2) 1.0000 + 1.0000i	99
	(1) 1.0000	
	(2) 1.0000 + 1.0000i	
Simpson's 1/3	(1) 1.0000 (2) 1.0000 + 1.0000i	9

All the integrations took less than one second on a fast Windows computer. Even with only 9 points, the Simpson's 1/3 rule estimate was equal to the exact values.