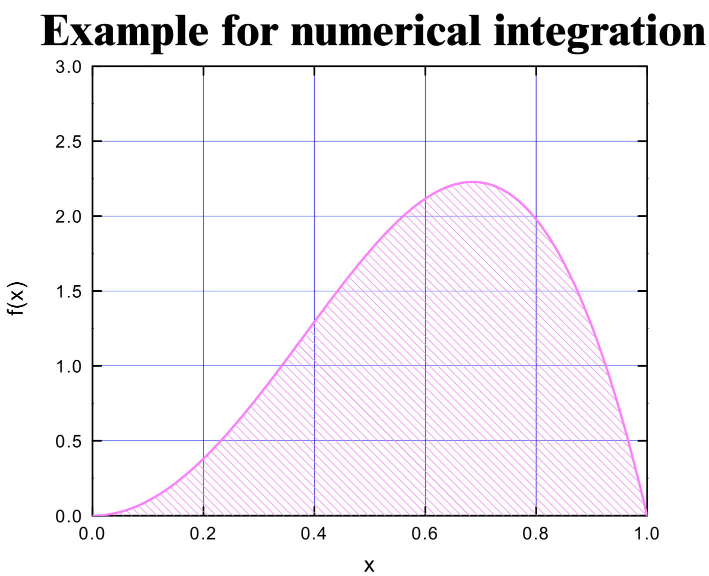
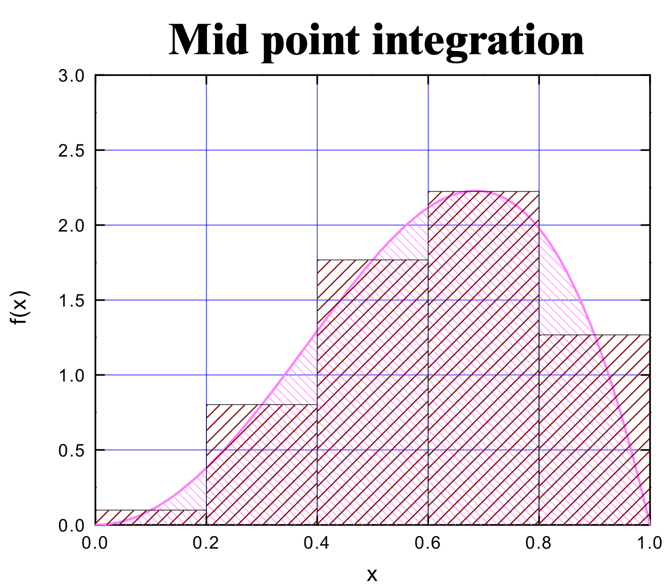
April 5, 2006

Notes on numerical analysis

It is *very* frequently the case that some sort of numerical work is needed to complete an analysis of a physics problem. For example, consider the integration of the following function $f(x)$:



The easiest method of approximating the integral, is the mid-point formula, which divides the interval $x_{\min} \leq x \leq x_{\max}$ into N regularly spaced sampling points $(n - \frac{1}{2})h$, $n = 1, 2, \cdots N$, and $h = (x_{\max} - x_{\min})/N$.

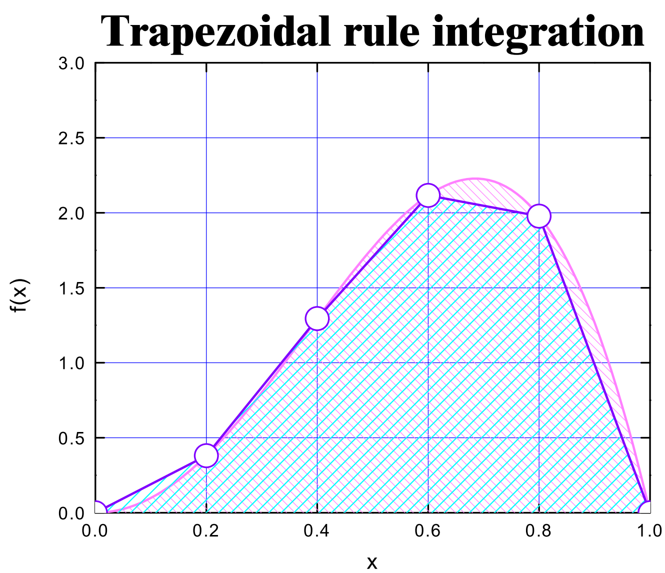


In this example, $N = 5$ and $h = 0.2$.

The mid-point algorithm for approximating the integral is:

$$\int_a^b f(x)dx \approx h \sum_{n=1}^{N} f(a + (n - \frac{1}{2})h). \tag{1}$$

At the next level of approximation, there is the trapezoidal rule which evaluates the function at the end points of the N intervals to estimate the area as the sum of trapezoidal areas.



In this example, $N = 5$ and $h = 0.2$.

The trapezoidal rule algorithm for approximating the integral is:

$$\int_a^b f(x)dx \approx \frac{h}{2} \sum_{n=1}^{N} \left\{ f(a + (n-1)h) + f(a + nh) \right\}. \tag{2}$$

There is a very large class of methods which can be derived from a Taylor series expansion:

$$\Phi(\mathbf{r} + \mathbf{u}) = \Phi(\mathbf{r}) + \mathbf{u} \cdot \nabla \Phi(\mathbf{r}) + \frac{1}{2!}(\mathbf{u} \cdot \nabla)^2 \Phi(\mathbf{r}) + \frac{1}{3!}(\mathbf{u} \cdot \nabla)^3 \Phi(\mathbf{r}) + \frac{1}{4!}(\mathbf{u} \cdot \nabla)^4 \Phi(\mathbf{r}) + \cdots. \tag{3}$$

This expansion shows how the value of a function at a given point is related to its values at neighboring points and its derivatives. We can use the Taylor series to approximate numerical derivatives. For example, the first derivative of a function $f(x)$ can be approximated by

$$\frac{df(x)}{dx} \approx \frac{f(x+h) - f(x-h)}{2h} + O(h^2). \tag{4}$$

The second derivative of the function can be approximated by

$$\frac{d^2 f(x)}{dx^2} \approx \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} + O(h^2). \tag{5}$$

In a similar way, we can also derive higher order integration algorithms. For example, Simpson's rule for integrating with an even number of intervals is given by:

$$\int_a^b f(x)dx \approx \frac{h}{3} \sum_{n=1}^{N/2} \left\{ f(a + (2n-2)h) + 4f(a + (2n-1)h) + f(a + 2nh) \right\}. \tag{6}$$

Here it is assumed that N is even and that $b = a + Nh$. The result follows from considering approximating $f(x)$ within each interval $-h \leq x \leq h$ as

$$f(x) \approx f(0) + x\frac{df(0)}{dx} + \frac{1}{2}x^2 \frac{d^2 f(0)}{dx^2} + \ldots, \tag{7}$$

with the further approximation

$$f(x) \approx f(0) + x\left(\frac{f(h) - f(-1)}{2h}\right) + \frac{1}{2}x^2 \left(\frac{f(h) + f(-h) - 2f(0)}{h^2}\right) + \ldots. \tag{8}$$

Using this last expression to perform the integral, we obtain

$$\int_{-h}^{h} f(x)dx = 2hf(0) + 0 + \frac{2h^3}{3}\left(\frac{f(h) + f(-h) - 2f(0)}{h^2}\right) = \frac{h}{3}\left(f(-h) + f(h) + 4f(0)\right). \tag{9}$$

We can also use the difference formula Eq. (5) for solving differential equations. For example suppose we have a differential equation of the form

$$\frac{d^2 f}{dx^2} = A(x), \tag{10}$$

where $A(x)$ is a known function. Then we can rewrite Eq. (5) to find $f(x+h)$ in terms of $A(x), f(x-h)$, and $f(x)$:

$$f(x+h) \approx h^2 A(x) + 2f(x) - f(x-h). \tag{11}$$

A more accurate method that can also be used for eigenvalue problems is discussed in the notes "numerov.pdf".