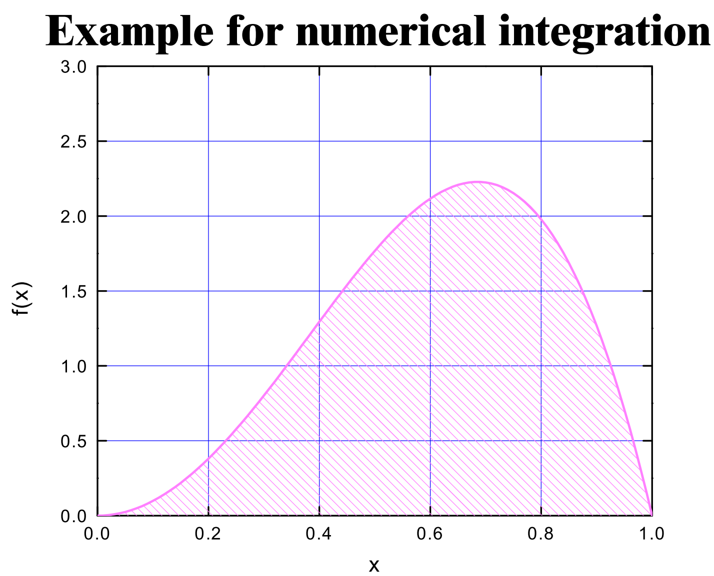
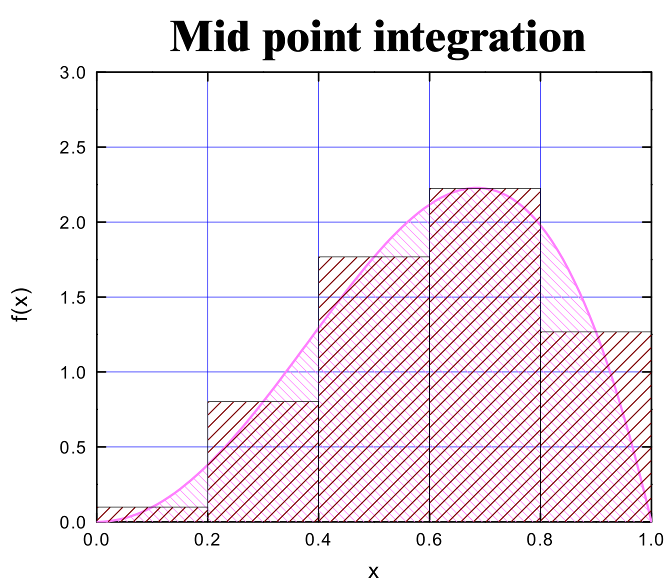
February 27, 2002

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 $x_{\min} \le x \le x_{\max}$ into N regularly spaced sampling points $(n - \frac{1}{2})h$, $n = 1, 2, \cdots N$, and $h = (x_{\max} - x_{\min})/N$.

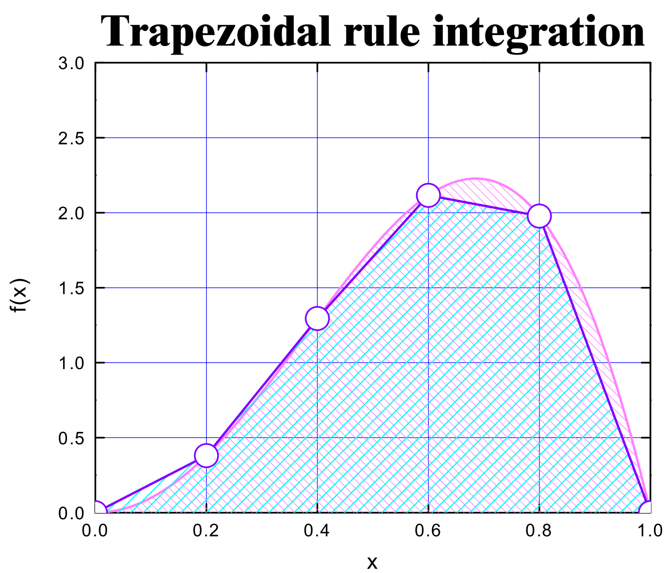


In this example, $N = 5$ and $h = 0.2$.

The mid-point algorithm for approximating the integral is:

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

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:

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

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

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

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

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

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:

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