Numerical integration of functions
(Reference: Chapter 4 in W. H. Preuss, *et al.*, Numerical Recipes in Fortran, 2nd ed., Cambridge University Press, 1992)

Learning objectives

1. Review of methods for numerical integration
2. Develop problem solution skills using computers and numerical methods
3. Develop programming skills using FORTRAN

   FORTRAN elements in this module
   - input/output
   - loops
   - use of function routines

Introduction

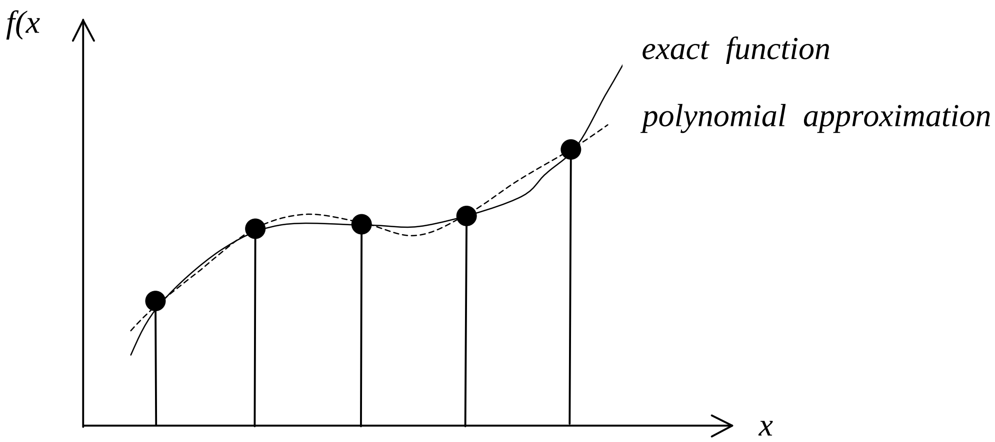
Evaluation of a definite integral

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

by formal methods is often difficult or impossible, even if the function *f(x)* has a relatively simple analytical form. For such cases, and for the more general integration problem where we have a few a few values of *f(x)* available at distinct base-points arguments x_i, *i=0, 1,…, n*, some other approach is required. An obvious alternative is to find a function *g(x)* that is both a suitable approximation of *f(x)* and simple to integrate formally. Then Eq. (1) can be estimated as

$$\int_a^b g(x)dx \tag{2}$$

One possibility is to apply interpolation polynomials to the known points of the function, and then carry out the integration of the polynomials. In the figure below, such a procedure is illustrated. Here, the function *f(x)* is shown by the solid curve, and some discrete points at equally spaced intervals are indicated by dots. Now, if we apply a polynomial to the discrete points, we may come up with an approximation of the function *f(x)* indicated by the dashed curve.

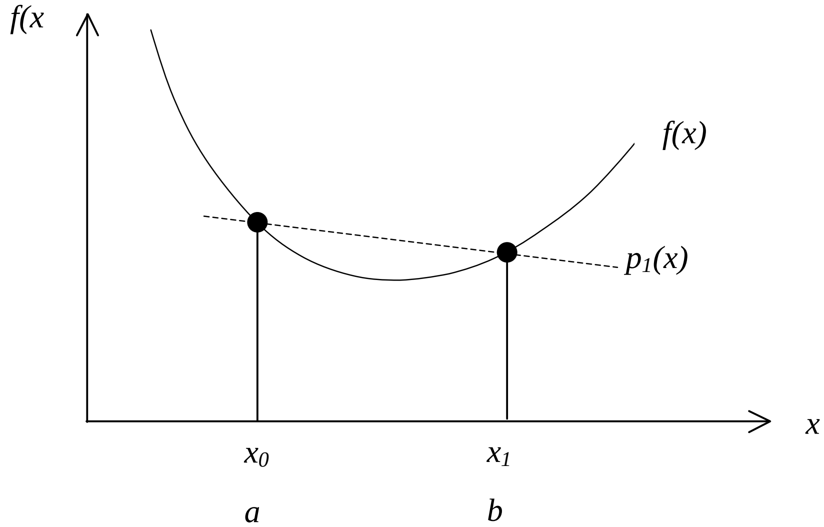


Note that even though the polynomial fits exactly at the 5 discrete points, the area under the dashed line will not be the same as the area under the solid line. However, often a positive error in one segment may cancel a negative error in another segment, so that the total error may be small. This is why integration often is called a smoothing process.

Text books on numerical integration often focus on formulas for approximation. This is not surprising since there are so many possibilities for selecting the degree of interpolation polynomial, spacing between points, and location of points. Normally, we classify the methods into two groups, one that uses equally spaced points (Newton-Cotes formulas), and another that uses unequally spaced points (Gaussian quadrature formulas). We will consider some of the simplest and most common methods in the first group, namely the trapezoidal method and the Simpson's formula.

Trapezoidal formula

The method is illustrated in the figure below. Here, the exact function, *f(x),* is indicated by the solid line, and the first order polynomial approximation (straight line) is indicated by the dashed line, passing through two points on the function, at x_0 and x_1.



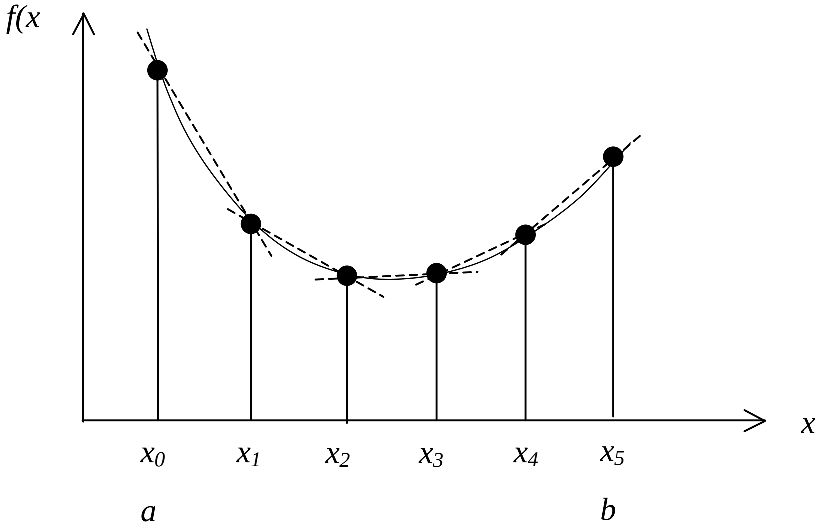
The first-order approximation formula for a straight line is of course

$$p_1(x) = f(x_0) + \left[f(x_1) - f(x_0)\right]\frac{(x - x_0)}{(x_1 - x_0)} \tag{3}$$

Integration of the approximation may then be carried out

$$\begin{aligned}\int_a^b f(x)dx \approx \int_{x_0}^{x_1} p_1(x)dx &= \int_{x_0}^{x_1} \left\{ f(x_0) + \left[f(x_1) - f(x_0)\right]\frac{(x - x_0)}{(x_1 - x_0)} \right\} dx \\ &= \frac{1}{2}(x_1 - x_0)\left[f(x_0) + f(x_1)\right]\end{aligned} \tag{4}$$

Now, consider integration over a series of intervals, as illustrated with 5 intervals in the figure below. The function is approximated with stright lines between pairs of points.



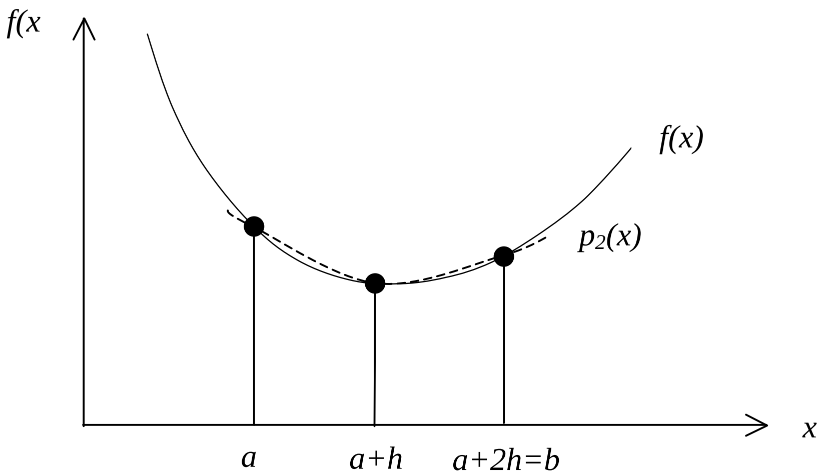
We may apply Eq. (4) to each sub-interval, and take the sum the sub-areas to get the total area under the function from *a* to *b*:

$$A_i = = \frac{1}{2}(x_i - x_{i-1})[f(x_i) + f(x_{i-1})] \quad (5)$$

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} A_i = \frac{1}{2}\sum_{i=1}^{n}(x_i - x_{i-1})[f(x_i) + f(x_{i-1})] \quad (6)$$

Simpson's formula

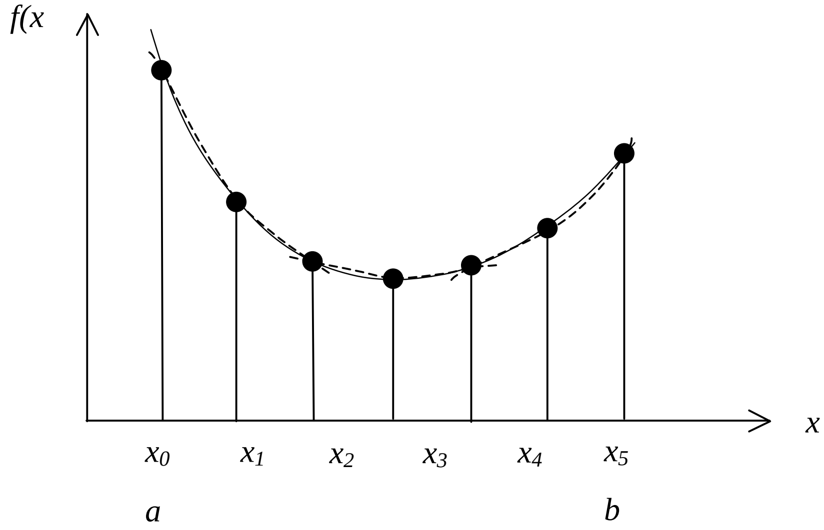
Simson's formula is similar to the trapezoidal rule in dividing the total interval into many smaller intervals and aproximating the area under them, but different in that it fits a parabola to three pont of two adjoining intervals. Thus, in the figure below is shown two sub-intervals, with three points that the second order polynomial $p_2(x)$ is fitted to.



The Simpson's formula may then be derived as:

$$\int_a^{a+2h} f(x)dx \approx \frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right] \tag{7}$$

For an integration interval [*a*,*b*], subdivided into *n* intervals, as illustrated with 6 intervals in the figure below, a parabola is fitted to pairs of intervals.



The total integral over the 6 intervals, by application of Eq. (7) three times, is

$$\begin{aligned}\int_a^b f(x)dx &\approx = \frac{h}{3}\left[f(a) + 4f(x_1) + f(x_2)\right] \\ &+ \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right] \\ &+ \frac{h}{3}\left[f(x_4) + 4f(x_5) + f(b)\right] \\ &= \frac{h}{3}\left[f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + 4f(x_5) + f(b)\right]\end{aligned} \tag{8}$$

In general, for *n* intervals, Simpson's formula becomes:

$$\begin{aligned}\int_a^b f(x)dx \approx \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + ... \\ + 2f(a-2h) + 4f(b-h) + f(b)]\end{aligned} \tag{9}$$

where the interval length *h=(b-a)/n.*

Integration exercise

1. Make a FORTRAN program that uses the two methods above to determine the integrals of the functions FX1(X), FX2(X), FX3(X) and FX4(X). The program should consist of a main program and 6 function routines (2 for the methods and 4 for the functions that are to be integrated) . The main program will ask you to type on the screen which method is to be used (TRA or SIM), the lower and upper interval values, and the number of intervals to be used. The computed results should be written to the output file OUT.DAT. The FORTRAN program is to be organized so that after reading the input values from the screen, it calls one of the function routines, TRA(A,B,N,FX) or SIM(A,B,N,FX). From these, function values are obtained by calling the function routines FX1(X), FX2(X), FX3(X), and FX4(X), and then the integrated values are computed.
2. Run the program using the functions $f_1(x)=x^2$, $f_2(x)=x^4$, $f_3(x)=1/(1+x)$, and $f_4(x)=(1+x^2)^{0,5}$. Use lower and upper limits of $a=0$ and $b=1$, and the number of intervals is $n=100$. Compare the results from the two methods with the exact results for all four functions.