6. Numerical Integration

Given a function \( f(x) \) defined on the interval \([a, b]\), if the anti-derivative \( F(x) = \int f(x) \, dx \) of \( f(x) \) is known to us, then computing the value of the definite integral

\[
I(f; a, b) \equiv \int_{a}^{b} f(x) \, dx \quad (6.1)
\]

is straightforward; \( I(f; a, b) \) is equal to \( F(b) - F(a) \). If the anti-derivative of the given function does not exist or is not available, an approximation method has to be used to approximate \( I(f; a, b) \). This chapter is concerned with the second case, i.e., developing numerical methods to approximate the definite integral of a function whose anti-derivative is unknown to us.

One way to approximate the value of \( I(f; a, b) \) is to use an \((n+1)\)-point quadrature rule or formula:

\[
Q_n(f) = a_0 f(x_0) + a_1 f(x_1) + \cdots + a_n f(x_n) = \sum_{i=0}^{n} a_i f_i \quad (6.2)
\]

where \( f_i \equiv f(x_i) \), and \( a_i \)'s are constants to be determined. Hence, an \((n+1)\)-point quadrature formula is a strategy in forming a linear combination of the values of the integrand \( f(x) \) at \( n+1 \) quadrature points \( x_i, 0 \leq i \leq n \), so that the value of the linear combination \( Q_n(f) \) would be close to \( I(f; a, b) \).

This is usually done by replacing the integrand \( f(x) \) with the polynomial \( p_n(x) \) which interpolates \( f(x) \) at the \( n+1 \) quadrature points \( x_0, x_1, \ldots, x_n \) and then integrate \( p_n(x) \). In this case,

\[
Q_n(f) = I(p_n, a, b)
\]

We then use \( Q_n(f) \) to approximate \( I(f; a, b) \). Note that \( p_n(x) \) can be put in the following form:

\[
p_n(x) = l_0(x) f_0 + l_1(x) f_1 + \cdots + l_n(x) f_n
\]

where \( l_i(x) \) are Lagrange polynomials of degree \( n \) defined in (4.6). Therefore, we have

\[
Q_n(f) = I(p_n, a, b)
\]

\[
= \int_{a}^{b} (f_0 l_0(x) + \cdots + f_n l_n(x)) \, dx
\]

\[
= \sum_{i=0}^{n} f_i \int_{a}^{b} l_i(x) \, dx
\]
\[ i = 0 \]

where

\[ a_i \equiv \int_a^b l_i(x)dx \quad (6.3) \]

The values of \( a_i \)'s depend on \( x_i \)'s. A quadrature rule is completely characterized by the location of the quadrature points. To define a quadrature rule, all one has to do is to specify the strategy in choosing the quadrature points. The simplest approach in choosing the quadrature points is the Newton-Cotes (uniform) rule:

\[ x_i \equiv a + i \cdot h, \quad i = 0, 1, ..., n \]

where \( h = (b-a)/n \).

If \( n = 1 \) in (6.2) and (6.3), it can be shown that

\[ I(p_1; a, b) = \frac{(b-a)}{2} f_0 + \frac{(b-a)}{2} f_1 \]
\[ = \frac{(b-a)}{2} [f(a) + f(b)] \quad (6.4) \]

This is the well known Trapezoidal rule.

If \( n = 2 \) in (6.2) and (6.3), it can be shown that

\[ I(p_2; a, b) = \frac{h}{3} [f_0 + 4f_1 + f_2] \]
\[ = \frac{h}{3} [f(a) + 4f((a+b)/2) + f(b)] \quad (6.5) \]

where \( h = (b-a)/2 \). (6.5) is the well known Simpson’s 1/3 rule.

One certainly would like to know the error \( E_n(f) \) between an \( (n+1) \)-point quadrature and \( I(f; a, b) \). This error term can be expressed as follows:

\[ E_n(f) \equiv I(f; a, b) - Q_n(f) \]
\[ = I(f; a, b) - I(p_n; a, b) \]
\[ = I(f - p_n; a, b) \]
\[ = \int_a^b [f(x) - p_n(x)] dx \quad (6.6) \]
The integrand \( f(x) - p_n(x) \) in (6.6) can be expressed as:

\[
f(x) - p_n(x) = f[x_0, x_1, \ldots, x_n, x] \psi_{n+1}(x) \tag{6.7}
\]

where \( f[x_0, x_1, \ldots, x_n, x] \) is the \((n+1)\)st divided difference of \( f \) at \( x_0, x_1, \ldots, x_n, \) and \( x \), and \( \psi_{n+1}(x) \) is a polynomial of degree \( n+1 \) whose roots are the quadrature points \( x_i \):

\[
\psi_{n+1}(x) = (x - x_0)(x - x_1) \cdots (x - x_n) = \prod_{i=0}^{n} (x - x_i) \tag{6.8}
\]

The proof of (6.7) follows. Note that the Newton form of the polynomial \( p_{n+1}(t) \) that interpolates \( x_0, x_1, \ldots, x_n, \) and \( x \) is:

\[
p_{n+1}(t) = p_n(t) + f[x_0, x_1, \ldots, x_n, x](t - x_0)(t - x_1) \cdots (t - x_n)
\]

Since the value of \( p_{n+1}(t) \) at \( x \) is the same as that of \( f(t) \) at \( x \):

\[
p_{n+1}(x) = f(x)
\]

and

\[
p_{n+1}(x) = p_n(x) + f[x_0, x_1, \ldots, x_n, x](x - x_0)(x - x_1) \cdots (x - x_n)
\]

therefore,

\[
f(x) - p_n(x) = f[x_0, x_1, \ldots, x_n, x](x - x_0)(x - x_1) \cdots (x - x_n)
\]

and (6.7) is proved.

Using (6.6) and (6.7), we have

\[
E_n(f) = \int_a^b f[x_0, x_1, \ldots, x_n, x] \psi_{n+1}(x) \, dx
\]

If \( f(x) \) is \( n \)-times continuously differentiable, we have

\[
f[x_0, x_1, \ldots, x_n, x] = \frac{f^n(\theta)}{n!}
\]

for some \( \theta \) between \( a \) and \( b \). Therefore, if \( f^n(\theta) \) is bounded above by some \( M \),

\[
|f^n(\theta)| \leq M
\]

on \([a, b]\) then

\[
E_n(f) \leq \frac{M}{n!} \int_a^b \psi_{n+1}(x) \, dx \tag{6.9}
\]
Note that \( \int_{a}^{b} \psi_{n+1}(x) \, dx \) is a constant and is computable.