Chapter 7 Numerical Integration

Reference

James F. Epperson (Revised Edition, 2007)
- Chapter 5

Content

7.1 Introduction
7.2 Basic Quadrature Rules
7.3 Composite Simpson’s Rule
7.4 Error Estimate in Simpson’s Rule
7.5 Improper Integrals with Singularities

7.1 Introduction
• The value of an integral is the area under a curve i.e. the integrand (Figure 7.1).

\[ f(x) \]

\[ f(b) \]

\[ f(a) \]

\[ x_0 = a \]

\[ x_n = b \]

\[ x \]

Figure 7.1

• In numerical integration we are interested to find methods of approximating an integral.
• Numerical integration methods are called quadrature rules.
• Definite integral is written as

\[ \int_a^b f(x) \, dx, \quad x \in [a, b]. \]  

(7.1)

• Some integral could not be solved analytically in closed form.
• We use approximation to \( I(f) \).
• \( I(f) \) is approximated by a \( n \)-point quadrature rule:

\[ I(f) \approx Q_n(f) = \sum_{i=1}^{n} \omega_i f(x_i), \quad x \in [a, b]. \]  

(7.2)

where the mesh points are \( a = x_0 < x_1 < x_2 \cdots < x_{n-1} < x_n = b \) and \( \omega_i \) is the weight/coefficient.
• The objective of quadrature rules is to choose nodes/abscissas \( x_i \) and weights \( \omega_i \) so that a certain level of accuracy is achieved.
• **Open quadrature** rule if \( a < x_0 \) & \( x_n < b \). Usually \( a \) and \( b \) are at infinity.
• **Closed quadrature** rule \( a = x_0 \) & \( x_n = b \).

7.2 Basic Quadrature Rules
These are (open and closed) Newton-Cotes quadratures with \( x \in [a, b] \).

(a) Mid-point rule:

\[
I(f) = M(f) = (b - a)f\left(\frac{a + b}{2}\right). \tag{7.3}
\]

(b) Trapezoid rule:

Let \( p_1 \) - linear polynomial that interpolates \( f \) at 2 points, \( x = a \) and \( x = b \).

From Chapter 2, the first order linear polynomial is written as:

\[
p_1(x) = \frac{x - a}{b - a} f(b) + \frac{b - x}{b - a} f(a)
\]

Integrating \( p_1 \),

\[
I(p_1) = \int_a^b p_1(x) \, dx
\]

\[
= \int_a^b \left[ \frac{x - a}{b - a} f(b) + \frac{b - x}{b - a} f(a) \right] \, dx
\]

\[
= \frac{f(b)}{b - a} \int_a^b (x - a) \, dx + \frac{f(a)}{b - a} \int_a^b (b - x) \, dx
\]

\[
= \frac{1}{2} (b - a) [f(a) + f(b)]
\]

Thus, the basic trapezoid rule is

\[
T_1(f) = \frac{(b - a)}{2} [f(a) + f(b)]. \tag{7.4}
\]

Error in this approximation is

\[
I(f) - T_1(f) = \Delta T_1(f) = -\frac{1}{12} (b - a)^3 f''(\xi).
\]

The error is \( \propto (b - a) \), thus we subdivide the interval such that

\[
a = x_0 < x_1 < x_2 \cdots < x_i-1 < x_i \cdots < x_{n-1} < x_n = b.
\]

Then at each subinterval apply the basic trapezoid rule (7.4):
Chapter 7 Numerical Integration

\[ I(f) = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x) \, dx \]

\[ \approx \sum_{i=1}^{n} T_i(f) \]

\[ = \sum_{i=1}^{n} \frac{1}{2} (x_i - x_{i-1}) [f(x_{i-1}) + f(x_i)] \]

\[ = T_n(f) \] \hfill (7.6)

where \( a = x_{i-1} \) and \( b = x_i \).

- If we use uniform grid with step size \( h = x_i - x_{i-1} \) then the **composite trapezoid rule** is given as

\[ T_n(f) = \frac{h}{2} \left[ f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + f(x_n) \right] \]

\[ = \frac{h}{2} \left[ f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n) \right] \]

\[ = \frac{h}{2} \left[ f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right] \] \hfill (7.7)

- Rate of convergence \( \sim O(h^2) \).

**Example 7.1 (MH Chapter 8 Section 8.3.1 Example 8.2, page 346)**

\[ I = \int_{0}^{1} e^{-x^2} \, dx \]

Use mid-point rule,

\[ M(f) = (1-0)f\left(\frac{1+0}{2}\right) \]

\[ = f(0.5) \]

\[ = e^{-0.25} = 0.778801 \]

Use basic trapezoid rule,

\[ T_1(f) = \frac{(1-0)}{2} [f(1)+f(0)] \]

\[ = \frac{1}{2} [1 + e^{-1}] = 0.683940 \]
• (c) Simpson’s rule:

Let \( p_2 \) - second order quadratic polynomial that interpolates \( f \) at 3 points:

\[
x_0 = a, \ x_2 = b \ & \ x_1 = c = \frac{a + b}{2}.
\]

• Define the basic Simpson’s rule as

\[
S_2(f) = l(p_2) = \int_a^b \left[ L_0(x)f(a) + L_1(x)f(c) + L_2(x)f(b) \right] \, dx
\]

where Lagrange functions are

\[
L_0(x) = \frac{(x - c)(x - b)}{(a - c)(a - b)}
\]

\[
L_1(x) = \frac{(x - a)(x - b)}{(c - a)(c - b)}
\]

\[
L_2(x) = \frac{(x - a)(x - c)}{(b - a)(b - c)}.
\]

• Quadrature rule:

\[
S_2(f) = Af(a) + Cf(c) + Bf(b)
\]

where

\[
A = \int_a^b L_0(x) \, dx, \quad C = \int_a^b L_1(x) \, dx, \quad B = \int_a^b L_2(x) \, dx
\]

Define \( h = b - c = c - a = \frac{b - a}{2} \)

\[
A = \int_a^a 2h L_0(x) \, dx
\]

\[
C = \int_a^{2h} L_1(x) \, dx
\]

\[
B = \int_a^{2h} L_2(x) \, dx
\]

Then,

\[
A = \frac{1}{2h^2} \int_a^{2h} \left[ x - (a + h) \right] \left[ x - (a + 2h) \right] \, dx, \ \text{use} \ u = x - a - h
\]
\[
\frac{h}{3}
\]

Similarly,

\[B = A = \frac{h}{3}, \quad C = \frac{4}{3} h\]

\[\therefore S_2(f) = \frac{h}{3} [f(a) + 4f(c) + f(b)]\]

**Basic Simpson’s rule or the Simpson’s 1/3 rule:**

\[S_2(f) = \frac{(b - a)}{6} \left[ f(a) + 4f\left(\frac{a + b}{2}\right) + f(b) \right].\] (7.8)

**Example 7.2**

Continue from Example 7.1.

\[S_2(f) = \frac{1}{6} \left( e^0 + 4e^{-0.25} + e^{-1} \right)\]

\[= 0.747180\]

Analytic value = 0.746824

Simpson’s rule is **more accurate**.

### 7.3 Composite Simpson’s Rule

- Basic Simpson’s rule applied to pairs of subinterval.
- **Composite Simpson’s Rule:**

\[S_n(f) = \sum_{i=1}^{n/2} \frac{h_i}{3} \left[ f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}) \right].\] (7.9)

where

\[h_i = \frac{(x_{2i} - x_{2i-2})}{2}\]

- Rate of convergence \(\sim O(h^4)\).

### 7.4 Error Estimate in Simpson’s Rule

- The error in \(S_2(f)\)
\[ I(f) - S_2(f) = \Delta S_2(f) = -\frac{1}{90} \left( \frac{b-a}{2} \right)^5 f^{(4)}(\xi) \]  
(7.10)

where \( a \) and \( b \) are the lower and upper integration limits respectively with \( a < b \), and \( \xi \in [a,b] \).

- When the grid is uniform, \( x_{i+1} - x_i = \frac{b-a}{n} = h \) then

\[ I(f) - S_2(f) = \Delta S_2(f) = -\frac{(b-a)h^4}{180} f^{(4)}(\xi). \]  
(7.11)

**Example 7.3 JE Chapter 5 Section 5.3 Example 5.6, page 260.**

Given \( f(x) = e^x \) and interval \([0,1]\). We want the error \( \Delta S_2 \leq 10^{-6} \). What is \( h \)?

From Equation (7.10), the absolute error is written as

\[ |E_n(f)| = |I(f) - S_2(f)| = |\Delta S_2(f)| = \frac{(b-a)h^4}{180} |f^{(4)}(\xi)| \leq 10^{-6}. \]

This means that

\[ \frac{(b-a)h^4}{180} \max_{x \in [0,1]} |f^{(4)}(\xi)| \leq 10^{-6}. \]

Since \( f^{(4)}(x) = e^x \) then \( \max_{x \in [0,1]} |f^{(4)}(\xi)| = e^1. \)

Putting \( a = 0 \) and \( b = 1 \), then

\[ \frac{e}{180} h^4 \leq 10^{-6}. \]

Solving for \( h \),

\[ h \leq 0.09021. \]

**7.5 Improper Integrals with Singularities**

- Improper integrals are:

  (i) limit /limits of the integration is/are infinite,
  (ii) integrand has a singular point/some singular points.

- An improper integral with infinite limits is written as
We want to evaluate an improper integral in which the integrand $f(x)$ has a singularity at some point $c$ in the range of integration $a$ to $b$, for example

$$I(f) = \int_a^b f(x) \, dx, \quad x \in [a, b],$$

or

$$I(f) = \int_0^b f(x) \, dx, \quad x \in [0, b],$$

or

$$I(f) = \int_a^\infty f(x) \, dx, \quad x \in [a, \infty].$$

We write the integral (see Figure 7.2) as

$$I = \int_a^b f(x) \, dx = I_1 + I_2$$

where

$$I_1 = \int_a^c f(x) \, dx = \lim_{\varepsilon \to +0} \int_a^{c+\varepsilon} f(x) \, dx$$

(from the left)

$$I_2 = \int_c^b f(x) \, dx = \lim_{\varepsilon \to +0} \int_c^{b-\varepsilon} f(x) \, dx$$

(from the right)

$I_1$ and $I_2$ are evaluated with smaller values of $\varepsilon$ until values of $I_1$ and $I_2$ are not significantly changed. Thus the process has converged.
Example 7.4

Integrate \( \int_{0}^{3} \frac{e^{2x}}{\sqrt{x}} \, dx \).

Solution:

Step 1

Notice that the integrand has a singularity at \( x = 0 \).

Step 2

One way to avoid the singularity is to integrate by parts:

\[ \int u \, dv = uv - \int v \, du. \]

Step 3

Please complete the solution as an exercise.