SME 3023 Applied Numerical Methods

Numerical Integration

Abu Hasan Abdullah

Faculty of Mechanical Engineering

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1 Introduction
Outline

1. Introduction
2. Engineering Applications
Outline

1. Introduction

2. Engineering Applications

3. Methods

4. Newton-Cotes Quadrature
   - Rectangular Rule
   - Trapezoidal Rule
   - Simpson’s One-Third Rule
   - Simpson’s Three-Eighths Rule
Outline

1 Introduction

2 Engineering Applications

3 Methods

4 Newton-Cotes Quadrature
   • Rectangular Rule
   • Trapezoidal Rule
   • Simpson’s One-Third Rule
   • Simpson’s Three-Eighths Rule

5 Gauss Quadrature
   • Gauss-Legendre Formula
   • Gauss-Chebyshev Formula
   • Gauss-Hermite Formula
Outline

1. Introduction

2. Engineering Applications

3. Methods

4. Newton-Cotes Quadrature
   - Rectangular Rule
   - Trapezoidal Rule
   - Simpson’s One-Third Rule
   - Simpson’s Three-Eighths Rule

5. Gauss Quadrature
   - Gauss-Legendre Formula
   - Gauss-Chebyshev Formula
   - Gauss-Hermite Formula

6. Integration Using Matlab
Outline

1. Introduction
2. Engineering Applications
3. Methods
4. Newton-Cotes Quadrature
   - Rectangular Rule
   - Trapezoidal Rule
   - Simpson’s One-Third Rule
   - Simpson’s Three-Eighths Rule
5. Gauss Quadrature
   - Gauss-Legendre Formula
   - Gauss-Chebyshev Formula
   - Gauss-Hermite Formula
6. Integration Using Matlab
7. Bibliography
One of the major use of integral calculus was the calculation of areas and volumes of irregularly shaped region.

Many engineering problems require the evaluation of the integral

\[ I = \int_{a}^{b} f(x) \, dx \]  

where \( f(x) \) is integrand and \( a \) and \( b \) are limits of integration.

If \( f(x) \) is continuous, finite and well behaved over the range of integration \( a \leq x \leq b \), integral \( I \) can be evaluated analytically.

Numerical integration, a.k.a. numerical quadrature, is an approximation of definite integrals and used in cases where

- \( f(x) \) is a complicated continuous function that is difficult or impossible to integrate in closed form.
- \( f(x) \) is not known in analytical form; it may be known in tabular form, where values of \( x \) and \( f(x) \) are available at a number of discrete point in \( a \leq x \leq b \) range.
- limits of integration may be infinite.
- \( f(x) \) may be discontinuous or may become infinite at some point in range \( a \leq x \leq b \).
Integral of function $f(x)$ between limits $a$ and $b$ denotes the area under the curve of $f(x)$ between limits $a$ and $b$, see Figure 1.

*Riemann sums* are used to define the integral: the integral will be approximated by a weighted sum of integrand values at a finite number of sample points in the interval of integration—see Figure 2.

Figure 1: Integral as area under the curve.

Figure 2: Riemann sum
This leads us to the *n-point quadrature rule*

\[ Q_n = \sum_{i=1}^{n} w_i f(x_i) \]

where \( a = x_1 < x_2 < \ldots < x_n = b \). Points \( x_i \) at which \( f(x) \) is evaluated are called *nodes* or *abscissas*, the multipliers \( w_i \) are called *weights* or *coefficient*.
Problem Statement:
The variation of torque of an engine with the angular displacement of the crank is shown in Table 2.

1. Use a graphical method to determine the energy generated during a cycle by integrating the torque-displacement function over a cycle.
   **Hint:** Work = (Torque) × (Angular displacement)

2. Write a short Matlab M-file to solve part (1). Comment on possible agreement, or otherwise, between the two results.
**Problem Statement:** continued...

<table>
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<th>Crank angle $\theta$ (deg)</th>
<th>Torque $T$ (lb-in)</th>
<th>Crank angle $\theta$ (deg)</th>
<th>Torque $T$ (lb-in)</th>
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<td>630</td>
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</tr>
<tr>
<td>360</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2: Variation of engine torque with crank angle

![Graph](image.png)

**Figure 3:** Torque vs. Angular Displacement.
**Problem Statement:**
A semi-infinite solid body, initially at temperature $T_i$, is suddenly exposed to a fluid at temperature $T_0$ at the face $x = 0$ as shown in Figure 4. If the diffusivity of the material $\alpha$ is constant, the unsteady state temperature distribution in the body, $T(x, t)$, is governed by

$$\frac{d^2 \theta}{d\eta^2} + 2\eta \frac{d\theta}{d\eta} = 0$$

subject to

$$\theta(\eta) \to 0 \quad \text{as} \quad \eta \to \infty$$

$$\theta(0) = 1$$
**Problem Statement: continued...**

where

\[ \theta = \frac{T - T_i}{T_0 - T_i} \]

and

\[ \eta = \frac{x}{2\sqrt{\alpha t}} \]

Determine the temperature distribution in the body.

*Figure 4: Semi-infinite solid.*
Problem Statement:
The axial displacement $du$ of an elemental length $dx$ of the bar, shown in Figure 5, under a load $P$ is given by

$$\frac{du}{dx} = \frac{\sigma}{E} = \frac{P}{EA}$$

where $E$ is Young’s modulus and $A$ is the cross-sectional area.

Determine the axial displacement of the bar for the following data: $P = 5000$ lb, $l = 10$ in, $E = 30 \times 10^6(1 - 0.01x - 0.0005x^2)$ psi and $A = A_0e^{-0.1x} = 2e^{-0.1x}$ in$^2$. 

Figure 5: Nonuniform bar under axial load.
# Methods

## Newton-Cotes Quadrature
1. **Rectangular Rule**
2. **Trapezoidal Rule**
3. **Simpson’s $\frac{1}{3}$ Rule**
4. **Simpson’s $\frac{3}{8}$ Rule**

## Gauss Quadrature
1. **Gauss-Legendre Formula**
2. **Gauss-Chebyshev Formula**
3. **Gauss-Hermite Formula**
Newton-Cotes Quadrature

The most commonly used numerical integration methods, based on replacing a complicated function or tabular data by some *approximating function* that can be integrated easily

\[ I = \int_{a}^{b} f(x) \, dx = \int_{a}^{b} p_n(x) \, dx \]  

(2)

where \( p_n \) is the approximating function, usually taken as an \( n \)-th degree polynomial

\[ p_n(x) = a_n x^n + a_{n-1} x^{n-1} + \ldots + a_2 x^2 + a_1 x + a_0 \]  

(3)

and \( a_n, a_{n-1}, \ldots a_1, a_0 \) are determined. Simple polynomials commonly used include

- \( p_0(x) = a_0 \) a constant line
- \( p_1(x) = a_1 x + a_0 \) a straight line
- \( p_2(x) = a_2 x^2 + a_1 x + a_0 \) a parabolic curve
- \( p_3(x) = a_3 x^3 + a_2 x^2 + a_1 x + a_0 \) a cubic curve

Approximation of \( f(x) \) using some of these polynomials are shown in Figure 6.
Figure 6: Different types of approximation of $f(x)$. 
The function or data of $f(x)$ can also be approximated using a *series of piecewise polynomials*, see Figure 7.

- Range of integration, $a \leq x \leq b$, is divided into a finite number, $n$, of equal intervals. Width of each interval is

$$h = \Delta x = \frac{b - a}{n}$$

(4)

- Discrete points or nodes in the range of integration is given by

$$x_i = a + ih; i = 0, 1, 2, \ldots, n$$

(5)

![Figure 7](image_url)

(a) Approximation of $f(x)$ by piecewise polynomials.
Newton-Cotes Quadrature

Rectangular Rule

- If values of $f(x)$ is approximated by its values at the beginning of each interval, the area under the curve $f(x)$ in the interval $x_i \leq x \leq x_{i+1}$ is taken as $f_i h$ and the integral $I$ is evaluated as

$$I = \int_a^b f(x) \, dx \approx h \left( \sum_{i=0}^{n-1} f_i \right)$$  \hspace{1cm} (6)

- If values of $f(x)$ is approximated by its values at the end of each interval, the area under the curve $f(x)$ in the interval $x_i \leq x \leq x_{i+1}$ is taken as $f_{i+1} h$ and the integral $I$ is evaluated as

$$I = \int_a^b f(x) \, dx \approx h \left( \sum_{i=0}^{n-1} f_{i+1} \right) \equiv h \left( \sum_{i=1}^{n} f_i \right)$$  \hspace{1cm} (7)
For monotonically increasing function, Eq. (6) underestimates and Eq. (7) overestimates the actual value of the integral, see Figure 8. An improvement in accuracy of the piecewise-constant approximation can be achieved by using the average value of $f_i$ and $f_{i+1}$ in the interval $x_i \leq x \leq x_{i+1}$, shown in Figure 9, in which the integral is evaluated as

$$I = \int_a^b f(x) \, dx \approx h \sum_{i=0}^{n-1} \left( \frac{f_i + f_{i+1}}{2} \right)$$

(8)

Figure 8: Under- and over-estimation of integral $I$
Newton-Cotes Quadrature

Rectangular Rule

Figure 9: Approximation of $f(x)$ by $\frac{1}{2} (f_i + f_{i+1})$ in $x_i \leq x \leq x_{i+1}$
Newton-Cotes Quadrature

Trapezoidal Rule

- Extensively used in engineering applications. Simplicity in developing computer program. Applies for equally spaced base points only.
- Approximation of $f(x)$ by piecewise polynomial of order one $p_1(x) = a_1x + a_0$ which is a straight line. Area under the curve is equal to the area of the trapezoid, thus the name!
- Consider an arbitrary function $f(x)$ shown in Figure 10. An area bounded by $a = x_1$ and $b = x_2$ is required. We assume the integral is approximately equal to area enclosed by linear function and $x$-axis, then

$$I = \int_{a=x_1}^{b=x_2} f(x)\,dx \approx \int_{a=x_1}^{b=x_2} F(x)\,dx \tag{9}$$

Figure 10: Integral evaluation using trapezoidal quadrature.
Evidently, the simplest form for the approximating function, $F(x)$, is the first-order polynomial

$$F(x) = a_0 + a_1x$$  \hspace{1cm} (10)

Substituting Eq. (10) into Eq. (9) and integrating, yields

$$I = \int_{x_1}^{x_2} (a_0 + a_1x)dx = \left[ a_0x + \frac{1}{2}a_1x^2 \right]_{x_1}^{x_2} = a_0(x_2 - x_1) + \frac{1}{2}a_1(x_2^2 - x_1^2)$$  \hspace{1cm} (11)

Eq. (11) is subject to conditions

- at $x = x_1$ \quad $F(x_1) = f(x_1)$
- at $x = x_2$ \quad $F(x_2) = f(x_2)$

Substituting the above conditions into Eq. (10) yields

$$f(x_1) = a_0 + a_1x_1$$  \hspace{1cm} (12a)

$$f(x_2) = a_0 + a_1x_2$$  \hspace{1cm} (12b)
Newton-Cotes Quadrature

Trapezoidal Rule

And solving Eqs. (12) for unknowns $a_0$ and $a_1$ gives

$$a_0 = \frac{1}{x_2 - x_1} [x_2 f(x_1) - x_1 f(x_2)]$$  \hspace{1cm} (13a)$$

$$a_1 = \frac{1}{x_2 - x_1} [-f(x_1) + f(x_2)]$$  \hspace{1cm} (13b)$$

Substituting Eqs. (13) into Eq.(11) yields

$$I = \frac{1}{2} (x_2 - x_1)[f(x_1) + f(x_2)]$$  \hspace{1cm} (14)$$

and if we set $x_2 - x_1 = h$ then Eq. (14) becomes

$$I = \frac{1}{2} h[f(x_1) + f(x_2)]$$  \hspace{1cm} (15)$$
Newton-Cotes Quadrature

Trapezoidal Rule

- Better accuracy if more intermediate nodes are used between $a = x_1$ and $b = x_2$ and Eq. (15) re-written in a global form

\[
I = \frac{1}{2} h [f(x_1) + 2f(x_1 + h) + 2f(x_1 + 2h) + \cdots + f(x_2)]
\]  

(16)

where $h$ is the (equally spaced) increment between two adjacent nodes.

- In general, the integral is evaluated as

\[
I = \int_a^b f(x) \, dx \approx \frac{1}{2} h [f_0 + 2f_1 + 2f_2 + \cdots + 2f_{n-1} + f_n]
\]  

(17)
Examples

1. Evaluate the following integral using the trapezoidal quadrature and $h = 0.1$

$$I = \int_{1}^{1.6} e^{x^2} \, dx$$

2. Determine the value of the integral $I = \int_{a}^{b} f(x) \, dx$, where

$$f(x) = 0.84885406 + 31.51924706x - 137.66731262x^2$$

$$+ 240.55831238x^3 - 171.45245361x^4 + 41.95066071x^5$$

with $a = 0.0$ and $b = 1.5$ using trapezoidal quadrature with different intervals.
Newton-Cotes Quadrature

Simpson’s One-Third Rule

- Accuracy of the trapezoidal rule can be improved by increasing number of segments $n$ or reducing step size $h$; but the latter leads to increase in round-off error.
- Another way to get more accurate estimate of integral is to use higher order polynomials for approximating the function $f(x)$.
- Makes use of parabola or second-order polynomial

$$p_2(x) = a_2x^2 + a_1x + a_0$$  \hspace{1cm} (18)

... to estimate the integral

$$I = \int_a^b f(x) \, dx$$  \hspace{1cm} (19)

- Constants $a_0$, $a_1$ and $a_2$ can be determined by making the approximating polynomial, Eq. (18), pass through three consecutive $x_i$, see Figure 11.
Figure 11: Simpson’s one-third rule.
Newton-Cotes Quadrature
Simpson’s One-Third Rule

- Take the origin at \( x_i \) (\( x = 0 \) at \( x_i \)) so that \( x_{i-1} \) and \( x_{i+1} \) correspond to \( -h \) and \( +h \), respectively, and apply them to the polynomial. For

  \[
  x_{i-1}: \quad p_2(x=-h) = f_{i-1} = a_2(-h)^2 + a_1(-h) + a_0 \quad (20)
  \]
  \[
  x: \quad p_2(x=0) = f_i = a_2(0)^2 + a_1(0) + a_0 \quad (21)
  \]
  \[
  x_{i+1}: \quad p_2(x=+h) = f_{i+1} = a_2(h)^2 + a_1(h) + a_0 \quad (22)
  \]

- Solving for \( a_0 \), \( a_1 \) and \( a_2 \) using Eqs. (20)–(22) yields

  \[
  a_2 = \frac{f_{i-1} - 2f_i + f_{i+1}}{2h^2} \quad a_1 = \frac{f_{i+1} - f_{i-1}}{2h} \quad a_0 = f_i \quad (23)
  \]

- Area \( \bar{I} \) under the second-order polynomial \( p_2(x) \) between \( x_{i-1} \) and \( x_{i+1} \) is given by

  \[
  \bar{I} = \int_{x_{i-1}}^{x_{i+1}} p_2(x) \, dx = \int_{-h}^{+h} (a_2x^2 + a_1x + a_0) \, dx \\
  = \left[ \frac{a_2}{3}(x^3) \right]_{-h}^{+h} + \left[ \frac{a_1}{2}(x^2) \right]_{-h}^{+h} + a_0(x) \bigg|_{-h}^{+h} = \frac{2}{3}a_2h^3 + 2a_0h \quad (24)
  \]
Substituting for $a_0$, $a_1$ and $a_2$ from Eq. (23), Eq. (22) gives

$$\bar{I} = \frac{2}{3} h^3 \left( \frac{f_{i-1} - 2f_i + f_{i+1}}{2h^2} \right) + 2hf_i$$

$$= \frac{1}{3} h (f_{i-1} + 4f_i + f_{i+1})$$

(25)

The term “$\frac{1}{3}$” in Simpson’s one-third rule refers to the factor “$\frac{1}{3}$” in Eq. (25)

For multistage application, we need to divide the range $a \leq x \leq b$ into $n$ segments of equal width $h = \frac{b-a}{n}$, with $n$ being **EVEN** so that Eq. (25) can be applied for groups of two segments.

Integral in Eq. (19) can be evaluated thus

$$I = \int_a^b f(x) \, dx \approx \sum_{j=1}^{n/2} (\bar{I})_j$$

(26)

with $\bar{I}$ given by Eq. (25) and $i = 2j - 1$
Eqs. (25) and (26) lead to

\[
I \approx \frac{1}{3} h \left[ f_0 + \left( 4 \sum_{i=1,3,5,\ldots}^{n-1} f_i \right) + \left( 2 \sum_{i=2,4,6,\ldots}^{n-2} f_i \right) + f_n \right]
\]

(27)
Examples

Determine the value of the integral $I = \int_{a}^{b} f(x)dx$, where

$$f(x) = 0.84885406 + 31.51924706x - 137.66731262x^2$$
$$+ 240.55831238x^3 - 171.45245361x^4 + 41.95066071x^5$$

with $a = 0.0$ and $b = 1.5$ using Simpson’s $\frac{1}{3}$ rule with different intervals.
Newton-Cotes Quadrature

Simpson’s Three-Eighths Rule

- Makes use of cubic function or third-order polynomial

\[ p_3(x) = a_3x^3 + a_2x^2 + a_1x + a_0 \]

(28)

to estimate the integral

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

- \(a_0, a_1, a_2\) and \(a_a\) are determined by making the approximating polynomial, Eq. (28), pass through FOUR consecutive points \(x_i\), see Figure 12

Figure 12: Simpson’s three-eighths rule.
Newton-Cotes Quadrature

Simpson’s Three-Eighths Rule

Take the origin at \( x_i \) \((x = 0\) at \( x_i \)) so that \( x_{i-1}, x_{i+1} \) and \( x_{i+2} \) correspond to \(-h, +h\) and \(+2h\), respectively, and apply them to the polynomial. For

\[
x_{i-1} : \quad p_3(x = -h) = f_{i-1} = a_3(-h)^3 + a_2(-h)^2 + a_1(-h) + a_0
\]  \tag{29}

\[
x_i : \quad p_3(x = 0) = f_i = a_0
\]  \tag{30}

\[
x_{i+1} : \quad p_3(x = +h) = f_{i+1} = a_3(h)^3 + a_2(h)^2 + a_1(h) + a_0
\]  \tag{31}

\[
x_{i+2} : \quad p_3(x = +2h) = f_{i+2} = a_3(2h)^3 + a_2(2h)^2 + a_1(2h) + a_0
\]  \tag{32}

Solving for \( a_0, a_1, a_2 \) and \( a_3 \) using Eqs. (29)–(32) yields

\[
a_0 = f_i
\]  \tag{33}

\[
a_1 = \frac{1}{6h}(-f_{i+2} + 6f_{i+1} - 3f_i - 2f_{i-1})
\]  \tag{34}

\[
a_2 = \frac{1}{2h^2}(f_{i-1} - 2f_i + f_{i+1})
\]  \tag{35}

\[
a_3 = \frac{1}{6h^3}(f_{i+2} - 3f_{i+1} + 3f_i - f_{i-1})
\]  \tag{36}
Newton-Cotes Quadrature

Simpson’s Three-Eighths Rule

- Area \( \bar{I} \) under the third-order polynomial \( p_3(x) \) between \( x_{i-1} \) and \( x_{i+2} \) is given by

\[
\bar{I} = \int_{x_{i-1}}^{x_{i+2}} p_3(x) \, dx = \int_{-h}^{+2h} (a_3 x^3 + a_2 x^2 + a_1 x + a_0) \, dx
\]

\[
= \frac{a_3}{4} (x^4) \bigg|_{-h}^{+2h} + \frac{a_2}{3} (x^3) \bigg|_{-h}^{+2h} + \frac{a_1}{2} (x^2) \bigg|_{-h}^{+2h} + a_0 (x) \bigg|_{-h}^{+2h}
\]

\[
= \frac{a_3}{4} (15h^4) + \frac{a_2}{3} (9h^3) + \frac{a_1}{2} (3h^2) + a_0 (3h)
\]  \((37)\)

- Substituting for \( a_0, a_1, a_2 \) and \( a_3 \) from Eqs. (33)–(36), Eq. (37) gives

\[
\bar{I} = \frac{15h^4}{4} \left( \frac{f_{i+2} - 3f_{i+1} + 3f_i - f_{i-1}}{6h^3} \right) + 3h^3 \left( \frac{f_{i+1} - 2f_i + f_{i-1}}{2h^2} \right)
\]

\[
+ \frac{3h^2}{2} \left( \frac{-f_{i+2} + 6f_{i+1} - 3f_i - 2f_{i-1}}{6h} \right) + 3hf_i
\]

\[
= \frac{3}{8} h \left[ f_{i+2} + 3f_{i+1} + 3f_i + f_{i-1} \right]
\]  \((38)\)

The term “\( \frac{3}{8} \)” in Simpson’s three-eighths rule refers to the factor “\( \frac{3}{8} \)” in Eq. (38)
Integral in Eq. (19) can be evaluated thus

$$I = \int_a^b f(x) \, dx \approx \sum_{j=1}^{n/3} (\bar{I})_j$$

(39)

with $\bar{I}$ given by Eq. (38) and $i = 3j - 2$

Eqs. (38) and (39) lead to

$$I \approx \frac{3}{8} h \left[ f_0 + \left( 3 \sum_{i=1,4,7,\ldots}^{n-2} (f_i + f_{i+1}) \right) + \left( 2 \sum_{i=3,6,9,\ldots}^{n-3} f_i \right) + f_n \right]$$

(40)
Examples

Determine the value of the integral $I = \int_{a}^{b} f(x)dx$, where

$$f(x) = 0.84885406 + 31.51924706x - 137.66731262x^2 + 240.55831238x^3 - 171.45245361x^4 + 41.95066071x^5$$

with $a = 0.0$ and $b = 1.5$ using Simpson’s $\frac{3}{8}$ rule with different step sizes.
Trapezoidal rule used to calculate area under the straight line connecting the function values at the ends of the integration intervals is

\[ I = \int_{a}^{b} f(x)dx \approx (b - a)\frac{f(a) + f(b)}{2} \]  

(41)

where \( a \) and \( b \) are limits of integration and \( (b - a) \) is the integration interval.

Because trapezoidal rule must pass through end points, there are cases such as Figure 13 where the formula results in large error.

Figure 13: Trapezoidal rule.
Gauss Quadrature

Suppose we take away the constraint of fixed based points and evaluate the area under a straight line joining any two points on the curve—we could define a straight line that would balance the positive and negative errors, Figure 14, to arrive at an improved estimate of the integral.

Figure 14: Improved integral estimate.

Figure 14 describes the Gauss quadrature—a class of techniques to implement a strategy which allows the evaluation of integrand at a number of specified, but unequal, intervals.
An $n$-point Gaussian quadrature is constructed to yield an exact result for interpolating polynomials $p(x)$ of degree $2n - 1$, by a suitable choice of $n$ points $x_i$ and $n$ weights $\omega_i$. It is stated as

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} p(x)dx = \sum_{i=1}^{n} w_i p(x_i) \approx \sum_{i=1}^{n} w_i f(x_i)$$  \hspace{1cm} (42)$$

where $w_i$ are weights, $x_i$ are specific values of $x$ called Gauss points at which integrand is evaluated. Accuracy is much higher than the Newton-Cotes formulae.

For any specified $n$, values $w_i$ and $x_i$ are chosen so that the formula will be exact for polynomials up to and including degree $2n - 1$

**Example:** When $n = 2$, the values $w_1$, $w_2$, $x_1$ and $x_2$ are selected so that formula will give the exact value of the integral for polynomials up to degree $2n - 1 = 2 \times 2 - 1 = 3$

As shown in Eq.(42) the domain of integration for this rule is conventionally taken as $[-1, 1]$ to simplify the mathematics and make formulation as general as possible. A change of variable is used to translate the original $[a, b]$ integration limits into $[-1, 1]$ form.
Assume that a new variable \( r \) is related to the original variable \( x \) in a linear fashion,

\[
x = c_0 + c_1 r
\]  
\[\text{Eq. (43)}\]

If lower limit, \( x = a \) corresponds to \( r = -1 \), these values can be substituted into Eq. (43) to yield

\[
a = c_0 + c_1 (-1) = c_0 - c_1
\]  
\[\text{Eq. (44)}\]

Similarly, upper limit, \( x = b \), corresponds to \( r = 1 \), to give

\[
b = c_0 + c_1 (1) = c_0 + c_1
\]  
\[\text{Eq. (45)}\]

Solving Eqs. (44) and (45) yields

\[
c_0 = \frac{b + a}{2}
\]  
\[\text{Eq. (46)}\]

and

\[
c_1 = \frac{b - a}{2}
\]  
\[\text{Eq. (47)}\]
Substituting Eqs. (46) and (47) into Eq. (43), yields

\[ x = \frac{(b + a) + (b - a)r}{2} \]  \hspace{1cm} (48)

and differentiating Eq. (48) gives

\[ dx = \frac{b - a}{2} dr \]  \hspace{1cm} (49)
A popular form of Gauss quadrature is the Gauss-Legendre formula which uses Legendre polynomial

\[ P_0(x) = 1 \]
\[ P_1(x) = x \]
\[ P_n(x) = \left( \frac{2n - 1}{n} \right) x P_{n-1}(x) - \left( \frac{n - 1}{n} \right) P_{n-2}(x); \quad n = 2, 3, 4, \ldots \]  

(50)

as the interpolating polynomial to approximate function \( f(x) \), and roots of Legendre polynomial to locate points at which the integrand is evaluated . . .

In general, any arbitrary \( n \)th-degree interpolating polynomials, \( p_n(x) \), . . . and in general, any arbitrary \( n \)th-degree interpolating polynomials, \( p_n(x) \), can be represented by a linear combination of Legendre polynomials as

\[ p_n(x) = \sum_{i=0}^{n} w_i P_i(x) \]  

(51)

where \( w_i \) are constants.
Two-point Gauss quadrature formula is given by Eq. (42) with \( n = 2 \)

\[
\int_{-1}^{1} f(x)dx = \sum_{i=1}^{2} w_i f(x_i) = w_1 f(x_1) + w_2 f(x_2)
\]  

(52)

Since \( n = 2 \), the formula should give exact value for polynomials of order 3 and below, and we extend this reasoning by assuming that it fits the integrals of \( f(x) = 1, x, x^2, x^3 \) functions.

Evaluation of \( w_1, w_2, x_1 \) and \( x_2 \) requires use of FOUR conditions.

**When\( f(x) = 1 \)**

\[
\int_{-1}^{1} f(x)dx = \int_{-1}^{1} 1 dx = 2 = w_1 f(x_1) + w_2 f(x_2) = w_1 + w_2
\]

(53)

**When\( f(x) = x \)**

\[
\int_{-1}^{1} f(x)dx = \int_{-1}^{1} x dx = \left[ \frac{x^2}{2} \right]_{-1}^{1} = 0 = w_1 f(x_1) + w_2 f(x_2) = w_1 x_1 + w_2 x_2
\]

(54)
Gauss Quadrature

Gauss-Legendre Formula

When $f(x) = x^2$

\[
\int_{-1}^{1} f(x) \, dx = \int_{-1}^{1} x^2 \, dx = \left[ \frac{x^3}{3} \right]_{-1}^{1} = \frac{2}{3}
\]

\[
= w_1 f(x_1) + w_2 f(x_2)
\]

\[
= w_1 x_1^2 + w_2 x_2^2
\] (55)

Since limits of integration, $-1$ and $+1$, are symmetric about $x = 0$, we expect $x_1$ and $x_2$ also to be symmetric about $x = 0$.

By setting $x_2 = -x_1$, we obtain the following, from Eqs. (54) and (53)

\[
w_1 = w_2 = 1
\]

and both satisfy Eq. (56), and Eq. (55) gives

\[
x_1^2 = \frac{1}{3}
\]

\[
\left\{ \begin{array}{l}
x_1 = + \frac{1}{\sqrt{3}} = +0.577350269189626 \\
x_2 = - \frac{1}{\sqrt{3}} = -0.577350269189626 = -x_1
\end{array} \right.
\]

When $f(x) = x^3$

\[
\int_{-1}^{1} f(x) \, dx = \int_{-1}^{1} x^3 \, dx = \left[ \frac{x^4}{4} \right]_{-1}^{1} = 0
\]

\[
= w_1 f(x_1) + w_2 f(x_2)
\]

\[
= w_1 x_1^3 + w_2 x_2^3
\] (56)
Higher-Point Gauss quadrature formulae can be developed in the general form

\[ I \approx \sum_{i=1}^{n} w_i f(x_i) = w_1 f(x_1) + w_2 f(x_2) + \ldots + w_n f(x_n) \]  \hspace{1cm} (57)

where \( n \) = number of points. Values for \( w \)'s and \( x \)'s for up to and including the five-point formula are summarized in Table 3.

### Table 3: Weights and Gauss points used in Gauss-Legendre formulae

<table>
<thead>
<tr>
<th>Points</th>
<th>Weights</th>
<th>Gauss Points</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>( w_1 = 1.0000000 )</td>
<td>( x_1 = -0.577350269 )</td>
</tr>
<tr>
<td></td>
<td>( w_2 = 1.0000000 )</td>
<td>( x_2 = +0.577350269 )</td>
</tr>
<tr>
<td>3</td>
<td>( w_1 = 0.5555556 )</td>
<td>( x_1 = -0.774596669 )</td>
</tr>
<tr>
<td></td>
<td>( w_2 = 0.8888889 )</td>
<td>( x_2 = -0.0 )</td>
</tr>
<tr>
<td></td>
<td>( w_3 = 0.5555556 )</td>
<td>( x_3 = +0.774596669 )</td>
</tr>
<tr>
<td>4</td>
<td>( w_1 = 0.3478548 )</td>
<td>( x_1 = -0.861136312 )</td>
</tr>
<tr>
<td></td>
<td>( w_2 = 0.6521452 )</td>
<td>( x_2 = -0.339981044 )</td>
</tr>
<tr>
<td></td>
<td>( w_3 = 0.6521452 )</td>
<td>( x_3 = +0.339981044 )</td>
</tr>
<tr>
<td></td>
<td>( w_4 = 0.3478548 )</td>
<td>( x_4 = +0.861136312 )</td>
</tr>
<tr>
<td>5</td>
<td>( w_1 = 0.2369269 )</td>
<td>( x_1 = -0.906179846 )</td>
</tr>
<tr>
<td></td>
<td>( w_2 = 0.4786287 )</td>
<td>( x_2 = -0.538469310 )</td>
</tr>
<tr>
<td></td>
<td>( w_3 = 0.5688889 )</td>
<td>( x_3 = 0.0 )</td>
</tr>
<tr>
<td></td>
<td>( w_4 = 0.4786287 )</td>
<td>( x_4 = +0.538469310 )</td>
</tr>
<tr>
<td></td>
<td>( w_5 = 0.2369269 )</td>
<td>( x_5 = +0.906179846 )</td>
</tr>
</tbody>
</table>
Examples:

1. Express a fifth-degree polynomial, \( p_5(x) \), in terms of Legendre polynomials.
2. Evaluate the integral

\[
I = \int_{0}^{2} ye^{2y} \, dy
\]

using the Gauss-Legendre quadrature.
3. Take a look at \texttt{gauss5.f} to study sample 5-point Gauss-Legendre formula written in Fortran. Modify it to find the solution of the example above.
Gauss Quadrature
Gauss-Chebyshev Formula

- Based on Chebyshev polynomials

\[
P_0(x) = 1 \\
P_1(x) = x \\
P_2(x) = 2x^2 - 1 \\
P_n(n) = 2xP_{n-1}(x) - P_{n-2}(x); \quad n = 3, 4, 5, \ldots \tag{58}
\]

- Used to evaluate integrals of the type

\[
\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx
\]

with the formula given by

\[
\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx = \sum_{i=1}^{n} n w_i f(x_i) \tag{59}
\]
Gauss Quadrature

Gauss-Chebyshev Formula

- Roots of the $n$th-degree Chebyshev polynomial are given by

$$x_i = \cos \left( \frac{(i - \frac{1}{2}) \pi}{n} \right); \quad i = 1, 2, \ldots, n$$  \hspace{1cm} (60)

- Weights are given by

$$w_i = \frac{\pi}{n}; \quad i = 1, 2, \ldots, n$$  \hspace{1cm} (61)
Gauss Quadrature

Gauss-Hermite Formula

- Based on Hermite polynomials
  
  \[ P_0(x) = 1 \]
  \[ P_1(x) = 2x \]
  \[ P_2(x) = 4x^2 - 2 \]
  \[ P_3(x) = 8x^3 - 12x \]
  \[ P_n(x) = 2xP_{n-1}(x) - 2(n-1)P_{n-2}(x); \quad n = 2, 3, 4, \ldots \] (62)

- Used to evaluate integrals of the type

  \[ \int_{-\infty}^{\infty} e^{-x^2} f(x) \, dx \]

  with the formula given by

  \[ \int_{-\infty}^{\infty} e^{-x^2} f(x) \, dx = \sum_{i=1}^{n} w_i f(x_i) \] (63)

- Values for roots of the \( n \)-th-degree Hermite polynomial, \( x_i \), and weights \( w_i \) for \( n = 2, 3, 4, 5 \) are readily tabulated
**Problem Statement:**
Use Matlab to integrate the following definite integral

\[ \int_{0}^{1} 3 \sin \frac{1}{2}x \, dx \]

**Solution:**

Matlab Session

```matlab
>> fx = '3*sin(x/2)'
>> r = quad(fx,0,1)
```
Problem Statement:
You are given a table of data representing a graph under a curve. The data are saved in a file, `expt1.dat`, as pairs of $x$ and $y$. Read these data into Matlab, plot the curve and integrate for area under the curve.

Solution:

Matlab Session

```matlab
>> load expt1.dat;
>> x = expt1(:,1);
>> y = expt1(:,2);
>> plot(x,y)
>> area = trapz(x,y)
```
**Problem Statement:**
You have a function in 3-D space such that

\[ z = f(x, y) = \sin x \times \cos y + 1 \]

that stretches in the ranges of \( 0 < x < \pi \) and \( -\pi < x < \pi \).

Find the volume under this function.

**Solution:**

**Step 1:** Create a Matlab function file, `myownfun.m`, to contain the function definition

```matlab
function z=myownfun(x,y)
% myownfun(x,y) and example function of
% two variables--must be able to handle
% vector x input
z = sin(x).*cos(y)+1
```

**Step 2:** Matlab session making use of `myownfun.m`

```
>> % set x-range
>> x = linspace(0,pi,20);
>> % set y-range
>> y = linspace(-pi,pi,20);
>> % create a grid of points
>> [xx,yy] = meshgrid(x,y);
>> % evaluate at ALL grid points
>> zz = myownfun(xx,yy);
>> % plot the surface
>> mesh(xx,yy,zz)
>> % compute volume
>> volume=dblquad(@(myownfun,0,pi,-pi,pi)
```


