CHAPTER 7e. DIFFERENTIATION AND INTEGRATION

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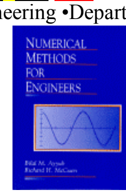

by

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ENCE 203 - Computation Methods in Civil Engineering II

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Numerical Integration

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- Gauss Quadrature
  - The methods for numerical integration (i.e., Trapezoidal and Simpson's rules) that were discussed previously are based on evenly spaced function value.
  - Consequently, the location of the base points used in these equations was *predetermined* or *fixed*.

Numerical Integration

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- Gauss Quadrature
  - For example, the trapezoidal rule is based on taking the area under the traight line connecting the function values at the ends of the integration interval.
  - In reference to Figure 1, the trapezoidal rule can be expressed as

$$I = \int_a^b f(x)dx \approx (b-a)\frac{f(b)+f(a)}{2} \qquad (1)$$

Numerical Integration

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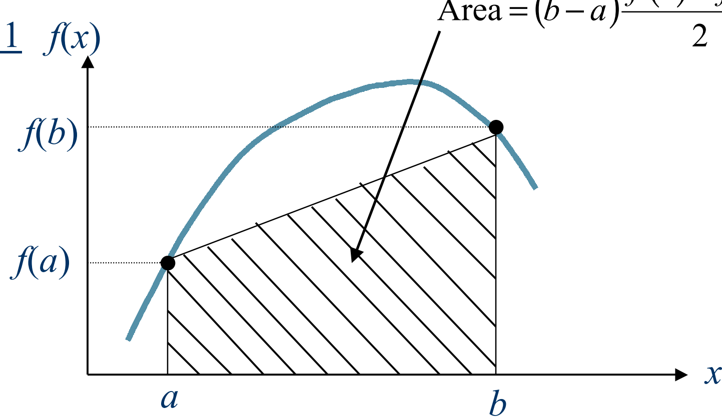
- Gauss Quadrature

$$\text{Area} = (b-a)\frac{f(b)+f(a)}{2}$$

Figure 1



Numerical Integration

■ Gauss Quadrature

– Because the trapezoidal rule requires that the line pass through the ends points (or called the pivotal points), there are cases where the formula results in a large error as shown in Figure 1.

– If we remove the constraint of fixed base points, then we can evaluate the area under a straight line that connects any two points on the curve (see Figure 2).

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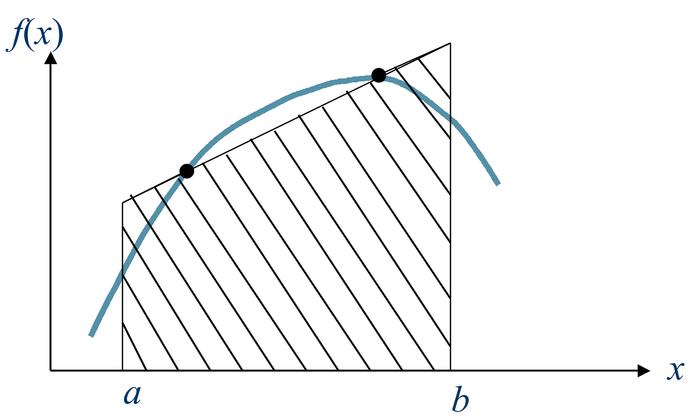
■ Gauss Quadrature

Figure 2



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Numerical Integration

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■ Gauss Quadrature

– If these two points are positioned wisely, then a straight line can defined that would balance the positive and negative errors as shown in Figure 2.

– In this case, the estimate of the integral will improve tremendously.

– This basic concept is the heart of the *Gauss Quadrature techniques*

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■ Gauss Quadrature

– Before describing Gauss's approach, it would be proper to derive the trapezoidal formula using the method of undetermined coefficients that will be employed in deriving the Gauss quadrature.

– Developing the trapezoidal method in this approach will make easier to understand the development of Gauss quadrature later on.

Numerical Integration

- Gauss Quadrature
  - Deriving Trapezoidal Rule using the Method of Undetermined Coefficients

$$I = \int_a^b f(x)dx \approx (b-a)\frac{f(b)+f(a)}{2} \qquad (1)$$

Eq 1 can be expressed as

$$I = \int_a^b f(x)dx \approx C_1 f(a) + C_2 f(b) \qquad (2)$$

Numerical Integration

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- Gauss Quadrature
  - Deriving Trapezoidal Rule using the Method of Undetermined Coefficients

    Where C_1 and C_2 are constant to be determined.

    We note that the trapezoidal rule should provide exact results when the function being integrated is a constant or straight line.

    Two simple equations that represent these cases are $f(x) = 1$ and $f(x) = x$.

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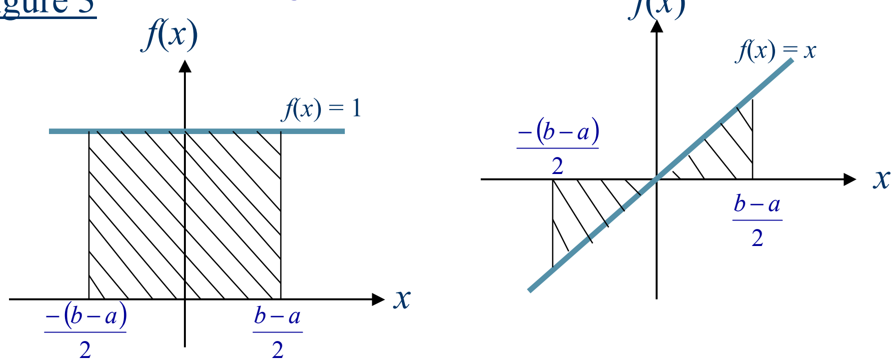
- Gauss Quadrature
  - Deriving Trapezoidal Rule

Figure 3



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- Gauss Quadrature
  - Deriving Trapezoidal Rule

    If $f(x) = 1$, then $f(a) = f(b) = 1$ in Equation 2

    And after changing the limits of integration of Eq. 2, the following equalities should hold:

$$\int_{-(b-1)/2}^{(b-a)/2} f(x)dx = C_1 f(a) + C_2 f(b)$$

$$= C_1(1) + C_2(1)$$

$$= C_1 + C_2$$

Numerical Integration

- Gauss Quadrature
  - Deriving Trapezoidal Rule

$$C_1 + C_2 = \int_{-(b-a)/2}^{(b-a)/2} f(x)dx = \int_{-(b-a)/2}^{(b-a)/2} (1)dx$$

$$C_1 + C_2 = x\Big|_{-(b-a)/2}^{(b-a)/2} = \frac{b-a}{2} + \frac{b-a}{2}$$

Therefore,

$$C_1 + C_2 = b - a \qquad (3)$$

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- Gauss Quadrature
  - Deriving Trapezoidal Rule

If $f(x) = x$, then $f(a) = -(b - a)/2$ and $f(b) = (b - a)/2$ in Equation 2.

And after changing the limits of integration of Eq. 2, the following equality should hold:

$$\int_{-(b-1)/2}^{(b-a)/2} f(x)dx = C_1 f(a) + C_2 f(b)$$

$$= C_1 \frac{-(b-a)}{2} + C_2 \frac{b-a}{2}$$

Numerical Integration

■ Gauss Quadrature

– Deriving Trapezoidal Rule

$$-C_1\frac{b-a}{2}+C_2\frac{b-a}{2}=\int_{-(b-a)/2}^{(b-a)/2} f(x)dx=\int_{-(b-a)/2}^{(b-a)/2} x dx$$

$$-C_1\frac{b-a}{2}+C_2\frac{b-a}{2}=\left.\frac{x^2}{2}\right|_{-(b-a)/2}^{(b-a)/2}=\frac{(b-a)^2}{8}-\frac{(b-a)^2}{8}$$

Therefore,

$$-C_1\frac{b-a}{2}+C_2\frac{b-a}{2}=0 \qquad (4)$$

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■ Gauss Quadrature

– Deriving Trapezoidal Rule

Equations 3 and 4 can be solved simultaneously for the constants C_1 and C_2 as follows:

$$C_1 \qquad + C_2 = b-a$$

$$-\frac{b-a}{2}C_1+\frac{b-a}{2}C_2=0$$

$$(b-a)(-C_1+C_2)=0$$

Numerical Integration

■ Gauss Quadrature

– Deriving Trapezoidal Rule

But $(b-a)$ cannot be zero, therefore,

$$-C_1 + C_2 = 0 \Rightarrow C_2 = C_1$$

$$C_1 + C_2 = b - a$$

$$C_1 + C_1 = b - a$$

or

$$C_1 = \frac{b-a}{2} = C_2 \qquad (5)$$

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■ Gauss Quadrature

– Deriving Trapezoidal Rule

Substituting the obtained values of the constants C_1 and C_2 into Equation 2, yields the Trapezoidal formula

$$I = C_1 f(a) + C_2 f(b)$$

$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

or

$$I = (b-a)\frac{f(b)+f(a)}{2}$$ ← Trapezoidal Formula

Numerical Integration

■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

As was the case for the derivation of trapezoidal rule, two-point gauss quadrature formula can be developed in a similar manner using the following form:

$$I \approx C_1 f(x_1) + C_2 f(x_2) \qquad (6)$$

Numerical Integration

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■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

- However, in contrast to the trapezoidal rule that used fixed end points a and b, the function arguments x_1 and x_2 are not fixed at the end points, but rather are unknown at this point as shown in Figure 4.
- In this case, we have a total of four unknowns that need to be evaluated.

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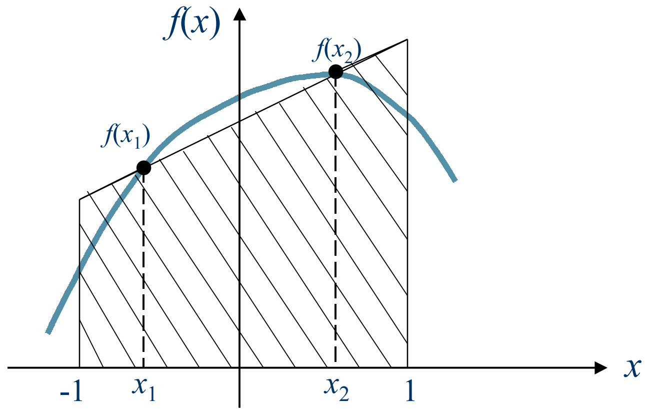
■ Gauss Quadrature

Figure 4



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■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

- Note that in the figure, the limits of the integration are from –1 to 1.
- This was intentionally done to simplify the mathematics and to make the formulation as general as possible as we will see later.

Numerical Integration

■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

• In order to determine the four unknowns C_1, C_2, x_1, and x_2, we need to define four conditions as follows:

Equation 6 should fit the integral with constant, linear, parabolic, and cubic functions, that is

Table 1

	Constant	Linear	Parabolic	Cubic
$f(x)$	1	x	x^2	x^3

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■ Gauss Quadrature

• With respect to Eq. 6 and Table 1, the following set of equations needs to be solved:

$$\left.\begin{aligned} C_1 f(x_1) + C_2 f(x_2) &= \int_{-1}^{1} (1)\, dx = 2 \\ C_1 f(x_1) + C_2 f(x_2) &= \int_{-1}^{1} x\, dx = 0 \\ C_1 f(x_1) + C_2 f(x_2) &= \int_{-1}^{1} x^2\, dx = \frac{2}{3} \\ C_1 f(x_1) + C_2 f(x_2) &= \int_{-1}^{1} x^3\, dx = 0 \end{aligned}\right. \qquad (7)$$

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■ Gauss Quadrature

- Eq. 7 can be expressed as follows:

$$C_1(1) + C_2(1) = 2 \qquad (8)$$

$$C_1 x_1 + C_2 x_2 = 0 \qquad (9)$$

$$C_1 x_1^2 + C_2 x_2^2 = \frac{2}{3} \qquad (10)$$

$$C_1 x_1^3 + C_2 x_2^3 = 0 \qquad (11)$$

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■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

- From Eq. 8 $C_2 = 2 - C_1$
- And by substituting C_2 into Eq. 9, yields

$$C_1 x_1 + (2 - C_1) x_2 = 0$$

or

$$x_1 = \frac{-(2 - C_1) x_2}{C_1} = \frac{(C_1 - 2) x_2}{C_1} \qquad (12)$$

Numerical Integration

■ Gauss Quadrature

- When x_1 of Eq. 12 is substituted in Equation 10, this equation (Eq.10) becomes

$$C_1 x_1^2 + C_2 x_2^2 = \frac{2}{3}$$

$$C_1 \frac{(C_1 - 2)^2 x_2^2}{C_1^2} + (2 - C_1)x_2^2 = \frac{2}{3}$$

Solving for x_2^2, gives

$$x_2^2 = \frac{C_1}{6 - 3C_1} \qquad (13)$$

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■ Gauss Quadrature

– Derivation of Two-Point Gauss Quadrature Formula

- Substituting x_1 of Eq. 12 into Eq. 11 gives

$$C_1 x_1^3 + C_2 x_2^3 = 0$$

$$C_1 \frac{(C_1 - 2)^3 x_2^3}{C_1^3} + (2 - C_1)x_2^3 = 0$$

which is equivalent to

$$x_2^3 (C_1 - 2)\left[(C_1 - 2)^2 - C_1^2\right] = 0 \qquad (14)$$

Numerical Integration

- Gauss Quadrature
  - Derivation of Two-Point Gauss Quadrature Formula
    - x_2 cannot be zero and C_1 cannot be 2 in Equation 14, therefore Equation 14 implies that

$$(C_1 - 2)^2 - C_1^2 = 0$$

$$C_1^2 - 4C_1 + 4 - C_1^2 = 0$$

$$-4C_1 = -4$$

or

$$C_1 = 1 \qquad (15)$$

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- Gauss Quadrature
  - Derivation of Two-Point Gauss Quadrature Formula
    - Substituting for C_1 in Eq.8 and in Eq.13 gives

$$C_2 = 1$$

$$x_2 = \sqrt{\frac{C_1}{6 - 3C_1}} = \sqrt{\frac{1}{6 - 3(1)}} = \frac{1}{\sqrt{3}} = 0.5773503$$

    - And from Eq. 11

$$x_1 = -x_2 = -\frac{1}{\sqrt{3}} = -0.5773503$$

Numerical Integration

■ Two-Point Gauss Quadrature Formula

$$I \approx \int_{-1}^{1} f(x)dx = C_1 f(x_1) + C_2 f(x_2)$$

$$I \approx \int_{-1}^{1} f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \qquad (16)$$

Numerical Integration

■ Higher-Point Gauss Quadrature Formulas

– Other higher point formulas can be developed in the same manner.

– As expected, the higher the Gauss Quadrature formula is , the higher the accuracy that can be obtained.

– The equations needed to determine the factors can be given in a compact form as

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- Higher-Point Gauss Quadrature Formulas

$$C_1x_1^0 + C_2x_2^0 + \cdots + C_nx_n^0 = \int_{-1}^{1} 1\,dx = 2$$

$$C_1x_1^1 + C_2x_2^1 + \cdots + C_nx_n^1 = \int_{-1}^{1} x\,dx = 0$$

$$C_1x_1^2 + C_2x_2^2 + \cdots + C_nx_n^2 = \int_{-1}^{1} x^2\,dx = 0$$

$$\vdots \qquad (17)$$

$$C_1x_1^2 + C_2x_2^2 + \cdots + C_nx_n^2 = \frac{(+1)^{k+1} - (-1)^{k+1}}{k+1}$$

$$= \begin{cases} 0 & \text{if } k \text{ is odd} \\ \dfrac{2}{\mathrm{k}+1} & \text{if } k \text{ is even} \end{cases}$$

$$C_1x_1^{2n-1} + C_2x_2^{2n-1} + \cdots + C_nx_n^{2n-1} = \frac{(+1)^{2n} - (-1)^{2n}}{2n} = 0$$

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- Higher-Point Gauss Quadrature Formulas

The higher-point formula can be developed in the general form

$$I = \int_{-1}^{1} f(x)dx = C_1 f(x_1) + C_2 f(x_2) + \cdots + C_n f(x_n) \qquad (18)$$

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Table 2
Gauss Quadrature Weights and Coefficients

Number of Points	Weighting Factors	Function Arguments
2	$C_1 = 1.000000000$ $C_2 = 1.000000000$	$x_1 = -0.577350269$ $x_2 = 0.577350269$
3	$C_1 = 0.555555556$ $C_2 = 0.888888889$ $C_3 = 0.555555556$	$x_1 = -0.774596669$ $x_2 = 0.000000000$ $x_3 = 0.774596669$
4	$C_1 = 0.347854845$ $C_2 = 0.652145155$ $C_3 = 0.652145155$ $C_4 = 0.347854845$	$x_1 = -0.861136312$ $x_2 = -0.339981044$ $x_3 = 0.339981044$ $x_4 = 0.861136312$
5	$C_1 = 0.236926885$ $C_2 = 0.478628670$ $C_3 = 0.568888889$ $C_4 = 0.478628670$ $C_5 = 0.236926885$	$x_1 = -0.906179846$ $x_2 = -0.538469310$ $x_3 = 0.000000000$ $x_4 = 0.538469310$ $x_5 = 0.906179846$
6	$C_1 = 0.171324492$ $C_2 = 0.360761573$ $C_3 = 0.467913935$ $C_4 = 0.467913935$ $C_5 = 0.360761573$ $C_6 = 0.171324492$	$x_1 = -0.932469514$ $x_2 = -0.661209386$ $x_3 = -0.238619186$ $x_4 = 0.238619186$ $x_5 = 0.661209386$ $x_6 = 0.932469514$

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- How to Apply Gauss Quadrature
  - Transformation of variables
    - It was noticed in Eqs.16 and 18 that the limits of integration are from –1 to 1.
    - This was done intentionally to simplify the mathematics and to make the formulation as general as possible.
    - A simple change of variable can be used to translate other limits of integration into this form.

Numerical Integration

- How to Apply Gauss Quadrature
  - Transformation of variables
    - This can done by assuming a new variable w is related to the original variable x in a linear fashion as

$$x = A + Bx_G \qquad (19)$$

    - If the lower limit, $x = a$, this corresponds to

$$x_G = -1$$

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- How to Apply Gauss Quadrature
  - Transformation of variables
    - These values can be substituted into Eq. 19 to give

$$x = A + Bx_G$$
$$a = A + B(-1) \qquad (20)$$

    - Similarly, the upper limit $x = b$ correspond to

$$x_G = 1$$

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- How to Apply Gauss Quadrature
  - Transformation of variables
    - These values can be substituted into Eq. 19 to give

$$x = A + Bx_G$$

$$b = A + B(1) \qquad (21)$$

    - Solving Eqs. 20 and 21 simultaneously, gives

$$A = \frac{b+a}{2} \quad \text{and} \quad B = \frac{b-a}{2} \qquad (22)$$

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- How to Apply Gauss Quadrature
  - Transformation of variables
    - Substituting for A and B into Eq. 19, yields the following transformation equation:

$$x = \frac{b+a}{2} + \frac{b-a}{2} x_G \qquad (23)$$

    - And this equation can be differentiated to give

$$dx = \frac{b-a}{2} dx_G \qquad (24)$$

Numerical Integration

Gauss Quadrature Transformation

Original Function		Transformed Function
$I \approx \int_a^b f(x)\,dx$ $x = \frac{b+a}{2} + \frac{b-a}{2}x_G$ $dx = \frac{b-a}{2}dx_G$	$\Longrightarrow$	$I \approx \int_{-1}^{1} f(x_G)\,dx_G$

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- Example 6

  Evaluate the following integral using 2, 3, and 4-point Gauss Quadrature. Compare your results with the true value of

  I = -0.346078:

$$\int_1^3 \frac{\cos x}{1+e^x}x^2\,dx$$

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■ Example 6 (cont'd)

We note that the limits of integration are from 1 to 3, therefore, $a = 1$ and $b = 3$.

So, using Eq. 23 will result in

$$x = \frac{b+a}{2} + \frac{b-a}{2} x_G = \frac{3+1}{2} + \frac{3-1}{2} x_G$$
$$= 2 + x_G$$

Therefore,

$$dx = dx_G$$

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■ Example 6 (cont'd)

And

$$\int_1^3 \frac{\cos x}{1+e^x} x^2 dx = \int_{-1}^{1} \frac{\cos(2+x_G)}{1+e^{2+x_G}} (2+x_G)^2 dx_G = \int_{-1}^{1} f(x_G) dx_G$$

For 2-Point Gauss Quadrature, the following equation applies

$$I = \int_{-1}^{1} f(x_G) dx_G = C_1 f(x_1) + C_2 f(x_2)$$

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■ Example 6 (cont'd)

Table 2 gives

$$C_1 = 1 \qquad x_1 = -0.577350$$
$$C_2 = 1 \qquad x_2 = 0.577350$$

We need to evaluate $f(x_G)$ for x_1 and x_2:

$$f(x_G) = \frac{\cos(2 + x_G)}{1 + e^{2+x_G}}(2 + x_G)^2$$

$$f(-0.57735) = \frac{\cos(2 - 0.57735)}{1 + e^{2-0.57735}}(2 - 0.57735)^2 = 0.058030$$

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■ Example 6 (cont'd)

$$f(0.57735) = \frac{\cos(2 + 0.57735)}{1 + e^{2+0.57735}}(2 + 0.57735)^2 = -0.396341$$

For two-point Gauss Quadrature:

$$\int_1^3 \frac{\cos x}{1 + e^x} x^2 = \int_{-1}^{1} f(x_G) dx_G = C_1 f(x_1) + C_2 f(x_2)$$
$$= (1)(0.058030) + (1)(-0.396341)$$
$$= \boxed{-0.338311}$$

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■ Example 6 (cont'd)

For 3-Point Gauss Quadrature, the following equation applies

$$I = \int_{-1}^{1} f(x_G)\,dx_G = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3)$$

Table 2 gives

$$\begin{aligned} C_1 &= 0.555555 & x_1 &= -0.774597 \\ C_2 &= 0.888888 & x_2 &= 0 \\ C_3 &= 0.555555 & x_3 &= 0.774597 \end{aligned}$$

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■ Example 6 (cont'd)

We need to evaluate $f(x_G)$ for x_1, x_2 and x_3:

$$f(x_G) = \frac{\cos(2 + x_G)}{1 + e^{2 + x_G}}(2 + x_G)^2$$

$$f(-0.774597) = \frac{\cos(2 - 0.774597)}{1 + e^{2 - 0.774597}}(2 - 0.774597)^2 = 0.115399$$

$$f(0) = \frac{\cos(2 + 0)}{1 + e^{2 + 0}}(2 + 0)^2 = -0.198424$$

$$f(0.774597) = \frac{\cos(2 + 0.774597)}{1 + e^{2 + 0.774597}}(2 + 0.774597)^2 = -0.421893$$

Numerical Integration

- Example 6 (cont'd)

  For three-point Gauss Quadrature:

$$\int_1^3 \frac{\cos x}{1+e^x} x^2 = \int_{-1}^{1} f(x_G)dx_G = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3)$$

$$= (0.555555)(0.115399) + (0.888888)(-0.198424) + (0.555555)(-0.421893)$$

$$= \boxed{-0.346651}$$

Numerical Integration

- Example 6 (cont'd)

  For 4-Point Gauss Quadrature, the following equation applies

$$I = \int_{-1}^{1} f(x_G)dx_G = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3) + C_4 f(x_4)$$

  Table 2 gives

$$\begin{array}{ll} C_1 = 0.347854 & x_1 = -0.861136 \\ C_2 = 0.652145 & x_2 = -0.339981 \\ C_3 = 0.652145 & x_3 = 0.339981 \\ C_4 = 0.347854 & x_4 = 0.861136 \end{array}$$

Numerical Integration

■ Example 6 (cont'd)

We need to evaluate $f(x_G)$ for x_1, x_2, x_3, and x_4:

$$f(x_G) = \frac{\cos(2 + x_G)}{1 + e^{2+x_G}}(2 + x_G)^2$$

$$f(-0.861136) = \frac{\cos(2 - 0.861136)}{1 + e^{2-0.861136}}(2 - 0.861136)^2 = 0.131684$$

$$f(-0.339981) = \frac{\cos(2 - 0.339981)}{1 + e^{2-0.339981}}(2 - 0.339981)^2 = -0.039228$$

$$f(0.339981) = \frac{\cos(2 + 0.339981)}{1 + e^{2+0.339981}}(2 + 0.339981)^2 = -0.334635$$

$$f(0.861136) = \frac{\cos(2 + 0.861136)}{1 + e^{2+0.861136}}(2 + 0.861136)^2 = -0.425632$$

Numerical Integration

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■ Example 6 (cont'd)

For four-point Gauss Quadrature:

$$\int_1^3 \frac{\cos x}{1 + e^x} x^2 = \int_{-1}^{1} f(x_G) dx_G = C_1 f(x_1) + C_2 f(x_2) + C_3 f(x_3) + C_4 f(x_3)$$

$$= (0.347854)(0.131684) + (0.652145)(-0.039228)$$

$$+ (0.652145)(-0.334635) + (0.347854)(-0.425632)$$

$$= \boxed{-0.346064}$$

Numerical Integration

- Example 6 (cont'd)

  Comparison:

	Gauss Quadrature			True
	$n = 2$	$n = 3$	$n = 4$	
I	-0.338311	-0.346651	-0.346064	-0.346078
% error	2.24	0.166	0.004	0.0

Numerical Integration $\int_1^3 \frac{\cos x}{1+e^x} x^2 dx$

- Comparison Among the Methods

	Gauss Quadrature			True
	$n = 2$	$n = 3$	$n = 4$	
I	-0.338311	-0.346651	-0.346064	-0.346078
% error	2.24	0.166	0.004	0.0

	Trapezoidal Rule			True
	$n = 3$	$n = 5$	$n = 9$	
I	-0.337049	-0.343924	-0.345543	-0.346078
% error	2.61	0.62	0.15	0.0

	Simpson's 3/8 Rule		True
	$n = 4$	$n = 7$	
I	-0.350335	-0.346135	-0.346078
% error	1.23	0.016	0.0

	Simpson's 1/3 Rule			True
	$n = 3$	$n = 5$	$n = 9$	
I	-0.356982	-0.346215	-0.346083	-0.346078
% error	3.151	0.040	0.001	0.0