9 – Numerical Integration

Numerical integration is a frequently-needed tool. Engineers and scientists typically visualize integration as the process of determining the area under a curve. This visualization tool will be employed here to describe four numerical integration methods:

- Rectilinear Rule
- Trapezoidal Rule
- Simpson's Rules: 1/3 and 3/8
- Gaussian-Quadrature Method.

The Gaussian Quadrature Method requires knowing the function that is being integrated. The other methods do not require the function but rather values of the function at regular values of the independent variable as might be obtained from tabular values, system measurements, regular evaluations of a very-difficult-to-analytically-integrate function, and many other sources.

9.1 - Rectilinear Rule

The Rectilinear Rule is a method for approximating the area under a curve given values of the function at regular intervals. The distance between each regularly-spaced value is called the panel width, h. The area of that corresponding panel is approximated by assuming the value of the function is constant over the width of the panel. Usually the starting value of the function is assumed to be the constant value of the function as shown in Figure 1. However, one could also use the ending or left-side value of the function for the panel height. For N values of the function, there are N-1 panels. The i^{th} panel has an area of $h*f(x_i)$. Summing the area of these panels gives the area approximation, I, to be

$$I \simeq h\sum_{i=0}^{N-1} f(x_i) \tag{9.1}$$

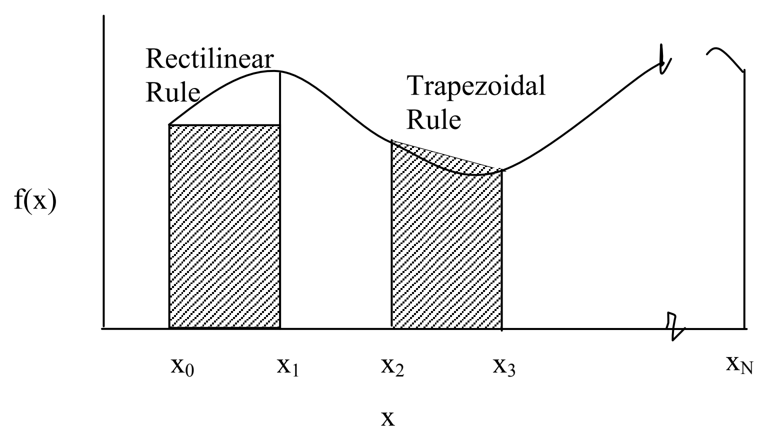

Figure 1 – Graphical Illustration of the Rectilinear and Trapezoid Rules

Since the Rectilinear Rule uses only one point to approximate the function being integrated, it is a zeroth order approximation of the area of each panel. The error in such an approximation is on the order of O(h), which is to say that the error in that approximation decreases proportionally with decreasing step size, h.

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9.2 – Trapezoidal Rule

The Trapezoidal Rule improves the Rectilinear Rule approximation by using the average height of the right and left side of the panel. This creates a trapezoid as shown in Figure 1. The approximation of the area from x_0 to x_N is then

$$I \simeq h\sum_{i=0}^{N-1}\frac{f(x_i)+f(x_{i+1})}{2} \tag{9.1}$$

Since the Trapezoidal Rule uses two points to approximate the function being integrated, it is a linear, or a first order, approximation of the area of each panel. The error in such an approximation is on the order of $O(h^2)$. Therefore, compared to the Rectilinear Rule, the Trapezoidal Rule approximation improves more rapidly with decreasing step size, h.

9.3 - Simpson's Integration

A much more accurate way than either the Rectilinear Rule or Trapezoidal Rule to determine areas is by Simpson's Rules. The two commonly used Simpson's Rules are

- 1/3 Rule
- 3/8 Rule.

Simpson's 1/3 Rule: This method is based on placing a cubic approximation of a function being integrated using Newton's Difference Equation. Figure 2 shows the four regularly-spaced data points through which a cubic approximation is passed. The cubic approximation is then integrated from x_0 to x_2 (not x_3) to yield the area of the first two panels shown in cross hatch. The method is then repeated for additional groups of two panels starting next at x_2.

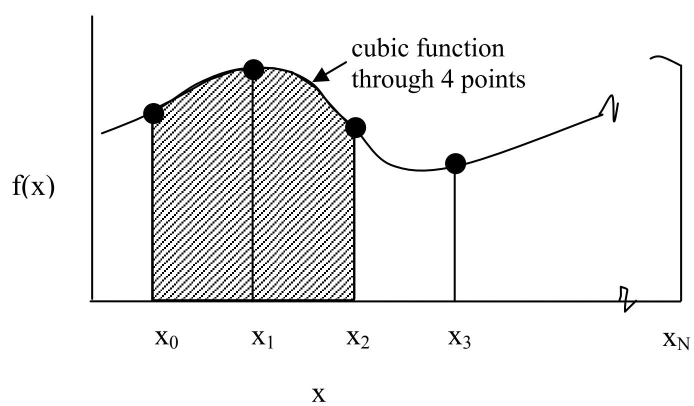

Figure 2 - A Plot Showing the Simpson's Rule Method

The derivation for the area of the first two panels is

$$I = \int_{x_0}^{x_2} f(x)dx \tag{9.2}$$

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where f(x) is approximated as a 3rd order function

$$f(x) \approx f(x_0) + \frac{\Delta f(x_0)(x - x_0)}{h} + \frac{\Delta^2 f(x_0)(x - x_0)(x - x_1)}{2!h^2} + \frac{\Delta^3 f(x_0)(x - x_0)(x - x_1)(x - x_2)}{3!h^3} \qquad (9.3)$$

The term α is introduced to simplify the integration

$$\alpha = \frac{(x - x_0)}{h} \qquad (9.4)$$

to give

$$I \approx h\int_0^2 \left(f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)\alpha(\alpha - 1)}{2!} + \frac{\Delta^3 f(x_0)\alpha(\alpha - 1)(\alpha - 2)}{3!} \right) d\alpha \qquad (9.5)$$

Integration gives

$$I \approx h\left[2f(x_0) + 2(f(x_1) - f(x_0)) + \frac{1}{3}(f(x_2) - 2f(x_1) + f(x_0)) \right] \qquad (9.6)$$

Terms are collected to give Simpson's 1/3 Rule.

$$I \approx \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2) \right] \qquad (9.7)$$

It is interesting to note that the value of x_3 vanishes from the result. That is, the value of $f(x_3)$ needed for the cubic approximation does not appear in the resulting equation for the area. This means that the accuracy of a cubic approximation is obtained with only the computation effort required for a quadratic approximation. This feature can be shown to occur for every odd power approximation (5th order approximation integrated from x_0 to x_4 or a 7th order approximation integrated from x_0 to x_6.) This conservation of effort makes Simpson 1/3 Rule Integration very useful and widely used. A more detailed derivation of Simpson's 1/3 Rule is shown in Example 9a.

Simpson's 3/8's Rule: The same idea as above for the 1/3 Rule is used to obtain Simpson's 3/8's Rule. However, the integration proceeds from α = 0 to 3 to yield

$$I \approx \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right] \qquad (9.8)$$

It is worth noting that Eq. (9.8) consists of the sum of eight estimates of the three panels' heights divided by 8. This gives a weighted average of the three panels' height. Multiplying by the term "3h" gives the area approximation for the three panels. The same feature occurs with the 1/3 Rule in which there are six approximations of the panels' heights. The factor 2h/6 has been reduced to h/3 in Eq. (9.7).

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Simpson's Rule Errors: The error in Simpson's Rules may be determined by adding an order of the error term to the above function approximations and carrying the terms through to Eqs. (9.7) and (9.8). Table 1 shows the magnitude of the errors for both a panel width h and for an interval a to b. Note that h = (b-a)/2 for the 1/3 Rule and (b-a)/3 for the 3/8 Rule.

Comparing the denominators over the interval shows that the error of the 1/3 Rule is slightly more than double the error over the same interval using the 3/8 Rule. However, this is not a fair comparison since one is not comparing a given set of panels of fixed h. What should be compared is the sequential use of 3 sets of two panels using the 1/3 Rule to two sets of three panels using the 3/8 Rule so as to integrate over the same six panels. However, even this is not a definitive measure of advantage because the computational effort for a given error is the goal and three applications of the 1/3 Rule do not equal the effort required for two applications of the 3/8 Rule. In practice, Simpson's 1/3 Rule is normally applied across the entire set of panels unless there are an odd number of panels in which case the last three panels are integrated using the Simpson's 3/8 Rule. In the case of equal-sized panels, Simpson's 3/8 Rule has an error 2.25 times larger than Simpson's 1/3 Rule assuming the same value of the fourth derivative. For a fixed interval divided into either two panels for Simpson's 1/3 Rule or three panels for Simpson's 3/8 Rule, the 3/8 Rule error is 3.38 times larger than the 1/3 Rule error assuming the fourth derivative is the same.

Table 1. Errors in Simpson Rule Integration

Rule	Minimum panels (2 or 3)	Over interval (a to b)
1/3	$-\frac{1}{90}h^5 f''''(\xi)$	$-\frac{(a-b)^5}{2^5 * 90} f''''(\xi)$
3/8	$-\frac{3}{80}h^5 f''''(\xi)$	$-\frac{(a-b)^5}{3^4 * 80} f''''(\xi)$

9.4 - Gaussian Quadrature Over the Interval -1 to +1

Gaussian Quadrature is a method of performing numerical integration of f(x) over the interval from -1 to +1. Unlike the previous methods, Gaussian Quadrature requires the function, not simply tabulated data. To gain an understanding of the concept behind the method, it is useful to first consider just the interval from 0 to 1 and to find a location x_0 and a coefficient c_0 such that the integral is approximated using the function

$$I \cong c_0 f(x_0) \tag{9.9}$$

The usefulness of such an approximation is that it requires no analytical integration, which is very useful especially for complicated functions. If the function for which the integral is needed is simply a constant such as f(x) = k, then a value of $c_0 = 1$ and any x_0 will provide an exact value of the integral as shown in Figure 3a. That is,

$$I = c_0 f(x_0) = f(x) = k = \int_{x=0}^{x=1} k\,dx = k \tag{9.10}$$

If this idea is extended to a function consisting of only a linear term, f(x) = kx, then many combinations of c_0 and x_0 could be used in Eq. (9.9) to exactly give the integral {viz. ($c_0 = 1$, $x_0 = 0.5$), ($c_0 = 0.5$, $x_0 = 1$), ..}. Therefore, setting $c_0 = 1$ and $x_0 = 0.5$ would satisfy any function of x containing both a constant and a linear term. Eq. (9.9) will exactly provide the value of the integral of a single quadratic term if $c_0 = 1$ and $x_0 = 1/\sqrt{3}$, but there is no way to use the equation to exactly integrate a function containing both a

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linear and a quadratic term. However, this problem is obviated if the interval is changed from -1 to +1 and Eq. (9.9) is modified to be

$$I \cong c_0 f(x_0) + c_1 f(x_1) \tag{9.11}$$

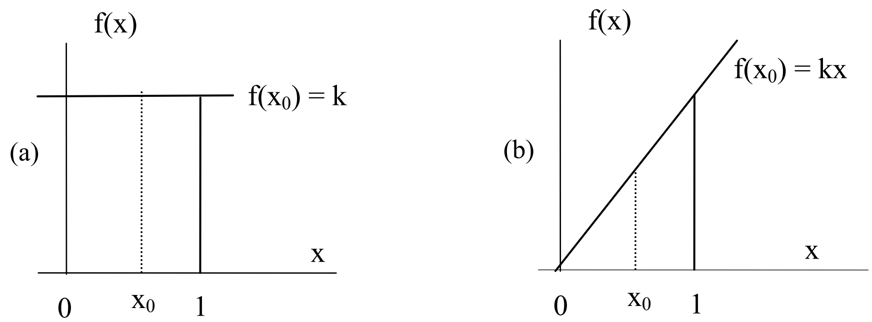

Figure 3. Constant and Linear Functions to be Integrated Using the Gaussian Quadrature Concept

The cleverness of this approach is that Eq. (9.11) will satisfy both the linear and quadratic terms as well as an additional cubic term since the net area of all odd power terms from -1 to + 1 is zero as shown in Figure 4.

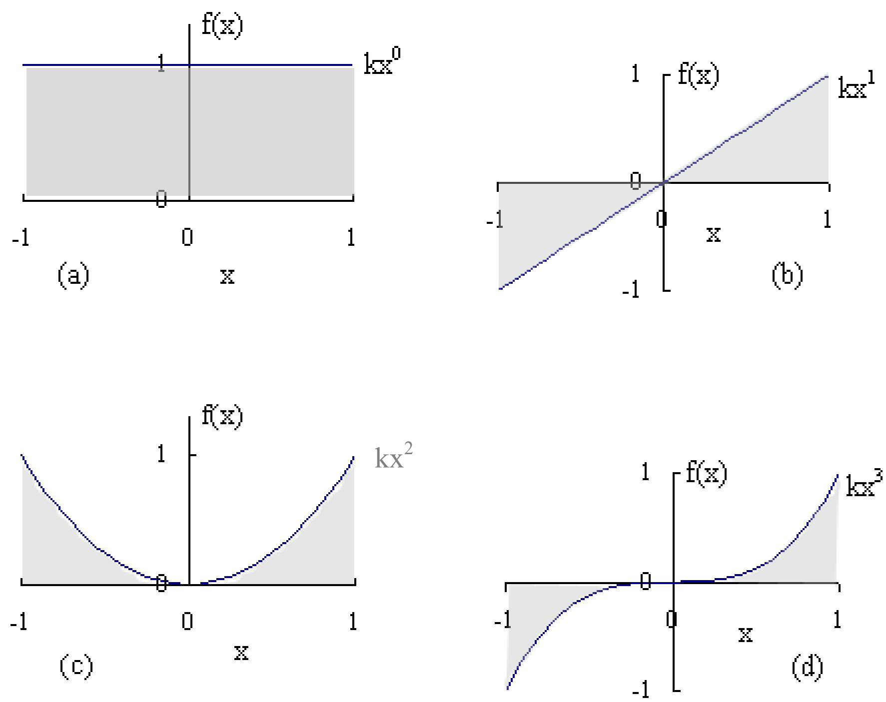

Figure 4. Third Order Polynomial Terms Used to Approximate the Integral of the Function from -1 to +1

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To get the linear and cubic terms to contribute no area, or zeroes in Eq. (9.11), one needs only to make certain that $x_0 = -x_1$ and $c_0 = c_1$. Since any x values will exactly represent constant terms if c_0 and c_1 are unity, the only unique condition that must be satisfied to exactly approximate all terms up to and including the cubic term is the one arising from the quadratic term. Therefore, the following values satisfy all these terms:

$$c_0 = c_1 = 1 \tag{9.12}$$

$$x_0 = -\frac{1}{\sqrt{3}} \tag{9.13}$$

$$x_1 = +\frac{1}{\sqrt{3}} \tag{9.14}$$

The use of these values in concert with Eq. (9.11) provides a cubic approximation of the area from -1 to +1 of any function and has an error of $O(h^4)$.

9.5 - Gaussian Quadrature over the Interval a to b

If one wants to integrate the function f(x) over an interval running from a to b using the Gaussian-Quadrature Method developed above, the variables must be translated to the equivalent range -1 to +1. The variable X will represent the translated x variable and its corresponding function will be F(X). The translation is most easily accomplished by recognizing the difference in the size of the variables based on their relative sizes as shown in Figure 5. This gives

$$\frac{dX}{dx} = \frac{2}{b-a} \tag{9.15}$$

Rearranging and integrating Eq. (9.15) yields

$$X = \frac{2}{b-a}x + c \tag{9.16}$$

The constant, c, may be found since when X = -1, x = a. Alternatively, c could be evaluated from X = 1, x = b. In either case

$$c = X - \frac{2}{b-a}x = -1 - \frac{2}{b-a}(a) = \frac{a-b-2a}{b-a} = \frac{a+b}{a-b} \tag{9.17}$$

Therefore,

$$X = \frac{2}{b-a}x + \frac{a+b}{a-b} \quad \text{and} \quad x = \frac{(b-a)}{2}X + \frac{a+b}{2} \tag{9.18}$$

The area is then

$$I = \int_{x=a}^{x=b} f(x)dx = \left(\frac{b-a}{2}\right)\int_{X=-1}^{X=1} F(X)dX \tag{9.19}$$

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$$\simeq \left(\frac{b-a}{2}\right)\left[f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right)+\frac{a+b}{2}\right) + f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)+\frac{a+b}{2}\right)\right] \tag{9.20}$$

where F(X) is the translated function to be evaluated at $\pm\frac{1}{\sqrt{3}}$ since

$$F\left(\frac{-1}{\sqrt{3}}\right) = f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right)+\frac{a+b}{2}\right)$$
$$F\left(\frac{1}{\sqrt{3}}\right) = f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right)+\frac{a+b}{2}\right) \tag{9.21}$$

In practice there is no need to actually ever perform the variable translation to generate a new function. One needs only to determine the locations of x corresponding to $X=\pm 1/\sqrt{3}$, evaluate f(x) at those locations, add the results, and multiply by the factor (b-a)/2 as indicated in Eq. (9.20).

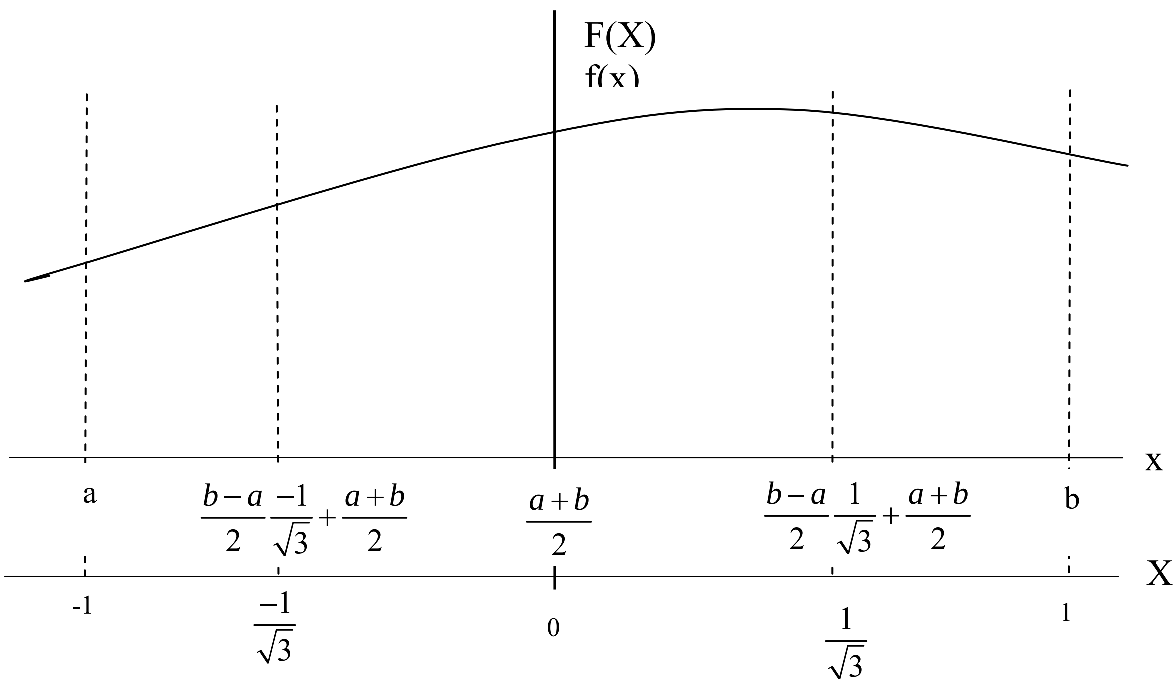

Figure 5. Translation of Variables in Preparation for Gaussian Quadrature over an Interval a to b.

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9.6 - Gaussian-Legendre: Higher Order Approximations

Higher order approximations may be achieved by adding additional terms to Eq. (9.11). Each additional term increases the approximation order by two. When the approximation order moves beyond cubic order, the more general name Gaussian-Legendre Integration is used. Table 1 shows for increasing approximation order the location of the c's and x's for evaluation in the interval –1 to +1 and the order of the error. The c values are commonly called weighting factors and their sum is always 2. Since the area to be determined has a width of 2, the integration may be thought of as 2 times a weighted average of the f(x)

$$I = 2f_{\text{Weighted Ave}}(x) \tag{9.22}$$

Table 1. Weighting Factors and Function Locations for Gaussian-Legendre Integration

Approx Order	Weighting Factors	Evaluation Locations	Order of Error
3	1	$-\sqrt{1/3} =$ - 0.577350269	$f^4(\xi)$
	1	$\sqrt{1/3} =$ 0.577350269	
5	5/9 =0.555555555	$-\sqrt{3/5} =$ - 0.774596669	$f^6(\xi)$
	8/9 =0.888888888	0	
	5/9 =0.555555555	$\sqrt{3/5} =$ 0.774596669	
7	0.347854845	$-\sqrt{\left(15+2\sqrt{30}\right)/35} =$ - 0.861136312*	$f^8(\xi)$
	0.652145155	$-\sqrt{\left(15-2\sqrt{30}\right)/35} =$ - 0.339981044*	
	0.652145155	$\sqrt{\left(15-2\sqrt{30}\right)/35} =$ 0. 339981044*	
	0.347854845	$\sqrt{\left(15+2\sqrt{30}\right)/35} =$ 0. 861136312*	
9	0.171324492	- 0.932469514	$f^{10}(\xi)$
	0.360761573	- 0.661209386	
	0.467913935	- 0.238619186	
	0.467913935	0.238619186	
	0.360761573	0.661209386	
	0.171324492	0.932469514	

* Roots to $x^4 - \frac{6}{7}x^2 + \frac{3}{35} = 0$

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Example 9a

Show all the steps in deriving Simpson's 1/3 Rule.

$$I \approx h\int_0^2 \left(f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)\alpha(\alpha-1)}{2!} + \frac{\Delta^3 f(x_0)\alpha(\alpha-1)(\alpha-2)}{3!} \right) d\alpha$$

$$I \approx h\left[2f(x_0) + \Delta f(x_0)\frac{\alpha^2}{2} + \frac{\Delta^2 f(x_0)\left(\frac{\alpha^3}{3} - \frac{\alpha^2}{2}\right)}{2} + \frac{\Delta^3 f(x_0)\left(\frac{\alpha^4}{4} - \frac{3\alpha^3}{3} + \frac{2\alpha^2}{2}\right)}{6} \right]_0^2$$

$$I \approx h\left[2f(x_0) + \Delta f(x_0)\frac{4}{2} + \frac{\Delta^2 f(x_0)\left(\frac{8}{3} - \frac{4}{2}\right)}{2} + \frac{\Delta^3 f(x_0)(\mathbf{4 - 8 + 4})}{6} \right]$$

$$I \approx h\left[2f(x_0) + 2\Delta f(x_0) + \frac{\Delta^2 f(x_0)}{3} \right]$$

$$I \approx \frac{h}{3}\left[6f(x_0) + 6\Delta f(x_0) + \Delta^2 f(x_0) \right]$$

$$I \approx \frac{h}{3}\left[6f(x_0) + 6(f(x_1) - f(x_0)) + (f(x_2) - 2f(x_1) + f(x_0)) \right]$$

$$I \approx \frac{h}{3}\left[f(x_0) + 4(f(x_1) + f(x_2) \right]$$

Note that the third order term in line 3 becomes zero. This means that $f(x_3)$ is never used in the 3rd-order approximation. That is, the accuracy of a 3rd-order approximation is achieved with the computational effort of a 2nd-order approximation.

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Example 9b

Estimate the

$$\int_2^4 (x^3 - 2x + 4)dx \tag{9.23}$$

using the Gauss Quadrature Method.

The answer is

$$I \cong [F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}})]*(4\text{-}2)/2 = F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}}) \tag{9.24}$$

Where the limits 2 to 4 have been translated to –1 and +1 as follows:

From Eq. (9.18) we know dX = dx. To translate X to x we need only to subtract 3 from x

$$X = x - 3 \tag{9.25}$$

Therefore, substituting for x into Eq. (9.23)

$$f(X) = [(X+3)^3 - 2(X+3) + 4] = X^3 + 9X^2 + 25X + 25 \tag{9.26}$$

Evaluating this function at $X = -\frac{1}{\sqrt{3}}$ and $\frac{1}{\sqrt{3}}$ and substituting into Eq. (9.24) gives the desired result

$$F(-\frac{1}{\sqrt{3}}) = -\frac{1}{3\sqrt{3}} + 3 - \frac{25}{\sqrt{3}} + 25 \tag{9.27}$$

$$F(\frac{1}{\sqrt{3}}) = \frac{1}{3\sqrt{3}} + 3 + \frac{25}{\sqrt{3}} + 25 \tag{9.28}$$

$$I = F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}}) = 56 \tag{9.29}$$

The student may confirm this answer is exact since the original function was cubic. The integration of cubic and lower order functions by the Gaussian Quadrature method will always be exact.

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Example 9c

Estimate the

$$\int_{-5}^{3}(x^2+4)dx \tag{9.30}$$

using the Gaussian-Quadrature method.

The answer is

$$I \cong [F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}})]*(3-(-5))/2 = [F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}})]*4 \tag{9.31}$$

where the limits -5 to 3 have been translated to –1 and +1 using Eq. (9.18)

$$F(X) = (4X-1)^2 + 4 = 16X^2 - 8X + 5 \tag{9.32}$$

Evaluating this function at X = $-\frac{1}{\sqrt{3}}$ and $\frac{1}{\sqrt{3}}$ and substituting into Eq. (9.31) gives the desired result

$$F(-\frac{1}{\sqrt{3}}) = \frac{16}{3} + \frac{8}{\sqrt{3}} + 5 \tag{9.33}$$

$$F(\frac{1}{\sqrt{3}}) = \frac{16}{3} - \frac{16}{\sqrt{3}} + 5 \tag{9.34}$$

$$I = [F(-\frac{1}{\sqrt{3}}) + F(\frac{1}{\sqrt{3}})]*4 = (2*16/3 + 10)*4 = 82.666. \tag{9.35}$$

The student may confirm this answer is exact since the original function was quadratic. The integration of cubic and lower order functions by the Gauss Quadrature method will always be exact.

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Example 9d

Use Eq. (9.11) and analytical integration of a polynomial to find four equations in the four unknowns: x_0, x_1, c_0, and c_1 from which the unknowns can be determined. What is the highest order polynomial that can fit the data using these four constants?

A cubic function requires four coefficients. Therefore, the values of c_0, c_1, x_0, and x_1 may fit up to a cubic equation. To find the four coefficients a term of each power of x from 0 to 3 must fit the coefficients. Therefore, the integrals of each of the following functions must satisfy Eq. (9.11):

$$f_0(x) = 1 \tag{9.36}$$

$$f_1(x) = x \tag{9.37}$$

$$f_2(x) = x^2 \tag{9.38}$$

$$f_3(x) = x^3 \tag{9.39}$$

Substituting each of the above functions into q. (9.11) and each to the analytically-determined integral from -1 to +1 gives

$$c_0(x_0^0) + c_1(x_1^0) = c_0 + c_1 = 2 \tag{9.40}$$

$$c_0(x_0) + c_1(x_1) = 0 \tag{9.41}$$

$$c_0(x_0^2) + c_1(x_1^2) = 2/3 \tag{9.42}$$

$$c_0(x_0^3) + c_1 f(x_1^3) = 0 \tag{9.43}$$

The formal solution would require the solution of a cubic equation but making some assumptions about the nature of the solution leads to the roots. The first assumption derives from the apparent symmetrical nature of the unknowns. From this we might reasonably assume that $c_o = c_1$ in which case they would each equal unity from Eq. (9.40) . Eq. (9.41) requires that $x_o = -x_1$. This assumption for the nature of the c's and the resulting conclusion for the nature of the x's satisfy Eq. (9.43) while Eq. (9.42) provides a means of evaluating the specific values of the x's. Furthermore, since Eq. (9.42) is a quadratic, the roots are of opposite sign but of equal magnitude. Therefore, the x's will be the +/- roots of the quadratic. This feature leads to the solution of Eq. (9.42)

$$c_0 = c_1 = 1 \qquad x_0 = -\frac{1}{\sqrt{3}} \qquad x_1 = \frac{1}{\sqrt{3}} \tag{9.44}$$

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Example 9e

Determine the values of the constants and x values in the equation

$$I = c_a f(x_a) + c_b f(x_b) + c_c f(x_c) \tag{9.45}$$

for 5th order Gaussian-Legendre integration.

The following condition must be met to satisfy the zeroth order term.

$$c_a + c_b + c_c = 2 \tag{9.46}$$

The terms in Eq. (9.45) must be symmetrical so as to satisfy the zero area terms arising from each odd power term; therefore, $x_b = 0$ and $x_a = - x_c$. The determination of the x_a and x_c and their corresponding coefficients is simplified if only the interval from 0 to 1 is considered. In that case the following equations must be satisfied for the quadratic and quartic terms

$$c_c x_c^2 = 1/3 \tag{9.47}$$

$$c_c x_c^4 = 1/5 \tag{9.48}$$

Solving for c and x gives

$$x = 1/\sqrt{5} \tag{9.49}$$

$$c = 5/9 \tag{9.50}$$

Therefore the integration from x = -1 to 1 is given by

$$I = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + c_b f(x_b) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

This equation satisfies order 1, 2, 3, and 4 terms in the function. To satisfy the zeroth–order term, the sum must be 2 times the constant value of the zeroth-order term. Therefore,

$$c \ = 8/9$$

Then, $x_b = 0$ to preserve the correct areas for all higher-order terms.

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Example 9f

Write the equations that must be satisfied for 7th order Gaussian-Legendre integration.

$$I = c_a f(x_a) + c_b f(x_b) + c_c f(x_c) + c_d f(x_d) \quad (9.51)$$

The solution will be symmetrical; therefore $x_a = - x_d$, $x_b = - x_c$, $c_a = c_d$, and $c_b = c_c$. For the interval x = 0 to 1,

The quadratic term requires that

$$c_c x_c^{\,2} + c_d x_d^{\,2} = 1/3 \quad (9.52)$$

The quartic term requires that

$$c_c x_c^{\,4} + c_d x_d^{\,4} = 1/5 \quad (9.53)$$

The sextic term requires that

$$c_c x_c^{\,6} + c_d x_d^{\,6} = 1/7 \quad (9.54)$$

The constant term requires that

$$c_c + c_d = 1 \quad (9.55)$$

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