Numerical Analysis

10th ed

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Beamer Presentation Slides
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Three-Point Formulas

THREE-POINT ENDPOINT FORMULA

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\xi_0),$$

where ξ_0 lies between x_0 and $x_0 + 2h$.

THREE-POINT MIDPOINT FORMULA

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1),$$

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Five-Point Formulas

FIVE-POINT MIDPOINT FORMULA

$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30}f^{(5)}(\xi),$$

where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

FIVE-POINT ENDPOINT FORMULA

$$\begin{aligned} f'(x_0) &= \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) \\ &\quad + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5}f^{(5)}(\xi), \end{aligned}$$

where ξ lies between x_0 and $x_0 + 4h$.

SECOND DERIVATIVE MIDPOINT FORMULA

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi),$$

for some ξ, where $x_0 - h < \xi < x_0 + h$. If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, and the approximation is $O(h^2)$.

NOTE: It is particularly important to pay attention to round-off error when approximating derivatives.

ERROR - INSTABILITY

The total error in the approximation,

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1),$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M.$$

To reduce the truncation error, $h^2 M/6$, we need to reduce h. But as h is reduced, the round-off error ε/h grows. In practice, then, it is seldom advantageous to let h be too small, because in that case the round-off error will dominate the calculations.

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas.

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size h.

Richardson's Extrapolation

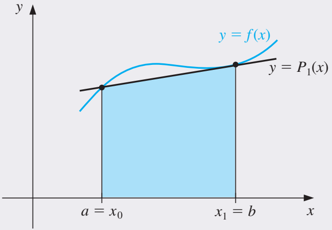
The YouTube video developed by Douglas Harder can serve as a good illustration of the Richardson's Extrapolation for students. Richardson's Extrapolation Video

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating $\int_a^b f(x)\,dx$ is called **numerical quadrature**. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

Trapezoidal Rule

$$\int_a^b f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

This is called the Trapezoidal rule because when f is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in the figure below.



Trapezoidal Rule

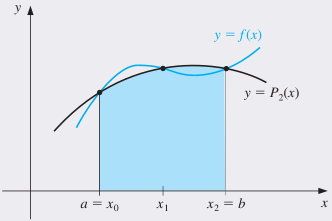
The YouTube video developed by Mathispower4u can serve as a good illustration of the Trapezoidal Rule for students.

Trapezoidal Rule Video

Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$.

$$\int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi).$$



Simpson's Rule

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

The YouTube video developed by Exam Solutions can serve as a good illustration of the Simpson's Rule for students.

▸ Simpson's Rule Video

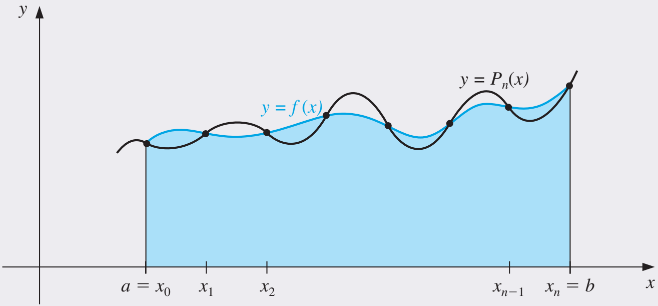
Definition

4.1 The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.

- Definition 4.1 implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.
- The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.
- The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

Closed Newton-Cotes Formulas

The $(n+1)$*-point closed Newton-Cotes formula* uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. (See Figure) It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes.



Theorem (4.2: Closed Newton-Cotes Formulas)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b-a)/n$. There exists $\xi \in (a,b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt,$$

if n is even and $f \in C^{n+2}[a,b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt,$$

if n is odd and $f \in C^{n+1}[a,b]$.

Common Closed Newton-Cotes Formulas

- $n=1$: Trapezoidal rule where $x_0 < \xi < x_1$

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0)+f(x_1)] - \frac{h^3}{12}f''(\xi).$$

- $n=2$: Simpson's rule where $x_0 < \xi < x_2$

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] - \frac{h^5}{90}f^{(4)}(\xi).$$

- $n=3$: Simpson's Three-Eighths where $x_0 < \xi < x_3$

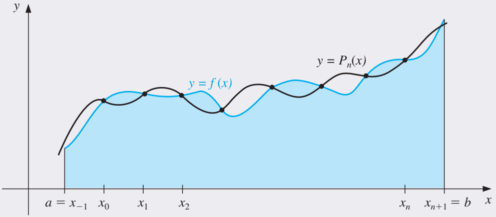
$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)] - \frac{3h^5}{80}f^{(4)}(\xi).$$

- $n=4$: where $x_0 < \xi < x_4$

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)] - \frac{8h^7}{945}f^{(6)}(\xi).$$

Open Newton-Cotes Formulas

The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as shown in the figure. Open formulas contain all the nodes used for the approximation within the open interval (a, b).



Common Open Newton-Cotes Formulas

- $n = 0$: Midpoint rule $\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi), \quad x_{-1} < \xi < x_1.$
- $n = 1$: $\int_{x_{-1}}^{x_2} f(x)\,dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(\xi), \quad x_{-1} < \xi < x_2.$
- $n = 2$:

$$\int_{x_{-1}}^{x_3} f(x)\,dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45}f^{(4)}(\xi), \quad x_{-1} < \xi < x_3.$$

- $n = 3$:

$$\int_{x_{-1}}^{x_4} f(x)\,dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95}{144}h^5 f^{(4)}(\xi),\ x_{-1} < \xi < x_4.$$

Theorem (4.3)

Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point open Newton-Cotes formula with $x_{-1} = a$, $x_{n+1} = b$, and $h = (b-a)/(n+2)$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt,$$

if n is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt,$$

if n is odd and $f \in C^{n+1}[a, b]$.

Theorem (4.4)

Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the ***Composite Simpson's rule*** *for n subintervals can be written with its error term as*

$$\int_a^b f(x)\, dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180} h^4 f^{(4)}(\mu).$$

Choose an even integer n. Subdivide the interval $[a, b]$ into n subintervals, and apply Simpson's rule on each consecutive pair of subintervals. (See Figure 4.7)

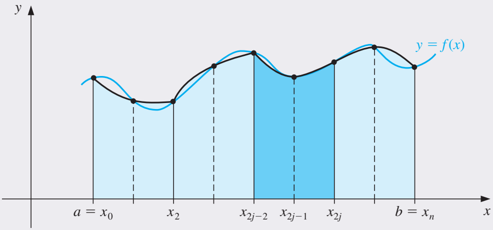


Figure: Figure 4.7

The error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule. However, these rates are not comparable because for standard Simpson's rule we have h fixed at $h = (b - a)/2$, but for Composite Simpson's rule we have $h = (b - a)/n$, for n an even integer. This permits us to considerably reduce the value of h.

Algorithm 4.1: COMPOSITE SIMPSON'S RULE

To approximate the integral $I = \int_a^b f(x)\,dx$:

INPUT endpoints a, b; even positive integer n.
OUTPUT approximation XI to I.
Step 1 Set $h = (b - a)/n$.
Step 2 Set $XI0 = f(a) + f(b)$;
$XI1 = 0$; (*Summation of* $f(x_{2i-1})$.)
$XI2 = 0$. (*Summation of* $f(x_{2i})$.)
Step 3 For $i = 1, \ldots, n - 1$ do Steps 4 and 5.
Step 4 Set $X = a + ih$.
Step 5 If i is even then set $XI2 = XI2 + f(X)$
else set $XI1 = XI1 + f(X)$.
Step 6 Set $XI = h(XI0 + 2 \cdot XI2 + 4 \cdot XI1)/3$.
Step 7 OUTPUT (XI);
STOP.

Theorem (4.5)

Let $f \in C^2[a,b]$, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the ***Composite Trapezoidal rule*** *for n subintervals can be written with its error term as*

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu).$$

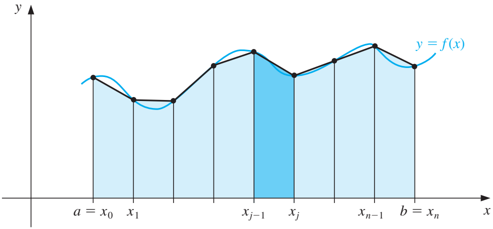
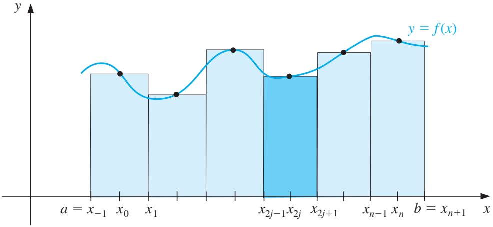


Figure 4.8

Theorem (4.6)

Let $f \in C^2[a,b]$, n be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$ for each $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ for which the ***Composite Midpoint rule****(see also composite midpoint rule) for $n+2$ subintervals can be written with its error term as*

$$\int_a^b f(x)\,dx = 2h\sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6}h^2 f''(\mu).$$



Recall from Section 4.2 that Richardson extrapolation can be performed on any approximation procedure whose truncation error is of the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants K_j and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$. In that section we gave demonstrations to illustrate how effective this techniques is when the approximation procedure has a truncation error with only even powers of h, that is, when the truncation error has the form.

$$\sum_{j=1}^{m-1} K_j h^{2j} + O(h^{2m}).$$

Because the Composite Trapezoidal rule has this form, it is an obvious candidate for extrapolation. This results in a technique known as **Romberg integration**.

To approximate the integral $\int_a^b f(x)\,dx$ we use the results of the Composite Trapezoidal Rule with $n = 1, 2, 4, 8, 16, \ldots$, and denote the resulting approximations, respectively, by $R_{1,1}$, $R_{2,1}$, $R_{3,1}$, etc. We then apply extrapolation in the manner given in Section 4.2, that is, we obtain $O(h^4)$ approximations $R_{2,2}$, $R_{3,2}$, $R_{4,2}$, etc, by

$$R_{k,2} = R_{k,1} + \frac{1}{3}(R_{k,1} - R_{k-1,1}), \quad \text{for } k = 2, 3, \ldots$$

Then $O(h^6)$ approximations $R_{3,3}$, $R_{4,3}$, $R_{5,3}$, etc, by

$$R_{k,3} = R_{k,2} + \frac{1}{15}(R_{k,2} - R_{k-1,2}), \quad \text{for } k = 3, 4, \ldots.$$

In general, after the appropriate $R_{k,j-1}$ approximations have been obtained, we determine the $O(h^{2j})$ approximations from

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1} - 1}(R_{k,j-1} - R_{k-1,j-1}), \quad \text{for } k = j, j+1, \ldots$$

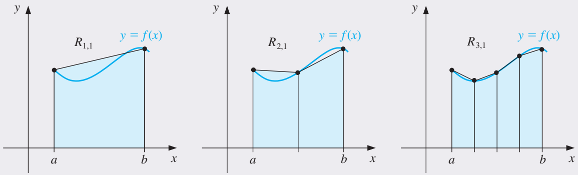


Figure: Figure 4.10 and Table 4.10

k	$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$		$O(h_k^{2n})$
1	$R_{1,1}$					
2	$R_{2,1}$	$R_{2,2}$				
3	$R_{3,1}$	$R_{3,2}$	$R_{3,3}$			
4	$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
n	$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\cdots$	$R_{n,n}$

Algorithm 4.2: ROMBERG INTEGRATION

To approximate the integral $I = \int_a^b f(x)\,dx$, select an integer $n > 0$.

INPUT endpoints a, b; integer n.
OUTPUT an array R. (*Compute R by rows; only the last 2 rows are saved in storage.*)
Step 1 Set $h = b - a$;
$R_{1,1} = \frac{h}{2}(f(a) + f(b))$.
Step 2 OUTPUT $(R_{1,1})$.
Step 3 For $i = 2, \ldots, n$ do Steps 4–8.
Step 4 Set $R_{2,1} = \frac{1}{2}\left[R_{1,1} + h\sum_{k=1}^{2^{i-2}} f(a + (k - 0.5)h)\right]$.
(*Approximation from Trapezoidal method.*)
Step 5 For $j = 2, \ldots, i$
set $R_{2,j} = R_{2,j-1} + \frac{R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1}$. (*Extrapolation.*)
Step 6 OUTPUT $(R_{2,j}$ for $j = 1, 2, \ldots, i)$.
Step 7 Set $h = h/2$.
Step 8 For $j = 1, 2, \ldots, i$ set $R_{1,j} = R_{2,j}$. (*Update row 1 of R.*)
Step 9 STOP.

- Composite formulas very effective in most situations, but suffer occasionally from requirement of equally-spaced nodes.
- Inappropriate when integrating a function on an interval containing regions with both large and small functional variation.
- How can we determine what technique should be applied on various portions of the interval of integration
- How accurate can we expect the final approximation to be?

An efficient technique for this type of problem should predict the amount of functional variation and adapt the step size as necessary. These methods are called **Adaptive quadrature methods**.

Algorithm 4.3: ADAPTIVE QUADRATURE

To approximate the integral $I = \int_a^b f(x)\,dx$ to within a given tolerance:

INPUT endpoints a, b; tolerance TOL; limit N to number of levels.
OUTPUT approximation APP or message that N is exceeded.
Step 1 Set $APP = 0$;
$i = 1$;
$TOL_i = 10\ TOL;\ a_i = a;\ h_i = (b-a)/2;\ FA_i = f(a);\ FC_i = f(a+h_i)$;
$FB_i = f(b)$;
$S_i = h_i(FA_i + 4FC_i + FB_i)/3$; (*Approx. from Simpson's for entire interval*)
$L_i = 1$.
Step 2 While $i > 0$ do Steps 3–5.
Step 3 Set $FD = f(a_i + h_i/2)$;
$FE = f(a_i + 3h_i/2)$;
$S1 = h_i(FA_i + 4FD + FC_i)/6$; (*Approximations from Simpson's method for halves of subintervals.*)
$S2 = h_i(FC_i + 4FE + FB_i)/6$; $v_1 = a_i$; (*Save data at this level.*)
$v_2 = FA_i;\ v_3 = FC_i;\ v_4 = FB_i;\ v_5 = h_i;\ v_6 = TOL_i;\ v_7 = S_i;\ v_8 = L_i$.
Step 4 Set $i = i - 1$. (*Delete the level.*)

Algorithm 4.3: ADAPTIVE QUADRATURE CONTINUED

Step 5 If $|S1 + S2 - v_7| < v_6$
then set $APP = APP + (S1 + S2)$
else
if $(v_8 \geq N)$
then
OUTPUT ('LEVEL EXCEEDED'); (*Procedure fails.*)
STOP.
else (*Add one level.*)
set $i = i + 1$; (*Data for right half subinterval.*)
$a_i = v_1 + v_5$; $FA_i = v_3$; $FC_i = FE$; $FB_i = v_4$;
$h_i = v_5/2$; $TOL_i = v_6/2$;
$S_i = S2$; $L_i = v_8 + 1$;
set $i = i + 1$; (*Data for left half subinterval.*)
$a_i = v_1$;
$FA_i = v_2$; $FC_i = FD$; $FB_i = v_3$;
$h_i = h_{i-1}$; $TOL_i = TOL_{i-1}$;
$S_i = S1$; $L_i = L_{i-1}$.

Step 6 OUTPUT (APP); (*APP approximates I to within TOL.*)
STOP.

Consider the Trapezoidal rule applied to determine the integrals of the functions whose graphs are shown in Figure 4.15.
The Trapezoidal rule approximates the integral of the function by integrating the linear function that joins the endpoints of the graph of the function.

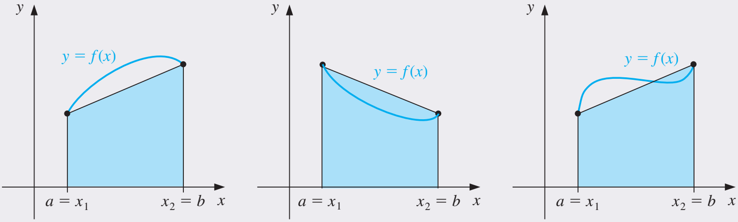


Figure: Figure 4.15

But this is not likely the best line for approximating the integral. Lines such as those shown in Figure 4.16 would likely give much better approximations in most cases.

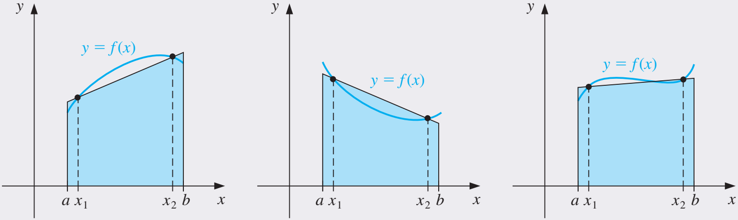


Figure: Figure 4.16

In Gaussian quadrature the points for evaluation are chosen in an optimal, rather than equally-spaced, way. The nodes $x_1, x_2, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, c_2, \ldots, c_n$, are chosen to minimize the expected error obtained in the approximation

$$\int_a^b f(x)\, dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

The YouTube video developed by Wen Shen can serve as a good illustration of the introduction to Gaussian Quadrature for students. ▸ Illustration Introducing Gaussian Quadrature

The nodes $x_1, x_2, \ldots, x_n$ needed to produce an integral approximation formula that gives exact results for any polynomial of degree less than $2n$ are the roots of the nth-degree Legendre polynomial. (See Theorem 4.7.)

Theorem (4.7)

Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers c_i are defined by

$$c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j}\, dx.$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\, dx = \sum_{i=1}^{n} c_i P(x_i).$$

Algorithm 4.4: SIMPSON'S DOUBLE INTEGRAL

To approximate the integral $I = \int_a^b \int_{c(x)}^{d(x)} f(x, y)\, dy\, dx$:

INPUT endpoints a, b: even positive integers m, n.
OUTPUT approximation J to I.
Step 1 Set $h = (b - a)/n$;
$J_1 = 0$; (*End terms.*) $J_2 = 0$; (*Even terms.*) $J_3 = 0$. (*Odd terms.*)
Step 2 For $i = 0, 1, \ldots, n$ do Steps 3–8.
Step 3 Set $x = a + ih$; (*Composite Simpson's method for* x.)
$HX = (d(x) - c(x))/m$;
$K_1 = f(x, c(x)) + f(x, d(x))$; (*End terms.*)
$K_2 = 0$; (*Even terms.*) $K_3 = 0$. (*Odd terms.*)
Step 4 For $j = 1, 2, \ldots, m - 1$ do Step 5 and 6.
Step 5 Set $y = c(x) + jHX$; $Q = f(x, y)$.
Step 6 If j is even then set $K_2 = K_2 + Q$ else set $K_3 = K_3 + Q$.
Step 7 Set $L = (K_1 + 2K_2 + 4K_3)HX/3$.
$\left(L \approx \int_{c(x_i)}^{d(x_i)} f(x_i, y)\, dy \quad \textit{by the Composite Simpson's method}.\right)$
Step 8 If $i = 0$ or $i = n$ then set $J_1 = J_1 + L$
else if i is even set $J_2 = J_2 + L$
else set $J_3 = J_3 + L$. (*End Step 2*)
Step 9 Set $J = h(J_1 + 2J_2 + 4J_3)/3$.
Step 10 OUTPUT (J);
STOP.

Algorithm 4.5: GAUSSIAN DOUBLE INTEGRAL

INPUT endpoints a, b; positive integers m, n.
(*The roots* $r_{i,j}$ *and coefficients* $c_{i,j}$ *need to be available for* $i = \max\{m, n\}$ *and for* $1 \leq j \leq i$.)

OUTPUT approximation J to I.

Step 1 Set $h_1 = (b - a)/2$;
$h_2 = (b + a)/2$;
$J = 0$.

Step 2 For $i = 1, 2, \ldots, m$ do Steps 3–5.

Step 3 Set $JX = 0$;
$x = h_1 r_{m,i} + h_2$; $d_1 = d(x)$; $c_1 = c(x)$;
$k_1 = (d_1 - c_1)/2$; $k_2 = (d_1 + c_1)/2$.

Step 4 For $j = 1, 2, \ldots, n$ do
set $y = k_1 r_{n,j} + k_2$;
$Q = f(x, y)$;
$JX = JX + c_{n,j} Q$.

Step 5 Set $J = J + c_{m,i} k_1 JX$. *(End Step 2)*

Step 6 Set $J = h_1 J$.

Step 7 OUTPUT (J);
STOP.

Algorithm 4.6: GAUSSIAN TRIPLE INTEGRAL

To approximate the integral $\int_a^b \int_{c(x)}^{d(x)} \int_{\alpha(x,y)}^{\beta(x,y)} f(x, y, z)\, dz\, dy\, dx$:

INPUT endpoints a, b; positive integers m, n, p.
 (*The roots* $r_{i,j}$ *and coefficients* $c_{i,j}$ *need to be available for* $i = \max\{n, m, p\}$ *and for* $1 \le j \le i$.)
OUTPUT approximation J to I.
Step 1 Set $h_1 = (b - a)/2$; $h_2 = (b + a)/2$; $J = 0$.
Step 2 For $i = 1, 2, \ldots, m$ do Steps 3–8.
 Step 3 Set $JX = 0$;
  $x = h_1 r_{m,i} + h_2$; $d_1 = d(x)$; $c_1 = c(x)$;
  $k_1 = (d_1 - c_1)/2$; $k_2 = (d_1 + c_1)/2$.
 Step 4 For $j = 1, 2, \ldots, n$ do Steps 5–7.
  Step 5 Set $JY = 0$;
   $y = k_1 r_{n,j} + k_2$; $\beta_1 = \beta(x, y)$; $\alpha_1 = \alpha(x, y)$;
   $l_1 = (\beta_1 - \alpha_1)/2$; $l_2 = (\beta_1 + \alpha_1)/2$.
  Step 6 For $k = 1, 2, \ldots, p$ do
   set $z = l_1 r_{p,k} + l_2$; $Q = f(x, y, z)$; $JY = JY + c_{p,k} Q$.
  Step 7 Set $JX = JX + c_{n,j} l_1 JY$. *(End Step 4)*
 Step 8 Set $J = J + c_{m,i} k_1 JX$. *(End Step 2)*
Step 9 Set $J = h_1 J$.
Step 10 OUTPUT (J);
 STOP.

Left Endpoint Singularity

Consider the situation when the integrand is unbounded at the left endpoint of the interval of integration, as shown in Figure 4.25. In this case we say that f has a **singularity** at the endpoint a. We will then show how other improper integrals can be reduced to problems of this form.

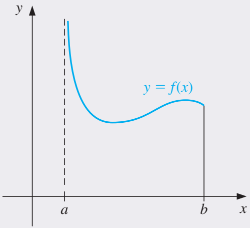


Figure: Figure 4.25

Left Endpoint Singularity

It is shown in calculus that the improper integral with a singularity at the left endpoint,

$$\int_a^b \frac{dx}{(x-a)^p},$$

converges if and only if $0 < p < 1$, and in this case, we define

$$\int_a^b \frac{1}{(x-a)^p}\,dx = \lim_{M \to a^+} \left. \frac{(x-a)^{1-p}}{1-p} \right|_{x=M}^{x=b} = \frac{(b-a)^{1-p}}{1-p}.$$

Right-Endpoint Singularity

To approximate the improper integral with a singularity at the right endpoint, we could develop a similar technique but expand in terms of the right endpoint b instead of the left endpoint a. Alternatively, we can make the substitution

$$z = -x, \qquad dz = -\,dx$$

to change the improper integral into one of the form

$$\int_a^b f(x)\,dx = \int_{-b}^{-a} f(-z)\,dz,$$

Right-Endpoint Singularity

which has its singularity at the left endpoint. Then we can apply the left endpoint singularity technique we have already developed.

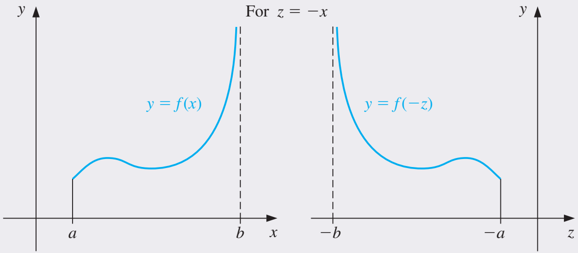


Figure: Figure 4.26

Infinite Singularity

The other type of improper integral involves infinite limits of integration. The basic integral of this type has the form

$$\int_a^{\infty} \frac{1}{x^p}\, dx,$$

for $p > 1$. This is converted to an integral with left endpoint singularity at 0 by making the integration substitution

$$t = x^{-1}, \quad dt = -x^{-2}\, dx, \quad \text{so} \quad dx = -x^2\, dt = -t^{-2}\, dt.$$

Then

$$\int_a^{\infty} \frac{1}{x^p}\, dx = \int_{1/a}^{0} -\frac{t^p}{t^2}\, dt = \int_0^{1/a} \frac{1}{t^{2-p}}\, dt.$$

Infinite Singularity

In a similar manner, the variable change $t = x^{-1}$ converts the improper integral $\int_a^\infty f(x)\, dx$ into one that has a left endpoint singularity at zero:

$$\int_a^\infty f(x)\, dx = \int_0^{1/a} t^{-2} f\left(\frac{1}{t}\right)\, dt.$$

It can now be approximated using a quadrature formula of the type described earlier.