Numerical Differentiation and Integration II

APM1137 - Numerical Analysis

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Composite Numerical Integration

The Newton-Cotes formulas are generally unsuitable for use over large integration intervals. Also, the Newton-Cotes formulas are based on interpolatory polynomials that use equally-spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials.

Here, we will use a piecewise approach to numerical integration that uses the low-order Newton-Cotes formulas.

Example

Use Simpson's rule to approximate $\int_0^4 e^x dx$ and compare this to the results obtained by adding the Simpson's rule approximations for $\int_0^2 e^x dx$ and $\int_2^4 e^x dx$. Compare these approximations to the sum of the Simpson's rule for $\int_0^1 e^x dx$, $\int_1^2 e^x dx$, $\int_2^3 e^x dx$, and $\int_3^4 e^x dx$

Solution

Recall Simpson's Rule

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

On [0,4], Simpson's rule uses $h = 2$ and gives

$$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958$$

Solution cont...

The exact answer in this case is $e^4 - e^0 = 53.59815$, and the error -3.17143 is far larger than we would normally accept.

On [0,2] and [2,4], use $h = 1$

$$\int_0^2 e^x dx + \int_2^1 e^x dx \approx \frac{1}{3}(e^0 + 4e + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4)$$
$$=53.86385$$

The error has been reduced to -0.26570.

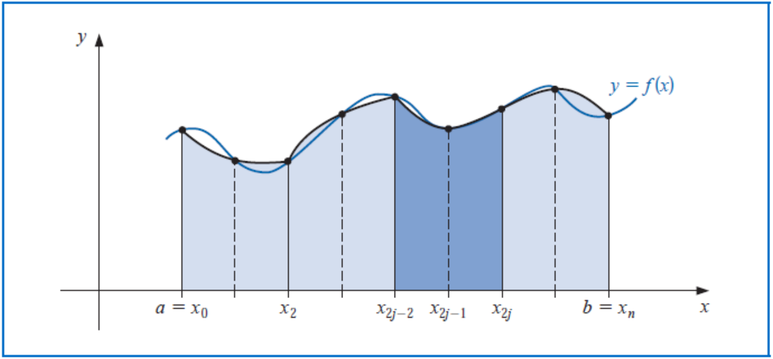
Solution cont...

on [0, 1],[1, 2],[3, 4], and [3, 4] use $h = \frac{1}{2}$

$$\int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx$$
$$\approx \frac{1}{6}(e^0 + 4e^{1/2} + e) + \frac{1}{6}(e + 4e^{3/2} + e^2)$$
$$+\frac{1}{6}(e^2 + 4e^{5/2} + e^3) + \frac{1}{6}(e^3 + 4e^{7/2} + e^4)$$
$$=53.61622$$

The error for this approximation has been reduced to -0.01807.

To generalize this procedure for an arbitrary integral $\int_a^b f(x)\,dx$, 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.)



With $h = (b-a)/n$ and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$, we have

$$\begin{aligned}\int_a^b f(x)dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)dx \\ &= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\}\end{aligned},$$

for some ξ_j with $x_{2j-2} < \xi_j < x_{2j}$, provided that $f \in C^4[a,b]$.

Using the fact that for each $j = 1, 2, \ldots, (n/2) - 1$ we have $f(x_{2j})$ appearing in the term corresponding to the interval $[x_{2j-2}, x_{2j}]$ and also in the term corresponding to the interval $[x_{2j}, x_{2j+2}]$, we can reduce this sum to

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right] - \frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

The error associated with this approximation is

$$E(f) = -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(4)}(\xi_j),$$

where $x_{2j-2} < \xi_j < x_{2j}$, for each $j = 1, 2, \ldots, n/2$.

If $f \in C^4[a,b]$, the Extreme Value Theorem 1.9 implies that $f^{(4)}$ assumes its maximum and minimum in $[a,b]$. Since

$$\min_{x\in[a,b]} f^{(4)}(x) \leq f^{(4)}(\xi_j) \leq \max_{x\in[a,b]} f^{(4)}(x),$$

we have

$$\frac{n}{2}\min_{x\in[a,b]} f^{(4)}(x) \leq \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \frac{n}{2}\max_{x\in[a,b]} f^{(4)}(x)$$

and

$$\min_{x\in[a,b]} f^{(4)}(x) \leq \frac{2}{n}\sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x\in[a,b]} f^{(4)}(x).$$

By the Intermediate Value Theorem 1.11, there is a $\mu \in (a, b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Thus

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu),$$

or, since $h = (b-a)/n$,

$$E(f) = -\frac{(b-a)}{180} h^4 f^{(4)}(\mu).$$

Theorem

Let $f \in C^4[a,b]$, n 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

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

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 $XI1 = XI1 + f(X)$.

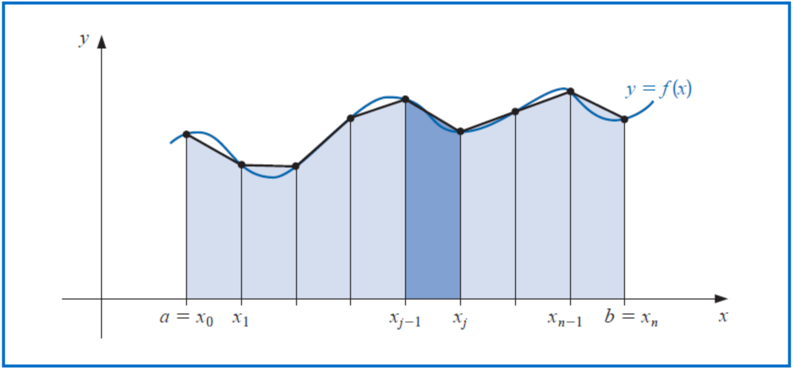
Step 6 Set $XI = h(XI0 + 2 \cdot XI2 + 4 \cdot XI1)/3$.

Step 7 OUTPUT (XI);
STOP.

Composite Trapezoidal Rule

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

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

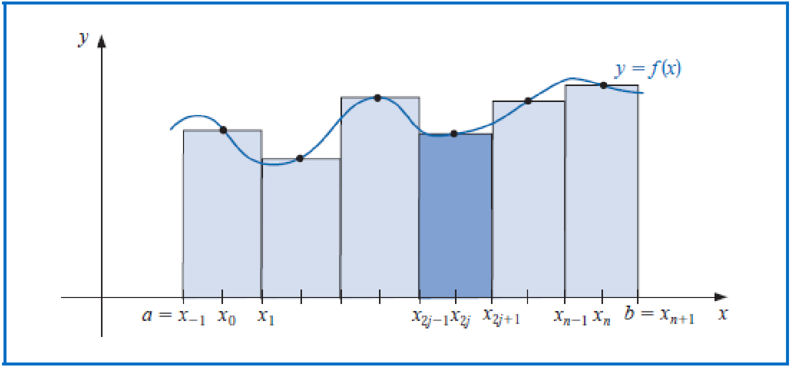

y
y = f(x)
a = x0
x1
xj−1
xj
xn−1
b = xn
x

Composite Midpoint Rule

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** for $n+2$ subintervals can be written with its error term as

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

∎


y
y = f(x)
a = x_{-1}
x_0
x_1
x_{2j-1}
x_{2j}
x_{2j+1}
x_{n-1}
x_n
b = x_{n+1}
x

Example

Determine values of h that will ensure an approximation error of less than 0.00002 when approximating $\int_0^\pi \sin x dx$ and employing (a) Composite Trapezoidal rule and (b) Composite Simpson's rule.

Solution

the error form for the Composite Trapezoidal rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left|\frac{\pi h^2}{12} f''(\mu)\right| = \left|\frac{\pi h^2}{12}(\sin \mu)\right| = \frac{\pi h^2}{12}|\sin \mu|$$

Solution cont...

$$\frac{\pi h^2}{12}|\sin\mu| \leq \frac{\pi h^2}{12} < 0.00002$$

Since $h = \pi/n$ implies that $n = \pi/h$, we need $\dfrac{\pi^3}{12n^2} < 0.00002$. This means that the Composite Trapezoidal rule requires $n \geq 360$.

Solution cont...

the error form for the Composite Simpson's rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left|\frac{\pi h^4}{180} f^{(4)}(\mu)\right| = \left|\frac{\pi h^4}{180}(\sin \mu)\right| = \frac{\pi h^4}{180}|\sin \mu|$$

$$\frac{\pi h^4}{180}|\sin \mu| \leq \frac{\pi h^4}{180} < 0.00002$$

Since $h = \pi/n$ implies that $n = \pi/h$, we need $\dfrac{\pi^5}{180n^4} < 0.00002$. This means that the Composite Simpson's rule requires $n \geq 18$.

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 to obtain $O(h^4)$ approximations $R_{2,2}, R_{3,2}, R_{4,2}$, etc., by

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

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

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

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

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

Example

Use the Composite Trapezoidal rule to find approximations to $\int_0^\pi \sin x dx$ with $n = 1, 2, 4, 8$, and 16. Then perform Romberg extrapolation on the results.

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0;$$

$$R_{2,1} = \frac{\pi}{4}\left[\sin 0 + 2\sin\frac{\pi}{2} + \sin \pi\right] = 1.57079633;$$

$$R_{3,1} = \frac{\pi}{8}\left[\sin 0 + 2\left(\sin\frac{\pi}{4} + \sin\frac{\pi}{2} + \sin\frac{3\pi}{4}\right) + \sin \pi\right] = 1.89611890;$$

$$R_{4,1} = \frac{\pi}{16}\left[\sin 0 + 2\left(\sin\frac{\pi}{8} + \sin\frac{\pi}{4} + \cdots + \sin\frac{3\pi}{4} + \sin\frac{7\pi}{8}\right) + \sin \pi\right] = 1.97423160;$$

$$R_{5,1} = \frac{\pi}{32}\left[\sin 0 + 2\left(\sin\frac{\pi}{16} + \sin\frac{\pi}{8} + \cdots + \sin\frac{7\pi}{8} + \sin\frac{15\pi}{16}\right) + \sin \pi\right] = 1.99357034.$$

The $O(h^4)$ approximations are

$$R_{2,2} = R_{2,1} + \frac{1}{3}(R_{2,1} - R_{1,1}) = 2.09439511; \quad R_{3,2} = R_{3,1} + \frac{1}{3}(R_{3,1} - R_{2,1}) = 2.00455976;$$

$$R_{4,2} = R_{4,1} + \frac{1}{3}(R_{4,1} - R_{3,1}) = 2.00026917; \quad R_{5,2} = R_{5,1} + \frac{1}{3}(R_{5,1} - R_{4,1}) = 2.00001659;$$

The $O(h^6)$ approximations are

$$R_{3,3} = R_{3,2} + \frac{1}{15}(R_{3,2} - R_{2,2}) = 1.99857073; \quad R_{4,3} = R_{4,2} + \frac{1}{15}(R_{4,2} - R_{3,2}) = 1.99998313;$$

$$R_{5,3} = R_{5,2} + \frac{1}{15}(R_{5,2} - R_{4,2}) = 1.99999975.$$

The two $O(h^8)$ approximations are

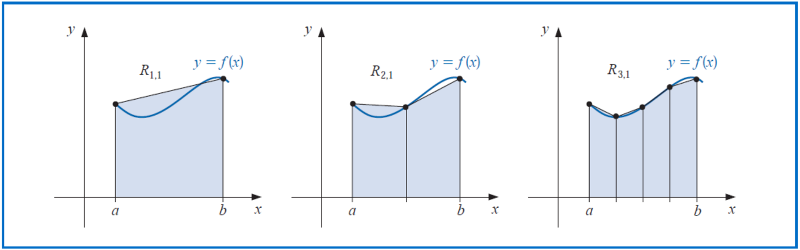
$$R_{4,4} = R_{4,3} + \frac{1}{63}(R_{4,3} - R_{3,3}) = 2.00000555; \quad R_{5,4} = R_{5,3} + \frac{1}{63}(R_{5,3} - R_{4,3}) = 2.00000001,$$

and the final $O(h^{10})$ approximation is

$$R_{5,5} = R_{5,4} + \frac{1}{255}(R_{5,4} - R_{4,4}) = 1.99999999.$$

These results are shown in Table 4.9. ■

0				
1.57079633	2.09439511			
1.89611890	2.00455976	1.99857073		
1.97423160	2.00026917	1.99998313	2.00000555	
1.99357034	2.00001659	1.99999975	2.00000001	1.99999999


y
$R_{1,1}$
$y = f(x)$
a
b
x
y
$R_{2,1}$
$y = f(x)$
a
b
x
y
$R_{3,1}$
$y = f(x)$
a
b
x

Extrapolation then is used to produce $O(h_k^{2j})$ approximations by

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

as shown in Table 4.10.

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

Romberg

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 $R_{2,j} = R_{2,j-1} + \dfrac{R_{2,j-1} - R_{1,j-1}}{4^{j-1}-1}$. (*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.*)

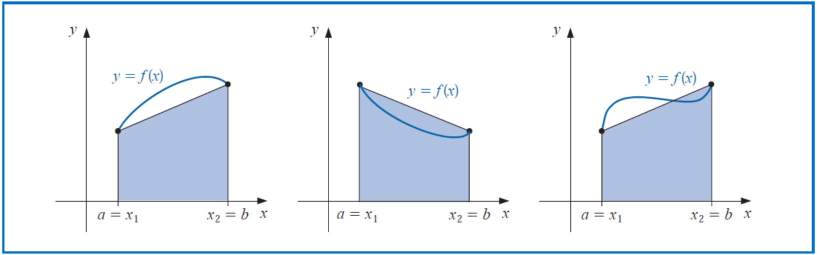
Step 9 STOP. ■

The algorithm requires a preset integer n to determine the number of rows to be generated. We could also set an error tolerance for the approximation and generate n, within some upper bound, until consecutive diagonal entries $R_{n-1,n-1}$ and $R_{n,n}$ agree to within the tolerance.

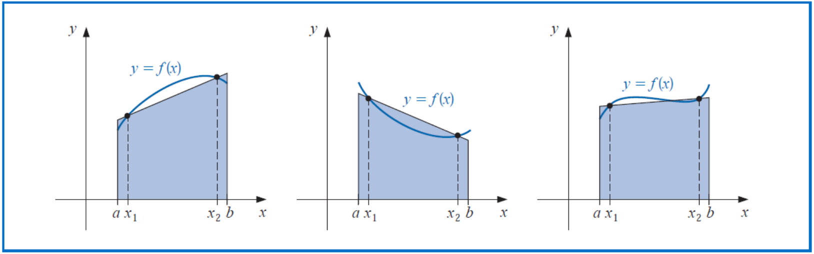
To guard against the possibility that two consecutive row elements agree with each other but not with the value of the integral being approximated, it is common to generate approximations until not only $|R_{n-1,n-1} - R_{n,n}|$ is within the tolerance, but also $|R_{n-2,n-2} - R_{n-1,n-1}|$. Although not a universal safeguard, this will ensure that two differently generated sets of approximations agree within the specified tolerance before $R_{n,n}$, is accepted as sufficiently accurate.

Gaussian Quadrature

Consider, for example, the Trapezoidal rule applied to determine the integrals of the functions whose graphs are shown



The Trapezoidal rule approximates the integral of the function by integrating the linear function that joins the endpoints of the graph of the function. But this is not likely the best line for approximating the integral. Lines such as those shown here would likely give much better approximations in most cases.



Gaussian quadrature chooses the points for evaluation 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

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

To measure this accuracy, we assume that the best choice of these values produces the exact result for the largest class of polynomials, that is, the choice that gives the greatest degree of precision.

Legendre Polynomials

The set that is relevant to our problem is the Legendre polynomials, a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots,\}$ with properties:

(i) For each $n, P_n(x)$ is a monic polynomial of degree n.

(ii) $\int_{-1}^{1} P(x)P_n(x)dx = 0$ whenever $P(x)$ is a polynomial of degree less than n

The first few Legendre Polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - \frac{1}{3},$$
$$P_3(x) = x^3 - \frac{3}{5}x, \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{3y}$$

The roots of these polynomials are distinct, lie in the interval (-1, 1), have a symmetry with respect to the origin, and, most importantly, are the correct choice for determining the parameters that give us the nodes and coefficients for our quadrature method.

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.

Theorem

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

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

The constants c_i needed for the quadrature rule can be generated from the equation in the theorem, but both these constants and the roots of the Legendre polynomials are extensively tabulated.

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

Example

Approximate $\int_{-1}^{1} e^x \cos x \, dx$ using Gaussian quadrature with $n = 3$.

Solution The entries in Table 4.12 give us

$$\begin{aligned}\int_{-1}^{1} e^x \cos x \, dx &\approx 0.\overline{5}e^{0.774596692} \cos 0.774596692 \\ &\quad + 0.\overline{8} \cos 0 + 0.\overline{5}e^{-0.774596692} \cos(-0.774596692) \\ &= 1.9333904.\end{aligned}$$

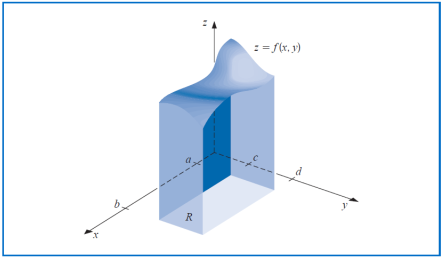
Integration by parts can be used to show that the true value of the integral is 1.9334214, so the absolute error is less than 3.2×10^{-5}. ■

Multiple Integrals

The techniques discussed in the previous sections can be modified for use in the approximation of multiple integrals. Consider the double integral

$$\int\int_R f(x,y)dA$$

where $R = \{(x,y) | a \leq x \leq b, c \leq y \leq d\}$, for some constants a, b, c, and d, is a rectangular region in the plane



The following illustration shows how the Composite Trapezoidal rule using two subintervals in each coordinate direction would be applied to this integral.

Writing the double integral as an iterated integral gives

$$\int\int_R f(x,y)dA = \int_a^b \left(\int_c^d f(x,y)dy \right) dx$$

To simplify notation, let $k = (d-c)/2$ and $h = (b-a)/2$. Apply the Composite Trapezoidal rule to the interior integral to obtain

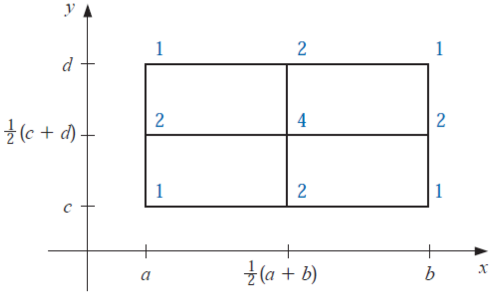
$$\int_c^d f(x,y)\,dy \approx \frac{k}{2}\left[f(x,c) + f(x,d) + 2f\left(x, \frac{c+d}{2}\right)\right].$$

This approximation is of order $O\left((d-c)^3\right)$. Then apply the Composite Trapezoidal rule again to approximate the integral of this function of x:

$$\begin{aligned}\int_a^b \left(\int_c^d f(x,y)\,dy\right) dx &\approx \int_a^b \left(\frac{d-c}{4}\right)\left[f(x,c) + 2f\left(x, \frac{c+d}{2}\right) + f(d)\right] dx \\ &= \frac{b-a}{4}\left(\frac{d-c}{4}\right)\left[f(a,c) + 2f\left(a, \frac{c+d}{2}\right) + f(a,d)\right]\end{aligned}$$

$$
\begin{aligned}
\int_a^b \left(\int_c^d f(x,y)\,dy\right) dx &\approx \int_a^b \left(\frac{d-c}{4}\right)\left[f(x,c) + 2f\left(x, \frac{c+d}{2}\right) + f(d)\right] dx \\
&= \frac{b-a}{4}\left(\frac{d-c}{4}\right)\left[f(a,c) + 2f\left(a, \frac{c+d}{2}\right) + f(a,d)\right] \\
&\quad + \frac{b-a}{4}\left(2\left(\frac{d-c}{4}\right)\left[f\left(\frac{a+b}{2}, c\right)\right.\right. \\
&\quad \left.\left. + 2f\left(\frac{a+b}{2}, \frac{c+d}{2}\right) + \left(\frac{a+b}{2}, d\right)\right]\right) \\
&\quad + \frac{b-a}{4}\left(\frac{d-c}{4}\right)\left[f(b,c) + 2f\left(b, \frac{c+d}{2}\right) + f(b,d)\right] \\
&= \frac{(b-a)(d-c)}{16}\left[f(a,c) + f(a,d) + f(b,c) + f(b,d)\right. \\
&\quad + 2\left(f\left(\frac{a+b}{2}, c\right) + f\left(\frac{a+b}{2}, d\right) + f\left(a, \frac{c+d}{2}\right)\right. \\
&\quad \left.\left. + f\left(b, \frac{c+d}{2}\right)\right) + 4f\left(\frac{a+b}{2}, \frac{c+d}{2}\right)\right]
\end{aligned}
$$

This approximation is of order $O\left((b-a)(d-c)\left[(b-a)^2+(d-c)^2\right]\right)$. Figure 4.19 shows a grid with the number of functional evaluations at each of the nodes used in the approximation. □



To apply the Composite Simpson's rule, we divide the region R by partitioning both $[a, b]$ and $[c, d]$ into an even number of subintervals. To simplify the notation, we choose even integers n and m and partition $[a, b]$ and $[c, d]$ with the evenly spaced mesh points $x_0, x_1, \ldots, x_n$ and $y_0, y_1, \ldots, y_m$, respectively. These subdivisions determine step sizes $h = (b - a)/n$ and $k = (d - c)/m$. Writing the double integral as the iterated integral

$$\iint_R f(x, y)\, dA = \int_a^b \left(\int_c^d f(x, y)\, dy \right) dx,$$

we first use the Composite Simpson's rule to approximate

$$\int_c^d f(x, y)\, dy,$$

treating x as a constant.

Let $y_j = c + jk$, for each $j = 0, 1, \ldots, m$. Then

$$\int_c^d f(x,y)\,dy = \frac{k}{3}\left[f(x,y_0) + 2\sum_{j=1}^{(m/2)-1} f(x,y_{2j}) + 4\sum_{j=1}^{m/2} f(x,y_{2j-1}) + f(x,y_m)\right] - \frac{(d-c)k^4}{180}\frac{\partial^4 f}{\partial y^4}(x,\mu),$$

for some μ in (c,d). Thus

$$\int_a^b \int_c^d f(x,y)\,dy\,dx = \frac{k}{3}\Bigg[\int_a^b f(x,y_0)\,dx + 2\sum_{j=1}^{(m/2)-1}\int_a^b f(x,y_{2j})\,dx + 4\sum_{j=1}^{m/2}\int_a^b f(x,y_{2j-1})\,dx + \int_a^b f(x,y_m)\,dx\Bigg] - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f}{\partial y^4}(x,\mu)\,dx.$$

Composite Simpson's rule is now employed on the integrals in this equation. Let $x_i = a + ih$, for each $i = 0, 1, \ldots, n$. Then for each $j = 0, 1, \ldots, m$, we have

$$\int_a^b f(x, y_j)\, dx = \frac{h}{3}\left[f(x_0, y_j) + 2 \sum_{i=1}^{(n/2)-1} f(x_{2i}, y_j) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}, y_j) + f(x_n, y_j) \right] - \frac{(b-a)h^4}{180} \frac{\partial^4 f}{\partial x^4}(\xi_j, y_j),$$

for some ξ_j in (a, b).

$$
\begin{aligned}
\int_a^b \int_c^d f(x,y)\,dy\,dx \approx \frac{hk}{9}\Bigg\{\Bigg[& f(x_0,y_0) + 2\sum_{i=1}^{(n/2)-1} f(x_{2i},y_0) \\
& + 4\sum_{i=1}^{n/2} f(x_{2i-1},y_0) + f(x_n,y_0)\Bigg] \\
& + 2\Bigg[\sum_{j=1}^{(m/2)-1} f(x_0,y_{2j}) + 2\sum_{j=1}^{(m/2)-1}\sum_{i=1}^{(n/2)-1} f(x_{2i},y_{2j}) \\
& + 4\sum_{j=1}^{(m/2)-1}\sum_{i=1}^{n/2} f(x_{2i-1},y_{2j}) + \sum_{j=1}^{(m/2)-1} f(x_n,y_{2j})\Bigg] \\
& + 4\Bigg[\sum_{j=1}^{m/2} f(x_0,y_{2j-1}) + 2\sum_{j=1}^{m/2}\sum_{i=1}^{(n/2)-1} f(x_{2i},y_{2j-1}) \\
& + 4\sum_{j=1}^{m/2}\sum_{i=1}^{n/2} f(x_{2i-1},y_{2j-1}) + \sum_{j=1}^{m/2} f(x_n,y_{2j-1})\Bigg] \\
& + \Bigg[f(x_0,y_m) + 2\sum_{i=1}^{(n/2)-1} f(x_{2i},y_m) + 4\sum_{i=1}^{n/2} f(x_{2i-1},y_m) + f(x_n,y_m)\Bigg]\Bigg\}.
\end{aligned}
$$

The error term E is given by

$$E = \frac{-k(b-a)h^4}{540}\left[\frac{\partial^4 f}{\partial x^4}(\xi_0, y_0) + 2\sum_{j=1}^{(m/2)-1}\frac{\partial^4 f}{\partial x^4}(\xi_{2j}, y_{2j}) + 4\sum_{j=1}^{m/2}\frac{\partial^4 f}{\partial x^4}(\xi_{2j-1}, y_{2j-1})\right.$$
$$\left. + \frac{\partial^4 f}{\partial x^4}(\xi_m, y_m)\right] - \frac{(d-c)k^4}{180}\int_a^b \frac{\partial^4 f}{\partial y^4}(x, \mu)\, dx.$$

If $\dfrac{\partial^4 f}{\partial y^4}(x,\mu)$ is continuous, with the Intermediate Value Theorem and the Weighted Mean Value Theorem, this can be simplified to

$$E = -\frac{(d-c)(b-a)}{180}\left[h^4\frac{\partial^4 f}{\partial y^4}(\overline{\eta}, \overline{\mu}) + k^4\frac{\partial^4 f}{\partial y^4}(\hat{\eta}, \hat{\mu})\right]$$

for some $(\overline{\eta}, \overline{\mu})$ and $(\hat{\eta}, \hat{\mu})$ in R

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 $L = (K_1 + 2K_2 + 4K_3)HX/3$.

$$\left(L \approx \int_{c(x_i)}^{d(x_i)} f(x_i, y)\, dy \quad \text{by the Composite Simpson's method.} \right)$$

Step 8 If $i = 0$ or $i = n$ then set $J_1 = J_1 + L$
else if i is even then set $J_2 = J_2 + L$
else set $J_3 = J_3 + L$.

Step 9 Set $J = h(J_1 + 2J_2 + 4J_3)/3$.

Step 10 OUTPUT (J);
STOP. ■

Gaussian Double Integral

To approximate the integral

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx :$$

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* $1 \le j \le i$.)

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 3–5.

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 $J = J + c_{m,i} k_1 JX$.

Step 6 Set $J = h_1 J$.

Step 7 OUTPUT (J);
STOP.

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 $1 \leq j \leq i$.)

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 3–8.

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 $JX = JX + c_{n,j} l_1 JY$.

Step 8 Set $J = J + c_{m,i} k_1 JX$.

Step 9 Set $J = h_1 J$.

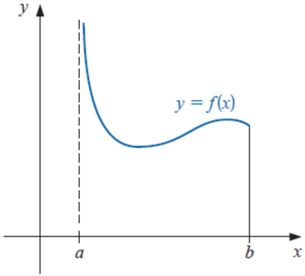
Step 10 OUTPUT (J);
STOP.

Improper Integrals

Improper integrals result when the notion of integration is extended either to an interval of integration on which the function is unbounded or to an interval with one or more infinite endpoints. In either circumstance, the normal rules of integral approximation must be modified.

Left Endpoint Singularity

We will first consider the situation when the integrand is unbounded at the left endpoint of the interval of integration, as shown in the figure. In this case we say that f has a singularity at the endpoint a.



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

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

If f is a function that can be written in the form

$$f(x) = \frac{g(x)}{(x-a)^p},$$

where $0 < p < 1$ and g is continuous on $[a, b]$, then the improper integral

$$\int_a^b f(x)dx$$

also exists.

also exists. We will approximate this integral using the Composite Simpson's rule, provided that $g \in C^5[a,b]$. In that case, we can construct the fourth Taylor polynomial, $P_4(x)$, for g about a,

$$P_4(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2!}(x-a)^2 + \frac{g'''(a)}{3!}(x-a)^3 + \frac{g^{(4)}(a)}{4!}(x-a)^4,$$

and write

$$\int_a^b f(x)\,dx = \int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\,dx + \int_a^b \frac{P_4(x)}{(x-a)^p}\,dx. \tag{4.44}$$

Because $P(x)$ is a polynomial, we can exactly determine the value of

$$\int_a^b \frac{P_4(x)}{(x-a)^p}\,dx = \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!}(x-a)^{k-p}\,dx = \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k+1-p)}(b-a)^{k+1-p}. \tag{4.45}$$

This is generally the dominant portion of the approximation, especially when the Taylor polynomial $P_4(x)$ agrees closely with $g(x)$ throughout the interval $[a,b]$.

To approximate the integral of f, we must add to this value the approximation of

$$\int_a^b \frac{g(x) - P_4(x)}{(x-a)^p}\, dx.$$

To determine this, we first define

$$G(x) = \begin{cases} \frac{g(x)-P_4(x)}{(x-a)^p}, & \text{if } a < x \leq b, \\ 0, & \text{if } x = a. \end{cases}$$

This gives us a continuous function on $[a, b]$. In fact, $0 < p < 1$ and $P_4^{(k)}(a)$ agrees with $g^{(k)}(a)$ for each $k = 0, 1, 2, 3, 4$, so we have $G \in C^4[a, b]$. This implies that the Composite Simpson's rule can be applied to approximate the integral of G on $[a, b]$. Adding this approximation to the value in Eq. (4.45) gives an approximation to the improper integral of f on $[a, b]$, within the accuracy of the Composite Simpson's rule approximation.

Use Composite Simpson's rule with $h = 0.25$ to approximate the value of the improper integral

$$\int_0^1 \frac{e^x}{\sqrt{x}}\, dx.$$

Solution The fourth Taylor polynomial for e^x about $x = 0$ is

$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24},$$

so the dominant portion of the approximation to $\int_0^1 \frac{e^x}{\sqrt{x}}\,dx$ is

$$\begin{aligned}
\int_0^1 \frac{P_4(x)}{\sqrt{x}}\,dx &= \int_0^1 \left(x^{-1/2} + x^{1/2} + \frac{1}{2}x^{3/2} + \frac{1}{6}x^{5/2} + \frac{1}{24}x^{7/2}\right)\,dx \\
&= \lim_{M\to 0^+}\left[2x^{1/2} + \frac{2}{3}x^{3/2} + \frac{1}{5}x^{5/2} + \frac{1}{21}x^{7/2} + \frac{1}{108}x^{9/2}\right]_M^1 \\
&= 2 + \frac{2}{3} + \frac{1}{5} + \frac{1}{21} + \frac{1}{108} \approx 2.9235450.
\end{aligned}$$

For the second portion of the approximation to $\int_0^1 \frac{e^x}{\sqrt{x}}\,dx$ we need to approximate $\int_0^1 G(x)\,dx$, where

$$G(x) = \begin{cases} \frac{1}{\sqrt{x}}(e^x - P_4(x)), & \text{if } 0 < x \le 1, \\ 0, & \text{if } x = 0. \end{cases}$$

Table 4.13 lists the values needed for the Composite Simpson's rule for this approximation.

Using these data and the Composite Simpson's rule gives

$$\int_0^1 G(x)\,dx \approx \frac{0.25}{3}[0 + 4(0.0000170) + 2(0.0004013) + 4(0.0026026) + 0.0099485]$$
$$= 0.0017691.$$

Hence

$$\int_0^1 \frac{e^x}{\sqrt{x}}\,dx \approx 2.9235450 + 0.0017691 = 2.9253141.$$

This result is accurate to within the accuracy of the Composite Simpson's rule approximation for the function G. Because $|G^{(4)}(x)| < 1$ on $[0, 1]$, the error is bounded by

$$\frac{1-0}{180}(0.25)^4 = 0.0000217. \qquad \blacksquare$$

Right Endpoint Singularity

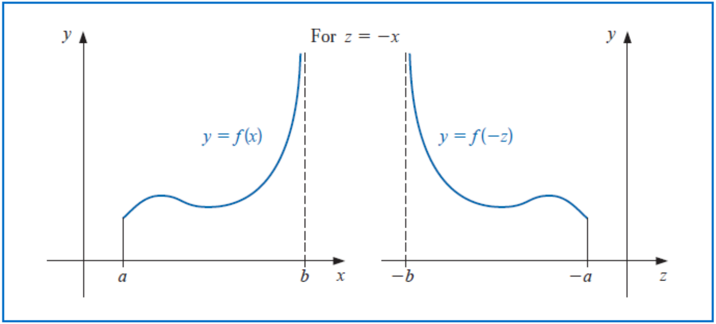
To approximate the improper integral with a singularity at the right endpoint, we could develop a similar technique but expand in terms of the right endpoint b instead of the left endpoint a. Alternatively, we can make the substitution

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

to change the improper integral into one of the form

$$\int_a^b f(x)\,dx = \int_{-b}^{-a} f(-z)\,dz, \tag{4.46}$$

which has its singularity at the left endpoint. Then we can apply the left endpoint singularity technique we have already developed. (See Figure 4.26.)



An improper integral with a singularity at c, where $a < c < b$, is treated as the sum of improper integrals with endpoint singularities since

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx.$$

Infinite Singularity

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

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

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:

$$\int_a^\infty f(x)\, dx = \int_0^{1/a} t^{-2} f\left(\frac{1}{t}\right)\, dt. \tag{4.47}$$

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

Example

Approximate the value of the improper integral

$$I = \int_1^\infty x^{-3/2} \sin \frac{1}{x}\, dx.$$

Solution We first make the variable change $t = x^{-1}$, which converts the infinite singularity into one with a left endpoint singularity. Then

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

and

$$I = \int_{x=1}^{x=\infty} x^{-3/2} \sin\frac{1}{x}\,dx = \int_{t=1}^{t=0} \left(\frac{1}{t}\right)^{-3/2} \sin t \left(-\frac{1}{t^2}\,dt\right) = \int_0^1 t^{-1/2} \sin t\,dt.$$

The fourth Taylor polynomial, $P_4(t)$, for $\sin t$ about 0 is

$$P_4(t) = t - \frac{1}{6}t^3,$$

so

$$G(t) = \begin{cases} \dfrac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}, & \text{if } 0 < t \leq 1 \\ 0, & \text{if } t = 0 \end{cases}$$

is in $C^4[0, 1]$, and we have

$$\begin{aligned} I &= \int_0^1 t^{-1/2}\left(t - \frac{1}{6}t^3\right) dt + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\, dt \\ &= \left[\frac{2}{3}t^{3/2} - \frac{1}{21}t^{7/2}\right]_0^1 + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\, dt \\ &= 0.61904761 + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{t^{1/2}}\, dt. \end{aligned}$$

The result from the Composite Simpson's rule with $n = 16$ for the remaining integral is 0.0014890097. This gives a final approximation of

$$I = 0.0014890097 + 0.61904761 = 0.62053661,$$

which is accurate to within 4.0×10^{-8}. ■