Simpsons Rule: $n = 3$, $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$, $h = \frac{b-a}{2}$.

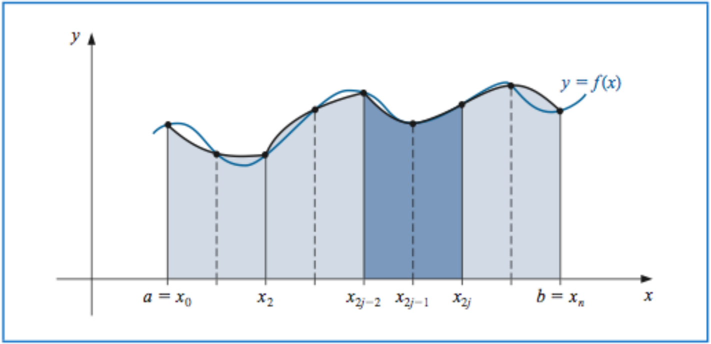
$$\int_a^b f(x)dx = \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right) - \frac{f^{(4)}(\xi)}{90}h^5.$$

Degree of precision $= 3$

Composite Simpsons Rule
$(n = 2m, x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx = \sum_{j=1}^{m} \int_{x_{2(j-1)}}^{x_{2j}} f(x)dx$$

$$= \sum_{j=1}^{m} \left(\frac{h}{3} \left(f(x_{2(j-1)}) + 4f(x_{2j-1}) + f(x_{2j}) \right) - \frac{f^{(4)}(\xi_j)}{90} h^5 \right).$$



Composite Simpsons Rule
$(n = 2m, x_j = a + j\,h, h = \frac{b-a}{n}, 0 \leq j \leq n)$

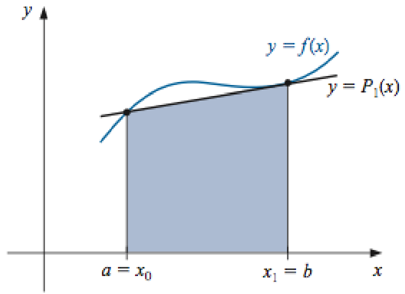
$$\int_a^b f(x)dx = \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right) - \frac{h^5}{90}\sum_{j=1}^{m} f^{(4)}(\xi_j)$$

$$= \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right) - \frac{h^5 m}{90} f^{(4)}(\mu)$$

$$= \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right) - \frac{(b-a)h^4}{180} f^{(4)}(\mu)$$

Trapezoidal Rule: $n = 1$, $x_0 = a, x_1 = b$, $h = b - a$.

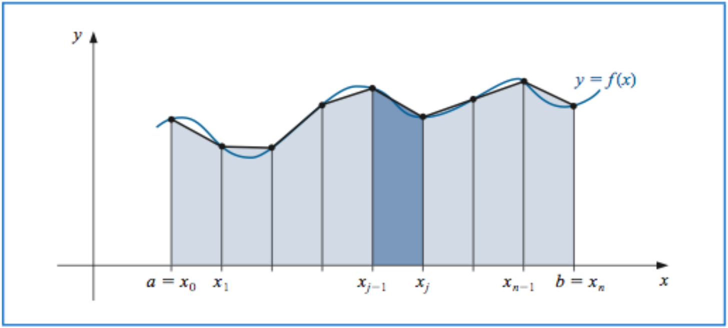
$$\int_a^b f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{f''(\xi)}{12}h^3.$$



Degree of precision $= 1$

Composite Trapezoidal Rule
$(x_j = a + j\,h, h = \frac{b-a}{n}, 0 \leq j \leq n)$

$$\int_a^b f(x)dx = \sum_{j=1}^{n} \int_{x_{j-1}}^{x_j} f(x)dx$$
$$= \sum_{i=1}^{n} \left(\frac{h}{2} \left(f(x_{j-1}) + f(x_j)\right) - \frac{f''(\xi_j)}{12} h^3 \right).$$



Composite Trapezoidal Rule
$(x_j = a + j\,h, h = \frac{b-a}{n}, 0 \leq j \leq n)$

$$\int_a^b f(x)dx = \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) - \frac{h^3}{12}\sum_{j=1}^{n} f''(\xi_j)$$

$$= \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) - \frac{h^3 n}{12} f''(\mu)$$

$$= \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) - \frac{(b-a)h^2}{12} f''(\mu)$$

For the same work, Composite Simpson yields twice as many correct digits.

Composite Simpsons Rule, example

Determine values of h for an approximation error $\leq \epsilon = 10^{-5}$ when approximating $\int_0^\pi \mathbf{sin}(x)\,dx$ with Composite Simpson.

Composite Simpsons Rule, example

Determine values of h for an approximation error $\leq \epsilon = 10^{-5}$ when approximating $\int_0^\pi \mathbf{sin}(x)\, dx$ with Composite Simpson.
Solution:

$$|f^{(4)}(\mu)| = |\mathbf{sin}(\mu)| \leq 1, \quad |\mathbf{Error}| = \left| \frac{\pi\, h^4}{180} f^{(4)}(\mu) \right| \leq \frac{\pi^5}{180 n^4}.$$

Choosing

$$\frac{\pi^5}{180 n^4} \leq \epsilon, \quad \text{leading to} \quad n \geq \pi \left(\frac{\pi}{180\epsilon} \right)^{\frac{1}{4}} \approx 20.3.$$

or $h = \frac{\pi}{2m}$ with $m \geq 11$.

Composite Simpsons Rule, example

Determine values of h for an approximation error $\leq \epsilon = 10^{-5}$ when approximating $\int_0^\pi \textbf{sin}(x)\, dx$ with Composite Simpson.
Solution:

$$|f^{(4)}(\mu)| = |\textbf{sin}(\mu)| \leq 1, \quad |\textbf{Error}| = \left| \frac{\pi\, h^4}{180} f^{(4)}(\mu) \right| \leq \frac{\pi^5}{180 n^4}.$$

Choosing

$$\frac{\pi^5}{180 n^4} \leq \epsilon, \quad \text{leading to} \quad n \geq \pi \left(\frac{\pi}{180 \epsilon} \right)^{\frac{1}{4}} \approx 20.3.$$

or $h = \frac{\pi}{2m}$ with $m \geq 11$. For $n = 2m = 22$,

$$\begin{aligned} 2 &= \int_0^\pi \textbf{sin}(x)\, dx \approx \frac{\pi}{3 \times 22} \left(2 \sum_{j=1}^{10} \textbf{sin}\left(\frac{j\pi}{11}\right) + 4 \sum_{j=1}^{11} \textbf{sin}\left(\frac{(2j-1)\pi}{22}\right) \right) \\ &\approx 2.0000046. \end{aligned}$$

$$\left(\int_0^\pi \textbf{sin}(x)\, dx \approx \frac{\pi}{2 \times 22} \left(2 \sum_{j=1}^{21} \textbf{sin}\left(\frac{j\pi}{22}\right) \right) \approx 1.9966. \text{ (Trapezoidal)} \right)$$

Composite Simpsons Rule: Round-Off Error Stability $(n = 2m, x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right) \stackrel{def}{=} \mathcal{I}(f).$$

Composite Simpsons Rule: Round-Off Error Stability $(n = 2m, x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right)$$

$$\stackrel{def}{=} \mathcal{I}(f).$$

Assume round-off error model:

$$f(x_i) = \widehat{f}(x_i) + e_i, \quad |e_i| \le \epsilon, \quad i = 0, 1, \cdots, n.$$

Composite Simpsons Rule: Round-Off Error Stability $(n = 2m, x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right)$$

$$\stackrel{def}{=} \mathcal{I}(f).$$

Assume round-off error model:

$$f(x_i) = \widehat{f}(x_i) + e_i, \quad |e_i| \le \epsilon, \quad i = 0, 1, \cdots, n.$$

$$\mathcal{I}(f) = \mathcal{I}(\widehat{f}) + \frac{h}{3}\left(e_0 + 2\sum_{j=1}^{m-1} e_{2j} + 4\sum_{j=1}^{m} e_{2j-1} + e_n\right).$$

$$|\mathcal{I}(f) - \mathcal{I}(\widehat{f})| \le \frac{h}{3}\left(|e_0| + 2\sum_{j=1}^{m-1} |e_{2j}| + 4\sum_{j=1}^{m} |e_{2j-1}| + |e_n|\right)$$

$$\le hn\epsilon = (b-a)\epsilon \quad \text{(numerically stable!!!)}$$

Composite Trapezoidal Rule: Round-Off Error Stability $(x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right)$$

$$\stackrel{def}{=} \mathcal{I}(f).$$

Composite Trapezoidal Rule: Round-Off Error Stability $(x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) \stackrel{def}{=} \mathcal{I}(f).$$

Assume round-off error model:

$$f(x_i) = \widehat{f}(x_i) + e_i, \quad |e_i| \le \epsilon, \quad i = 0, 1, \cdots, n.$$

Composite Trapezoidal Rule: Round-Off Error Stability $(x_j = a + j\,h, h = \frac{b-a}{n}, 0 \le j \le n)$

$$\int_a^b f(x)dx \approx \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) \stackrel{def}{=} \mathcal{I}(f).$$

Assume round-off error model:

$$f(x_i) = \widehat{f}(x_i) + e_i, \quad |e_i| \le \epsilon, \quad i = 0, 1, \cdots, n.$$

$$\mathcal{I}(f) = \mathcal{I}(\widehat{f}) + \frac{h}{2}\left(e_0 + 2\sum_{j=1}^{n-1} e_j + e_n\right).$$

$$|\mathcal{I}(f) - \mathcal{I}(\widehat{f})| \le \frac{h}{2}\left(|e_0| + 2\sum_{j=1}^{n-1} |e_j| + |e_n|\right)$$

$$\le h n \epsilon = (b-a)\epsilon \quad \text{(numerically stable!!!)}$$

Recursive Composite Trapezoidal: with $h_k = (b-a)/2^{k-1}$.

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

Recursive Composite Trapezoidal: with $h_k = (b-a)/2^{k-1}$.

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

$$\stackrel{book}{=\!=} \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) + \sum_{j=1}^{\infty} K_j h^{2j}.$$

$$\stackrel{def}{=\!=} \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h^{2j}, \quad \text{for} \quad n = 2^k.$$

Recursive Composite Trapezoidal: with $h_k = (b-a)/2^{k-1}$.

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

$$\stackrel{book}{=\!=} \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) + \sum_{j=1}^{\infty} K_j h^{2j}.$$

$$\stackrel{def}{=\!=} \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h^{2j}, \text{ for } n = 2^k.$$

$$\mathbf{R}_{1,1} = \frac{h_1}{2}(f(a) + f(b)) = \frac{b-a}{2}(f(a) + f(b)),$$

Recursive Composite Trapezoidal: with $h_k = (b-a)/2^{k-1}$.

$$\begin{aligned}
\int_a^b f(x)dx &\approx \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) - \frac{(b-a)h^2}{12} f''(\mu) \\
&\stackrel{book}{=\!=} \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) + \sum_{j=1}^{\infty} K_j h^{2j}. \\
&\stackrel{def}{=\!=} \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h^{2j}, \quad \text{for} \quad n = 2^k.
\end{aligned}$$

$$\begin{aligned}
\mathbf{R}_{1,1} &= \frac{h_1}{2}\left(f(a) + f(b)\right) = \frac{b-a}{2}\left(f(a) + f(b)\right), \\
\mathbf{R}_{2,1} &= \frac{h_2}{2}\left(f(a) + f(b) + 2f(a+h_2)\right) = \frac{1}{2}\left(\mathbf{R}_{1,1} + h_1 f(a+h_2)\right),
\end{aligned}$$

Recursive Composite Trapezoidal: with $h_k = (b-a)/2^{k-1}$.

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

$$\stackrel{book}{=\!=} \frac{h}{2}\left(f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right) + \sum_{j=1}^{\infty} K_j h^{2j}.$$

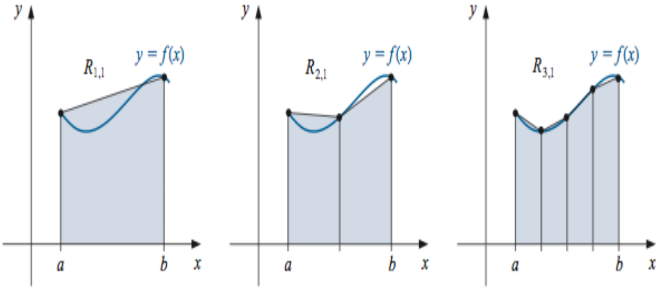
$$\stackrel{def}{=\!=} \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h^{2j}, \quad \text{for} \quad n = 2^k.$$

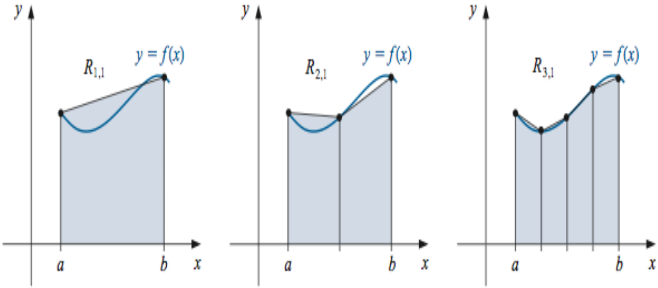
$$\mathbf{R}_{1,1} = \frac{h_1}{2}\left(f(a) + f(b)\right) = \frac{b-a}{2}\left(f(a) + f(b)\right),$$

$$\mathbf{R}_{2,1} = \frac{h_2}{2}\left(f(a) + f(b) + 2f(a+h_2)\right) = \frac{1}{2}\left(\mathbf{R}_{1,1} + h_1 f(a+h_2)\right),$$

$$\vdots \qquad \vdots$$

$$\mathbf{R}_{k,1} = \frac{1}{2}\left(\mathbf{R}_{k-1,1} + h_{k-1}\sum_{j=1}^{2^{k-2}} f(a + (2j-1)h_k)\right), \quad k = 2, \cdots, \log_2 n.$$


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



Romberg Extrapolation Table

$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$
$R_{1,1}$ $\searrow$ $\rightarrow$			
$R_{2,1}$ $\searrow$ $\rightarrow$	$R_{2,2}$ $\searrow$ $\rightarrow$		
$R_{3,1}$ $\searrow$	$R_{3,2}$ $\searrow$	$R_{3,3}$ $\searrow$	
$R_{4,1} \rightarrow$	$R_{4,2} \rightarrow$	$R_{4,3} \rightarrow$	$R_{4,4}$

Romberg Extrapolation for $\int_0^\pi \sin(x)\,dx$, $n = 1, 2, 2^2, 2^3, 2^4, 2^5$.

$$
\begin{aligned}
R_{1,1} &= \frac{\pi}{2}\left(\sin(0) + \sin(\pi)\right) = 0, \\
R_{2,1} &= \frac{1}{2}\left(R_{1,1} + \pi \sin(\frac{\pi}{2})\right) = 1.57079633, \\
R_{3,1} &= \frac{1}{2}\left(R_{2,1} + \frac{\pi}{2}\sum_{j=1}^{2} \sin(\frac{(2j-1)\pi}{4}\right) = 1.89611890, \\
R_{4,1} &= \frac{1}{2}\left(R_{3,1} + \frac{\pi}{4}\sum_{j=1}^{4} \sin(\frac{(2j-1)\pi}{8}\right) = 1.97423160, \\
R_{5,1} &= \frac{1}{2}\left(R_{4,1} + \frac{\pi}{8}\sum_{j=1}^{8} \sin(\frac{(2j-1)\pi}{16}\right) = 1.99357034, \\
R_{6,1} &= \frac{1}{2}\left(R_{5,1} + \frac{\pi}{16}\sum_{j=1}^{2^4} \sin(\frac{(2j-1)\pi}{32}\right) = 1.99839336.
\end{aligned}
$$

Romberg Extrapolation, $\int_0^\pi \sin(x)\, dx = 2$

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	1.9999999	
1.99839336	2.00000103	2.00000000	2.00000000	2.0000000	2.0000000

33 FUNCTION EVALUATIONS USED IN THE TABLE.

Recursive Composite Simpson:

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right) - \frac{(b-a)h^4}{12} f^{(4)}(\mu)$$

Recursive Composite Simpson:

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right)$$

$$-\frac{(b-a)h^4}{12} f^{(4)}(\mu)$$

$$\underset{\overline{\overline{\quad}}}{exists} \quad \frac{h}{3}\left(f(a) + 2\sum_{j=1}^{m-1} f(x_{2j}) + 4\sum_{j=1}^{m} f(x_{2j-1}) + f(b)\right)$$

$$+\sum_{j=2}^{\infty} K_j h^{2j}.$$

$$\stackrel{def}{=} \quad \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \quad \text{for} \quad n = 2^k.$$

Recursive Composite Simpson: with $h_k = (b-a)/2^{k-1}$.

$$\int_a^b f(x)dx \approx \quad \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \text{ for } \; n = 2^k.$$

Recursive Composite Simpson: with $h_k = (b-a)/2^{k-1}$.

$$\int_a^b f(x)dx \approx \quad \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \text{ for } n = 2^k.$$

$$\mathbf{R}_{1,1} \quad = \quad \frac{b-a}{6}\left(f(a) + 4\mathbf{S}_1 + f(b)\right), \quad \mathbf{S}_1 = f((a+b)/2),$$

Recursive Composite Simpson: with $h_k = (b-a)/2^{k-1}$.

$$\int_a^b f(x)dx \approx \quad \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \ \text{ for } \ n = 2^k.$$

$$\begin{aligned}
\mathbf{R}_{1,1} &= \frac{b-a}{6}\left(f(a) + 4\mathbf{S}_1 + f(b)\right), \quad \mathbf{S}_1 = f((a+b)/2), \\
\vdots & \quad \vdots \\
\mathbf{T}_k &= \sum_{j=1}^{2^{k-1}} f(a + (2j-1)h_k), \\
\mathbf{R}_{k,1} &= \frac{h_k}{3}\left(f(a) + 2\mathbf{S}_{k-1} + 4\mathbf{T}_k + f(b)\right), \\
\mathbf{S}_k &= \mathbf{S}_{k-1} + \mathbf{T}_k, \ k = 2, \cdots, \log_2 n.
\end{aligned}$$

Romberg Extrapolation Table, Simpson Rule

$$
\begin{array}{cccc}
O(h_k^4) & O(h_k^6) & O(h_k^8) & O(h_k^{10}) \\
\hline
R_{1,1} \searrow & & & \\
\quad \rightarrow & & & \\
R_{2,1} \searrow & R_{2,2} \searrow & & \\
\quad \rightarrow & \quad \rightarrow & & \\
R_{3,1} \searrow & R_{3,2} \searrow & R_{3,3} \searrow & \\
R_{4,1} \rightarrow & R_{4,2} \rightarrow & R_{4,3} \rightarrow & R_{4,4}
\end{array}
$$

Tricks of the Trade, $\int_a^b f(x)dx$

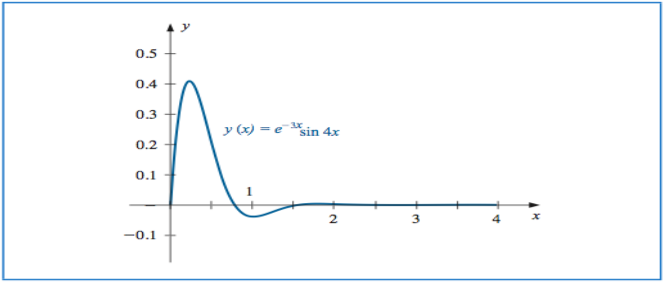
- Composite Simpson/Trapezoidal rules:
  - Adding more EQUI-SPACED points.
- Romberg extrapolation:
  - Obtain higher order rules from lower order rules.
- Adaptive quadratures:
  - Adding more points ONLY WHEN NECESSARY.

`quad` function of `matlab`: clever combination of all three.

Adaptive Quadrature Methods: step-size matters

$$y(x) = \mathbf{e}^{-3x}\mathbf{sin}\,4x.$$

- Oscillation for small x; nearly 0 for larger x.
  - Mechanical engineering (spring and shock absorber systems)
  - Electrical engineering (circuit simulations)

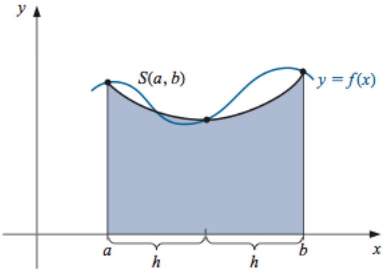


- $y(x)$ behaves different for small x and for large x.

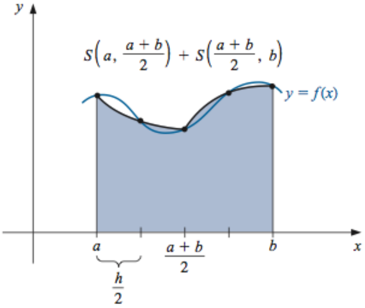
Adaptive Quadrature (I)

- $$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \xi \in (a,b),$$
  where $$S(a,b) = \frac{h}{3}\left(f(a) + 4f(a+h) + f(b)\right), \quad h = \frac{b-a}{2}.$$

Simpson on $[a, b]$



Composite Simpson



Adaptive Quadrature (II)

- $$\int_a^b f(x)dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \xi \in (a,b),$$

- $$\begin{aligned}\int_a^b f(x)dx &= \int_a^{\frac{a+b}{2}} f(x)dx + \int_{\frac{a+b}{2}}^b f(x)dx \\ &= S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) \\ &\quad -\frac{(h/2)^5}{90} f^{(4)}(\xi_1) - \frac{(h/2)^5}{90} f^{(4)}(\xi_2) \\ &= S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}),\end{aligned}$$

  where

  $$\xi_1 \in (a,\frac{a+b}{2}), \quad \xi_2 \in (\frac{a+b}{2},b), \quad \widehat{\xi} \in (a,b).$$

Adaptive Quadrature (III)

$$\begin{aligned}\int_a^b f(x)dx &= S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \\ &= S(a,b) - \frac{h^5}{90} f^{(4)}(\xi)\end{aligned}$$

Adaptive Quadrature (III)

$$\begin{aligned}\int_a^b f(x)dx &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \\ &= S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\widehat{\xi}).\end{aligned}$$

Adaptive Quadrature (III)

$$\begin{aligned}\int_a^b f(x)dx &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \\ &= S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\widehat{\xi}).\end{aligned}$$

$$\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \approx \frac{16}{15}\left(S(a,b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)\right),$$

Adaptive Quadrature (III)

$$\begin{aligned}\int_a^b f(x)dx &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \\ &= S(a,b) - \frac{h^5}{90} f^{(4)}(\xi) \approx S(a,b) - \frac{h^5}{90} f^{(4)}(\widehat{\xi}).\end{aligned}$$

$$\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi}) \approx \frac{16}{15}\left(S(a,b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)\right),$$

$$\left|\int_a^b f(x)dx - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)\right| = \left|\frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\widehat{\xi})\right|$$
$$\approx \frac{1}{15}\left|S(a,b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)\right|.$$

Adaptive Quadrature (IV)

- For a given tolerance τ,
  - $$\text{if} \quad \frac{1}{15}\left|S(a,b) - S(a,\frac{a+b}{2}) - S(\frac{a+b}{2},b)\right| \leq \tau,$$
    then $S(a,\frac{a+b}{2}) + S(\frac{a+b}{2},b)$ is sufficiently accurate approximation to $\int_a^b f(x)dx$;
  - otherwise recursively develop quadratures on $(a,\frac{a+b}{2})$ and $(\frac{a+b}{2},b)$, respectively.

AdaptQuad$(f, [a,b], \tau)$ for computing $\int_a^b f(x)\,dx$

- **compute** $S(a,b), S(a, \frac{a+b}{2}), S(\frac{a+b}{2}, b)$,
- **if**
$$\frac{1}{15}\left|S(a,b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)\right| \leq \tau,$$
return $S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b)$.
- **else return**
$$\textbf{AdaptQuad}(f, [a, \frac{a+b}{2}], \tau/2) + \textbf{AdaptQuad}(f, [\frac{a+b}{2}, b], \tau/2).$$

Adaptive Simpson (I)

```
function [Int,flg, fcnt,level] = AdaptSimpson(FunFcn,interv,tol,L)

a = interv(1);
b = interv(2);

%
% Evaluate the function at three nodal points
%
x = [a;(a + b)/2;b];
f = FunFcn(x);

fx      = [x, f];
simpson = ([1 4 1] * f)*(b-a)/6;
[Int,flg,fcnt,level] = AdaptSimpson2(FunFcn,tol,L,fx,simpson);
fcnt    = fcnt + 3;
level   = L - level + 1;
```

Adaptive Simpson (II)

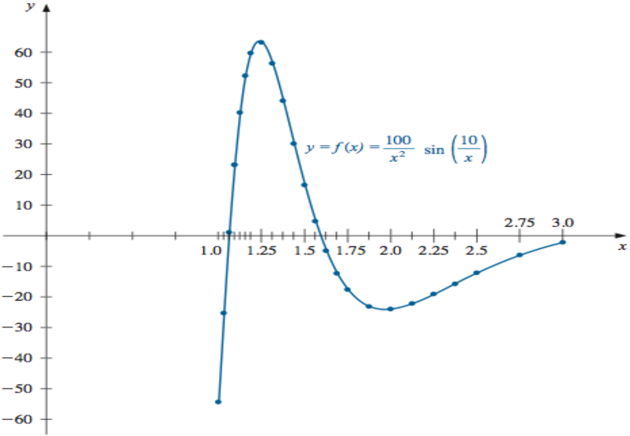
```
function [Int,flg,fcnt,level] = AdaptSimpson2(FunFcn,tol,L,fx,simpson)
%
% Recursive Adaptive Simpson's Rule
%
% Evaluate the function at three nodal points
%
xnew = [fx(1,1)+fx(2,1);fx(2,1)+fx(3,1)]/2;
fnew = FunFcn(xnew);
fcnt = 2;
h2   = (fx(3,1)-fx(1,1))/4;
simpson1 = sum([1 4 1] .* [fx(1,2) fnew(1) fx(2,2)])*h2/3;
simpson2 = sum([1 4 1] .* [fx(2,2) fnew(2) fx(3,2)])*h2/3;
Int      = simpson1+simpson2;
level    = L;
if (abs(Int-simpson)<15*tol)
    flg      = 0;
    return;
end
if (L == 1)
    flg = 1;
    return;
end
fx1  = [fx(1,1) fx(1,2);xnew(1) fnew(1); fx(2,1) fx(2,2)];
fx2  = [fx(2,1) fx(2,2);xnew(2) fnew(2); fx(3,1) fx(3,2)];
[Int1,flg1,fcnt1,level1] = AdaptSimpson2(FunFcnIn,tol/2,L-1,fx1,simpson1);
[Int2,flg2,fcnt2,level2] = AdaptSimpson2(FunFcnIn,tol/2,L-1,fx2,simpson2);
Int  = Int1 + Int2;
flg  = max(flg1, flg2);
fcnt = 2 + fcnt1 + fcnt2;
level= min(level1,level2);
```

Adaptive Simpson, example

- Integral $\int_1^3 f(x)\, dx$,

$$f(x) = \frac{100}{x^2} \mathbf{sin} \left(\frac{10}{x} \right).$$

- Tolerance $\tau = 10^{-4}$.



function $\mathtt{quad}(f, [a,b], \tau)$ of `matlab`

For a given tolerance τ,

- **composite Simpson**: $S(a,b), S(a,\frac{a+b}{2})$ and $S(\frac{a+b}{2},b)$.
- **Romberg extrapolation**:

$$\mathcal{Q}_1 = S(a,\frac{a+b}{2})+S(\frac{a+b}{2},b), \quad \mathcal{Q} = \mathcal{Q}_1+\frac{1}{15}\left(\mathcal{Q}_1 - S(a,b)\right).$$

- **if**

$$|\mathcal{Q}-\mathcal{Q}_1| \leq \tau,$$

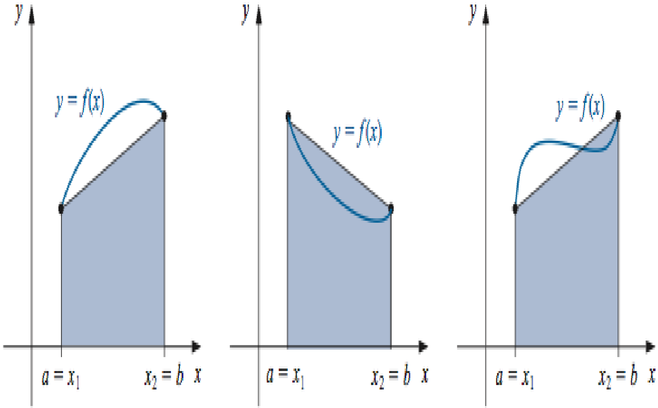
  return $\mathcal{Q}$

- **else return**

$$\mathtt{quad}(f,[a,\frac{a+b}{2}],\tau/2)+\mathtt{quad}(f,[\frac{a+b}{2},b],\tau/2).$$

Gaussian Quadrature (I)

- Trapezoidal rule with $x_1 = a, x_2 = b$ unlikely best node choices.



- Likely better node choices.

Gaussian Quadrature (II)

- Given $n > 0$, choose both distinct nodes $x_1, \cdots, x_n \in [-1, 1]$ and weights $c_1, \cdots, c_n$, so quadrature

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{j=1}^{n} c_j f(x_j), \tag{1}$$

gives the greatest degree of precision (**DoP**).

Gaussian Quadrature (II)

- Given $n > 0$, choose both distinct nodes $x_1, \cdots, x_n \in [-1, 1]$ and weights $c_1, \cdots, c_n$, so quadrature

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{j=1}^{n} c_j f(x_j), \qquad (1)$$

gives the greatest degree of precision (**DoP**).

- $2n$ total number of parameters in quadrature, could choose $2n$ monomials

$$f(x) = 1, x, x^2, \cdots, x^{2n-1}$$

in equation (1).

Gaussian Quadrature (II)

- Given $n > 0$, choose both distinct nodes $x_1, \cdots, x_n \in [-1, 1]$ and weights $c_1, \cdots, c_n$, so quadrature

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{j=1}^{n} c_j f(x_j), \tag{1}$$

  gives the greatest degree of precision (**DoP**).
- $2n$ total number of parameters in quadrature, could choose $2n$ monomials

$$f(x) = 1, x, x^2, \cdots, x^{2n-1}$$

  in equation (1).
- directly solving equation (1) can be very hard.

Gaussian Quadrature, $n = 2$ (I)

- Consider Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2).$$

Gaussian Quadrature, $n = 2$ (I)

- Consider Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2).$$

- Choose parameters c_1, c_2 and $x_1 < x_2$ so that Gaussian quadrature is exact for $f(x) = 1, x, x^2, x^3$:

$$\int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2),$$

Gaussian Quadrature, $n = 2$ (I)

- Consider Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2).$$

- Choose parameters c_1, c_2 and $x_1 < x_2$ so that Gaussian quadrature is exact for $f(x) = 1, x, x^2, x^3$:

$$\int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2), \quad \text{or}$$

$$2 = \int_{-1}^{1} 1\,dx = c_1 + c_2, \qquad 0 = \int_{-1}^{1} x\,dx = c_1\,x_1 + c_2\,x_2,$$

$$\frac{2}{3} = \int_{-1}^{1} x^2\,dx = c_1\,x_1^2 + c_2\,x_2^2, \qquad 0 = \int_{-1}^{1} x^3\,dx = c_1\,x_1^3 + c_2\,x_2^3.$$

Gaussian Quadrature, $n = 2$ (II)

- $x_1 < x_2$,
$$c_1\, x_1 = -c_2\, x_2, \quad c_1\, x_1^3 = -c_2\, x_2^3,$$
implying $x_1^2 = x_2^2$. Thus $x_1 = -x_2$ and $c_1 = c_2$.

Gaussian Quadrature, $n = 2$ (II)

- $x_1 < x_2$,
$$c_1\, x_1 = -c_2\, x_2, \quad c_1\, x_1^3 = -c_2\, x_2^3,$$
implying $x_1^2 = x_2^2$. Thus $x_1 = -x_2$ and $c_1 = c_2$.
-
$$c_1 + c_2 = 2, \quad c_1\, x_1^2 + c_2\, x_2^2 = \frac{2}{3},$$
which implies $c_1 = c_2 = 1$, $x_2 = \frac{1}{\sqrt{3}}$.
- Gaussian quadrature for $n = 2$
$$\int_{-1}^{1} f(x)\, dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}),$$
- exact for $f(x) = 1, x, x^2, x^3$, but not for $f(x) = x^4$.

- Legendre

- Legendre

- Legendre polynomials: $P_0(x) = 1, P_1(x) = x$.
  Bonnets recursive formula for $n \geq 1$:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

- Legendre

- Legendre polynomials: $P_0(x) = 1, P_1(x) = x$.
  Bonnets recursive formula for $n \geq 1$:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

n	$P_n(x)$
0	1
1	x
2	$\frac{1}{2}(3x^2 - 1)$
3	$\frac{1}{2}(5x^3 - 3x)$
4	$\frac{1}{8}(35x^4 - 30x^2 + 3)$
5	$\frac{1}{8}(63x^5 - 70x^3 + 15x)$

- $P_n(x)$ has degree exactly n.
- Legendre polynomials are orthogonal polynomials:

$$\int_{-1}^{1} P_m(x)\, P_n(x)\, dx = 0, \quad \text{whenever} \quad m < n.$$

- $P_n(x)$ has degree exactly n.
- Legendre polynomials are orthogonal polynomials:

$$\int_{-1}^{1} P_m(x)\, P_n(x)\, dx = 0, \quad \text{whenever} \quad m < n.$$

- Let $Q(x)$ be any polynomial of degree $< n$.
  Then $Q(x)$ is a linear combination of $P_0(x), P_1(x), \cdots, P_n(x)$:

$$Q(x) = \alpha_0\, P_0(x) + \alpha_1\, P_1(x) + \cdots + \alpha_{n-1}\, P_{n-1}(x).$$

- $P_n(x)$ has degree exactly n.
- Legendre polynomials are orthogonal polynomials:

$$\int_{-1}^{1} P_m(x)\, P_n(x)\, dx = 0, \quad \text{whenever} \quad m < n.$$

- Let $Q(x)$ be any polynomial of degree $< n$.
  Then $Q(x)$ is a linear combination of $P_0(x), P_1(x), \cdots, P_n(x)$:

$$Q(x) = \alpha_0\, P_0(x) + \alpha_1\, P_1(x) + \cdots + \alpha_{n-1}\, P_{n-1}(x).$$

$$\begin{aligned}
\int_{-1}^{1} Q(x) P_n(x)\, dx &= \alpha_0 \int_{-1}^{1} P_0(x) P_n(x)\, dx + \alpha_1 \int_{-1}^{1} P_1(x) P_n(x)\, dx \\
&\quad + \cdots + \alpha_{n-1} \int_{-1}^{1} P_{n-1}(x) P_n(x)\, dx \\
&= 0.
\end{aligned}$$

Gaussian Quadrature: Definition

- **Theorem**: $P_n(x)$ has exactly n distinct roots

$$-1 < x_1 < x_2 < \cdots < x_n < 1.$$

- **Define**: Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

Gaussian Quadrature: Definition

- **Theorem**: $P_n(x)$ has exactly n distinct roots

$$-1 < x_1 < x_2 < \cdots < x_n < 1.$$

- **Define**: Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

- **Choose**: for $i = 1, \cdots, n$,

$$c_i \stackrel{def}{=\!=} \int_{-1}^{1} L_i(x)\,dx = \int_{-1}^{1} \left(\prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \right) dx.$$

Gaussian Quadrature: Definition

- **Theorem**: $P_n(x)$ has exactly n distinct roots

$$-1 < x_1 < x_2 < \cdots < x_n < 1.$$

- **Define**: Gaussian quadrature

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

- **Choose**: for $i = 1, \cdots, n$,

$$c_i \stackrel{def}{=\!=} \int_{-1}^{1} L_i(x)\,dx = \int_{-1}^{1} \left(\prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \right) dx.$$

- Quadrature exact for polynomials of degree at most $n - 1$.

Theorem: DoP of Gaussian Quadrature $= 2n - 1$

- Gaussian quadrature, with roots of $P_n(x)$ $x_1, x_2, \cdots, x_n$:

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

Theorem: DoP of Gaussian Quadrature $= 2n - 1$

- Gaussian quadrature, with roots of $P_n(x)$ $x_1, x_2, \cdots, x_n$:

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

- **Let** $P(x)$ be any polynomial of degree at most $2n - 1$. Then

$$P(x) = Q(x)P_n(x) + R(x), \quad \text{(Polynomial Division)}$$

where $Q(x), R(x)$ polynomials of degree at most $n - 1$.

Theorem: DoP of Gaussian Quadrature $= 2n - 1$

- Gaussian quadrature, with roots of $P_n(x)$ $x_1, x_2, \cdots, x_n$:

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n),$$

- **Let** $P(x)$ be any polynomial of degree at most $2n - 1$. Then

$$P(x) = Q(x)P_n(x) + R(x), \quad \text{(Polynomial Division)}$$

where $Q(x), R(x)$ polynomials of degree at most $n - 1$.

$$\begin{aligned}
\int_{-1}^{1} P(x)\,dx &= \int_{-1}^{1} Q(x)P_n(x)\,dx + \int_{-1}^{1} R(x)\,dx \\
&= 0 + \int_{-1}^{1} R(x)\,dx \\
&= c_1 R(x_1) + c_2 R(x_2) + \cdots + c_n R(x_n) \quad \text{(quad exact for } R(x)) \\
&= c_1 P(x_1) + c_2 P(x_2) + \cdots + c_n P(x_n). \quad \text{(quad exact for } P(x))
\end{aligned}$$

$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$

- nodes and weights for $n = 2, 3, 4$

n	roots x_j	weights c_j
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

$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)$

- nodes and weights for $n = 2, 3, 4$

n	roots x_j	weights c_j
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

- **Example**: Approximate $\int_{-1}^{1} \mathbf{e}^x \mathbf{cos} x\,dx$ with $n = 3$.

$$\int_{-1}^{1} \mathbf{e}^x \mathbf{cos} x\,dx \approx 0.5555555556\mathbf{e}^{0.7745966692}\mathbf{cos}0.7745966692$$

$$+0.8888888889\mathbf{e}^{0.0}\mathbf{cos}0.0 + 0.5555555556\mathbf{e}^{-0.7745966692}\mathbf{cos}(-0.7745966692)$$

$$= 1.9333904 \quad (\text{absolute error} \approx 3 \times 10^{-5})$$