2021 Spring MAS 365
Chapter 4: Numerical Differentiation and Integration

Donghwan Kim

KAIST

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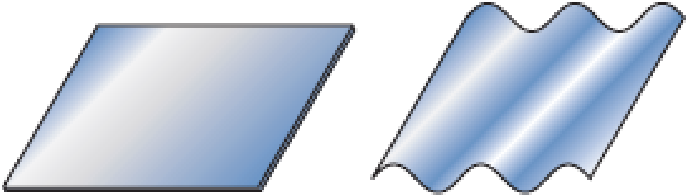
Introduction

Q. What is the length of the initial flat sheet required to make a 10m long corrugated sheet with the curve given by $f(x) = \sin x$ from $x = 0$ to $x = 10$?



- The initial length is

$$L = \int_0^{10} \sqrt{1 + (f'(x))^2}\, dx = \int_0^{10} \sqrt{1 + (\cos x)^2}\, dx.$$

1. 4.1 Numerical Differentiation
2. 4.2 Richardson's Extrapolation
3. 4.3 Elements of Numerical Integration
4. 4.4 Composite Numerical Integration
5. 4.7 Gaussian Quadrature

Numerical Differentiation

- The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

- So one simple way to approximate $f'(x_0)$ is

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

  for small values of h.

Numerical Differentiation (cont'd)

- Smaller h is not necessarily better numerically, due to round-off errors.

Goal Fit a polynomial to some set of the nodes, and use the derivative of that polynomial.

Two-Point Formulas

- Suppose $f \in C^2[a,b]$, $x_0 \in (a,b)$, $x_1 = x_0 + h \in [a,b]$ for some $h \neq 0$.

- Consider the first Lagrange polynomial $P_{0,1}(x)$ with its error term

$$f(x) = \underbrace{\frac{f(x_0)(x-x_0-h)}{-h} + \frac{f(x_0+h)(x-x_0)}{h}}_{P_{0,1}(x)} + \frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))$$

for some $\xi(x)$ between x_0 and x_1.

Two-Point Formulas (cont'd)

- Differentiating this gives

$$f'(x) = \frac{f(x_0+h)-f(x_0)}{h} + \frac{2(x-x_0)-h}{2} f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x))).$$

- When $x = x_0$, this reduces to

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2} f''(\xi).$$

Two-Point Formulas (cont'd)

- For small values of h,

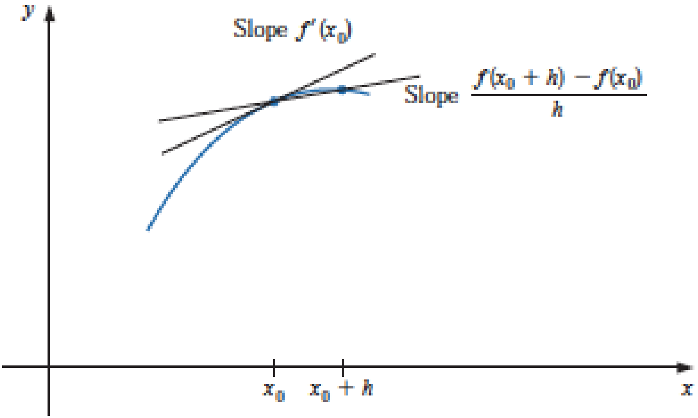
$$\frac{f(x_0+h)-f(x_0)}{h}$$

can be used to approximate $f'(x_0)$ with an error bounded by

$$\frac{M|h|}{2}, \quad \text{where } |f''(\xi)| \le M \text{ for } \xi \in (x_0, x_0+h).$$

- **Forward-difference formula** if $h > 0$.
- **Backward-difference formula** if $h < 0$.

Two-Point Formulas (cont'd)



- Let's consider more nodes to improve the accuracy.

$(n+1)$-Point Formula

- Suppose that $x_0, x_1, \ldots, x_n$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$.

$$f(x) = \sum_{k=0}^{n} f(x_k) L_k(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\cdots(x-x_n)$$

  for some $\xi(x)$ in I.

$(n+1)$-Point Formula (cont'd)

- Differentiating this gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} D_x\left[(x-x_0)\cdots(x-x_n)\right] + \frac{D_x[f^{(n+1)}(\xi(x))]}{(n+1)!}(x-x_0)\cdots(x-x_n).$$

- When $x = x_j$, this reduces to

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k).$$

- Usually consider three and five point formulas.

$(n+1)$-Point Formula (cont'd)

Theorem 1

Suppose that $x_0, x_1, \ldots, x_n$ *are* $(n+1)$ *distinct numbers in* $[a,b]$ *and that* $f \in C^{n+1}[a,b]$*. Then there exist distinct points* $\eta_1, \eta_2, \ldots, \eta_n$ *in* (a,b)*, and* $\xi(x)$ *in* (a,b) *such that*

$$f'(x) = \sum_{k=0}^{n} f(x_k) L'_k(x) + \frac{f^{(n+1)}(\xi)}{n!}(x-\eta_1)\cdots(x-\eta_n).$$

[E. Süli and D. Mayers, An Introduction to Numerical Analysis, 2003]

Three-Point Formulas

- Since $L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$, we have

$$L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)},$$

and

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}, \quad L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}.$$

- Hence, we have

$$\begin{aligned} f'(x_j) =& f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right] \\ &+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k). \end{aligned}$$

Three-Point Formulas (cont'd)

- Consider equally spaced nodes

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h \quad \text{for some } h \neq 0.$$

- Then,

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0),$$
$$f'(x_0+h) = \frac{1}{2h}\left[-f(x_0) + f(x_0+2h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1),$$
$$f'(x_0+2h) = \frac{1}{2h}\left[f(x_0) - 4f(x_0+h) + 3f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_2).$$

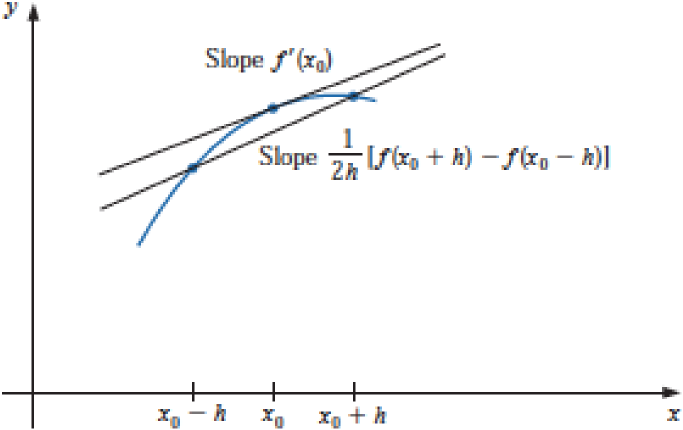
Three-Point Formulas (cont'd)

- Replacing $x_0 + h$ and $x_0 + 2h$ by x_0 yield

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

- Three-Point Endpoint Formula (the first and third)
- Three-Point Midpoint Formula (the second)

Three-Point Formulas (cont'd)



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

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

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

Numerical Differentiation

Ex Values for $f(x) = xe^x$ are given below. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$. The true value is $f'(2.0) = (2+1)e^2 = 22.167168$.

x	$f(x)$
1.8	10.9
1.9	12.7
2.0	14.8
2.1	17.1
2.2	19.9

Second Derivative Midpoint Formula

- Expand f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 + h$ and $x_0 - h$:

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4,$$
$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4,$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

Second Derivative Midpoint Formula (cont'd)

- Adding them yields

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})].$$

- By the Intermediate Value Theorem, we have

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

  for some ξ between $x_0 - h$ and $x_0 + h$.

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

Second Derivative Midpoint Formula (cont'd)

Ex Values for $f(x) = xe^x$ are given below. Approximate $f''(2.0)$. The true value is $f''(2.0) = 29.556224$.

x	$f(x)$
1.8	10.9
1.9	12.7
2.0	14.8
2.1	17.1
2.2	19.9

Round-Off Error Instability

- Recall the three-point midpoint formula:

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

- Consider the round-off errors:

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h) \quad \text{and} \quad f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h).$$

- If we assume that $|e(x_0 \pm h)| \leq \epsilon$, and that $|f^{(3)}(\xi_1)| \leq M$, we have

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \leq ?$$

Round-Off Error Instability (cont'd)

Ex. Consider using the values in the table to approximate $f'(0.900)$ by the three-point midpoint formula, where $f(x) = \sin x$. The true value is $f'(0.900) = \cos 0.900 = 0.62161$.

x	$\sin x$	x	$\sin x$
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

Round-Off Error Instability (cont'd)

- The formula

$$f'(0.900) \approx \frac{f(0.900+h) - f(0.900-h)}{2h}$$

with different values of h gives

h	Approximation to $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	−0.00011
0.020	0.62150	−0.00011
0.050	0.62140	−0.00021
0.100	0.62055	−0.00106

Round-Off Error Instability (cont'd)

- A minimum for

$$e(h) = \frac{\epsilon}{h} + \frac{h^2}{6}M$$

occurs at $h = \sqrt[3]{3\epsilon/M}$, where

$$M = \max_{x\in[0.800,1.00]} |f'''(x)| = \max_{x\in[0.800,1.00]} |\cos x| = \cos 0.8 \approx 0.69671.$$

Since values of f are given to five decimal places, we assume that $\epsilon = 5 \times 10^{-6}$. Therefore, we have

$$h = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \approx 0.028.$$

Richardson's Extrapolation

- Generate high-accuracy results using low-order formulas, when an approximation has an error term with a predictable form (one that depends on a parameter such as the step size h).

Richardson's Extrapolation (cont'd)

- Suppose that for each number $h \neq 0$ we have a formula $N_1(h)$ that approximates an unknown constant M, and

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots ,$$

for some collection of (unknown) constants $K_1, K_2, K_3, \ldots$.

The truncation error is $O(h)$, so if there is no large variation in magnitude among the constants $K_1, K_2, K_3, \ldots$

$$M - N_1(h) \approx K_1 h, .$$

Richardson's Extrapolation (cont'd)

Goal Find an easy way to combine these relatively inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error.

- Suppose, for example, we can combine the $N_1(h)$ formulas to produce an $O(h^2)$ approximation, $N_2(h)$, as

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots ,$$

for some unknown collection of constants $\hat{K}_2, \hat{K}_3, \ldots$

Richardson's Extrapolation (cont'd)

- Consider two $O(h)$ approximation formulas:

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$
$$M = N_1\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots$$

- Subtracting the first equation from twice the second one yields

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$

Richardson's Extrapolation (cont'd)

Ex. Consider the approximations to $f'(1.8)$ for $f(x) = \ln(x)$

$$h = 0.1 \ : \ f'(1.8) \approx 0.5406722, \quad \text{and} \quad h = 0.05 \ : \ f'(1.8) \approx 0.5479795$$

with the $O(h)$ truncation error. Use extrapolation on these values. The true value is $f'(1.8) = 0.\bar{5}$.

Richardson's Extrapolation (cont'd)

- Extrapolation can be applied whenever the truncation error has 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 $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$.

Richardson's Extrapolation (cont'd)

- Recall:

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]$$

- Continuing this procedure gives, for each $j = 2, 3, \ldots$, the $O(h^j)$ approximation:

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}$$

Richardson's Extrapolation (cont'd)

Ex. By Taylor's theorem, the centered-difference formula to approximate $f'(x_0)$ can expressed as

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f^{(3)}(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots .$$

Find approximations of order $O(h^2)$, $O(h^4)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

Richardson's Extrapolation (cont'd)

- When

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots ,$$

we have the $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}$$

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1: $N_1(h)$			
2: $N_1(\frac{h}{2})$	**3:** $N_2(h)$		
4: $N_1(\frac{h}{4})$	**5:** $N_2(\frac{h}{2})$	**6:** $N_3(h)$	
7: $N_1(\frac{h}{8})$	**8:** $N_2(\frac{h}{4})$	**9:** $N_3(\frac{h}{2})$	**10:** $N_4(h)$

- Round-off error in $N_1(h/2^k)$ will generally increase as k increases.

Numerical Quadrature

- When anti-derivative is not available, one can use **numerical quadrature** that replaces integration by summation as

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

  where $a \leq x_0 < x_1 < \cdots < x_n \leq b$.

- The methods of quadrature in this section are based on the interpolation polynomials studied in Chapter 3.

Numerical Quadrature (cont'd)

- Select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from $[a, b]$. then use the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x).$$

- Integrating it with its error term leads to

$$\int_a^b f(x)dx = \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x) dx + \int_a^b \prod_{i=0}^{n} (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!} dx.$$

- Trapezoidal rule: First Lagrange polynomial with equally-spaced nodes
- Simpson's rule: Second Lagrange polynomials with equally-spaced nodes

The Trapezoidal Rule

- Let $x_0 = a$, $x_1 = b$, $h = b - a$, and use the linear Lagrange polynomial:

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1).$$

- Then,

$$\begin{aligned}\int_a^b f(x)dx = &\int_{x_0}^{x_1} \left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)\right] dx \\ &+ \frac{1}{2}\int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)dx\end{aligned}$$

The Trapezoidal Rule (cont'd)

Theorem 2 (Weighted Mean Value Theorem for Integrals)

Suppose $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$, and $g(x)$ does not change sign on $[a,b]$. Then there exists a number c in (a,b) with

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx.$$

- The error term can be simplified as

$$\begin{aligned}
\int_{x_0}^{x_1} f''(\xi(x))(x-x_0)(x-x_1)dx &= f''(\xi)\int_{x_0}^{x_1}(x-x_0)(x-x_1)dx \\
&= f''(\xi)\left[\frac{x^3}{3} - \frac{x_1+x_0}{2}x^2 + x_0x_1x\right]_{x_0}^{x_1} \\
&= -\frac{h^3}{6}f''(\xi),
\end{aligned}$$

for some ξ in (x_0, x_1).

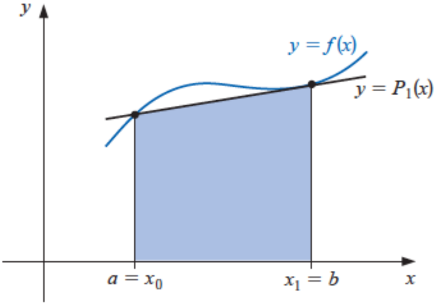
The Trapezoidal Rule (cont'd)

- Therefore,

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

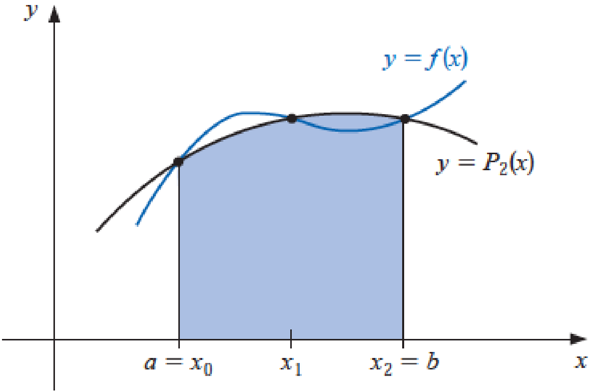
$$= \quad ? \quad - \frac{h^3}{12}f''(\xi).$$

- Exact result when ?.



Simpson's Rule

- Integrate over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_1 = a + h$, $x_2 = b$ where $h = (b - a)/2$.



Simpson's Rule (cont'd)

- We have

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right.$$
$$\left. + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$
$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)(x-x_2)}{6} f^{(3)}(\xi(x)) dx.$$

- Provides only an $O(h^4)$ error term involving $f^{(3)}$.
- One can find a higher-order error term involving $f^{(4)}$.

Trapezoidal and Simpson's Rules

Ex. Compare the Trapezoidal and Simpson's rule approximations to $\int_0^1 f(x)dx$ when $f(x)$ is (a) x, (b) x^2, (c) x^3, (d) x^4, (e) e^x.

$f(x)$	x	x^2	x^3	x^4	e^x
Exact	$1/2$	$1/3$	$1/4$	$1/5$	$e-1 \approx 1.7183$
Trapezoidal	?	?	?	?	?
Simpson's	?	?	?	?	?

Measuring Precision

Definition 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* $k = 0, 1, \ldots, n$.

- The Trapezoidal and Simpson's rules have degrees of precision ? and ?, 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 $n + 1$.

Selecting Nodes in Numerical Quadrature

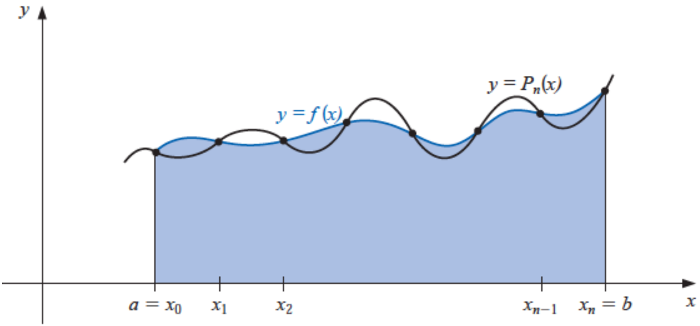
- Select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from $[a, b]$, and then use the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} f(x_i) L_i(x).$$

- Closed and Open Newton-Cotes Formulas

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 $h = (b-a)/n$.



Closed Newton-Cotes Formulas (cont'd)

Theorem 3

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* $f \in C^{n+1}[a, b]$*.*

Closed Newton-Cotes Formulas (cont'd)

- $n = 1$: Trapezoidal rule

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

- $n = 2$: Simpson's rule

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

- $n = 3$: Simpson's $\frac{3}{8}$ rule

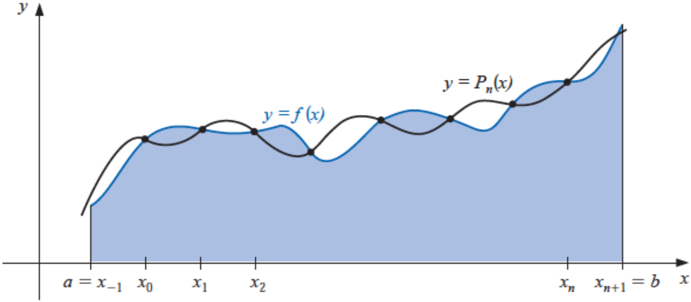
$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi)$$

- $n = 4$: Boole's rule

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

Open Newton-Cotes Formulas

- Do not include the endpoints of $[a, b]$ as nodes.



Open Newton-Cotes Formulas (cont'd)

- Use the nodes $x_i = x_0 + ih$ for each $i = 0, 1, \ldots, n$, where $h = (b-a)/(n+2)$ and $x_0 = a + h$.

- We have $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$. Then the formulas become

$$\int_a^b f(x)dx = \int_{x_{-1}}^{x_{n+1}} f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i),$$

where

$$a_i = \int_a^b L_i(x)dx.$$

Open Newton-Cotes Formulas (cont'd)

Theorem 4

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* $f \in C^{n+1}[a, b]$.

Open Newton-Cotes Formulas (cont'd)

- $n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)dx = 2hf(x_0) + h^3 3f''(\xi)$$

- $n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4}f''(\xi)$$

- $n = 2$:

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

- $n = 3$:

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

Closed and Open Newton-Cotes Formulas

Ex. Compare the results of the closed and open Newton-Cotes formulas when approximating

$$\int_0^{\pi/4} \sin x \, dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

n	0	1	2	3	4
Closed formulas		0.27768018	0.29293264	0.29291070	0.29289318
Error		0.01521303	0.00003942	0.00001748	0.00000004
Open formulas	0.30055887	0.29798754	0.29285866	0.29286923	
Error	0.00766565	0.00509432	0.00003456	0.00002399	

Composite Numerical Integration

- Newton-Cotes formulas are generally not suitable for use over large integration intervals. Why?

- Consider a *piecewise* approach to numerical integration with the low-order Newton-Cotes formulas.

Composite Numerical Integration (cont'd)

Ex. Compare the approximations resulted from applying Simpson's rule to both side of

$$\int_0^4 e^x \, dx = \int_0^2 e^x \, dx + \int_2^4 e^x \, dx$$

The exact solution is $\int_0^4 e^x \, dx = e^4 - e^0 = 53.59815$.

Sol. Simpson's rule gives

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

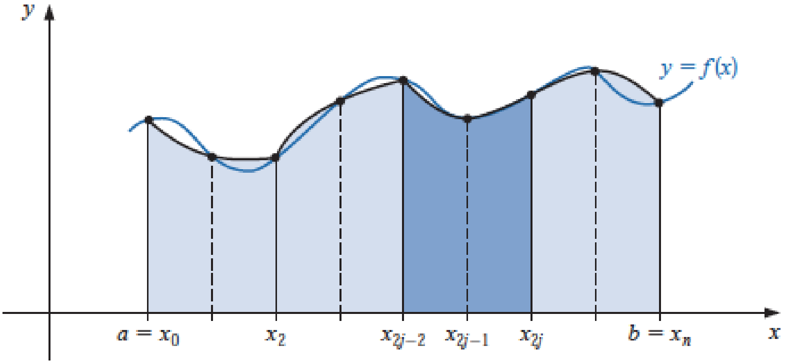
with the error -3.17143, and

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

with the error -0.26570.

Composite Simpson's Rule

- Choose an even integer n, subdivide the interval $[a, b]$ into n subintervals, and apply Simpson's rule on each consecutive pair of subintervals.



Composite Simpson's Rule (cont'd)

- With $h = (b-a)/n$ and $x_j = a + jh$ for $j = 0, 1, \ldots, n$, 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 between x_{2j-2} and x_{2j}, provided that $f \in C^4[a,b]$.

- This can be rewritten as

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

Composite Simpson's Rule (cont'd)

- Consider

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

- By the Intermediate Value Theorem, 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,

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

Composite Simpson's Rule (cont'd)

Theorem 5

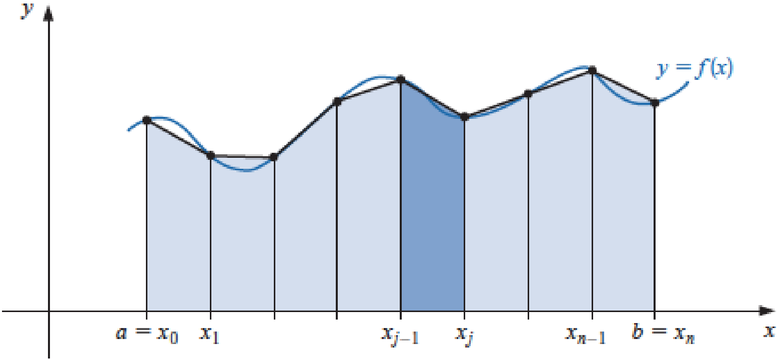
Let $f \in C^4[a,b]$, n be even, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the **Composite Simpson's rule** *for n subintervals can be written with its error term as*

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

- When $n = 2$, reduces to Simpson's rule:

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(a+h) + f(b)] - \frac{h^5}{90}f^{(4)}(\mu).$$

Composite Trapezoidal Rule



Composite Trapezoidal Rule (cont'd)

Theorem 6

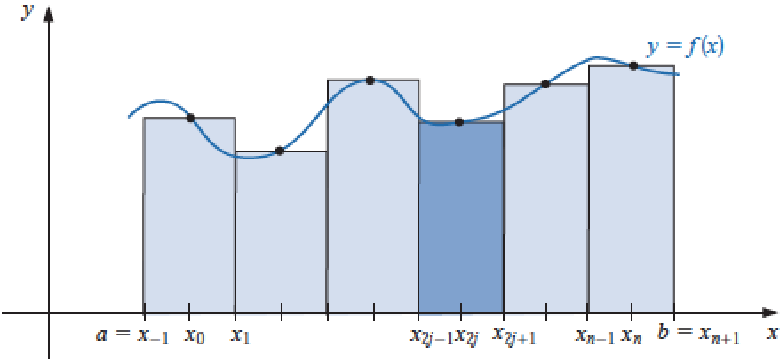
Let $f \in C^2[a,b]$, $h = (b-a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a,b)$ for which the **Composite Trapezoidal rule** *for n subintervals can be written with its error term as*

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

- When $n = 1$, reduces to Trapezoidal rule:

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

Composite Midpoint Rule



Composite Midpoint Rule (cont'd)

Theorem 7

Let $f \in C^2[a,b]$, n be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$, for each $j = -1, 0, 1, \ldots, n+1$. 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*

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

- When $n = 0$, reduces to Midpoint rule:

$$\int_a^b f(x)dx = 2hf(x_0) + \frac{h^3}{3} f''(\mu)$$

Composite Numerical Integration

Ex. Determine values of h that will ensure an error of less than 0.00002 when approximating $\int_0^\pi \sin x \, dx$ and employing

(a) Composite Trapezoidal rule

(b) Composite Simpson's rule

Sol. The error terms are

$$\left|\frac{\pi h^2}{12} f''(\mu)\right| = \frac{\pi h^2}{12} |\sin \mu| \quad \text{and} \quad \left|\frac{\pi h^4}{180} f^{(4)}(\mu)\right| = \frac{\pi h^4}{180} |\sin \mu|$$

Using $h = \pi/n$, we have

$$\frac{\pi^3}{12n^2} < 0.00002 \quad \text{and} \quad \frac{\pi^5}{180n^4} < 0.00002,$$

which gives

$$n > 359.04 \quad \text{and} \quad n > 17.07.$$

Round-Off Error Stability

- Consider the approximation

$$f(x_i) = \tilde{f}(x_i) + e_i, \quad \text{for each } i = 0, 1, \ldots, n,$$

where e_i denotes the round-off error.

Round-Off Error Stability (cont'd)

- The accumulated error in the Composite Simpson's rule is

$$e(h) = \left| \frac{h}{3} \left[e_0 + 2 \sum_{j=1}^{(n/2)-1} e_{2j} + 4 \sum_{j=1}^{n/2} e_{2j-1} + e_n \right] \right|$$
$$\leq \frac{h}{3} \left[|e_0| + 2 \sum_{j=1}^{(n/2)-1} |e_{2j}| + 4 \sum_{j=1}^{n/2} |e_{2j-1}| + |e_n| \right]$$

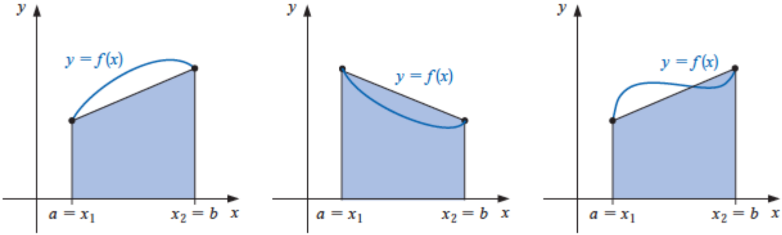
- If the round-off errors are uniformly bounded by ϵ, then

$$e(h) \leq ?$$

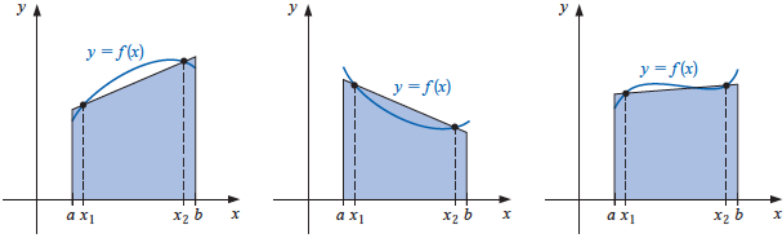
- Composite integration is ? with respect to round-off error.

Gaussian Quadrature

- Trapezoidal rule



- Better choice?



Gaussian Quadrature (cont'd)

- Choose nodes $x_1, \ldots, x_n$ in the interval $[a, b]$ and coefficients $c_1, \ldots, c_n$, so that they minimize the expected error in the approximation

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

Gaussian Quadrature (cont'd)

Definition 2

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 $k = 0, 1, \ldots, n$.*

- The class of polynomials of degree at most $2n - 1$ also contains $2n$ parameters. This is the largest class of polynomials for which it is reasonable to expect a formula to be exact.

Gaussian Quadrature (cont'd)

$n \rightarrow 2n-1$

Number of points	Newton-Cotes Closed	Newton-Cotes Open	Gaussian
1		1	1
2	1	1	3
3	3	3	5
4	3	3	7

Table: Degree of accuracy

Gaussian Quadrature (cont'd)

- Consider $n = 2$ and $[-1, 1]$. Suppose we want to determine c_1, c_2, x_1 and x_2 so that the integration formula

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

gives the exact result whenever $f(x)$ is a polynomial of degree $2 \times 2 - 1 = 3$ or less, that is, when

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

- Since

$$\int (a_0 + a_1 x + a_2 x^2 + a_3 x^3)dx$$
$$= a_0 \int 1dx + a_1 \int xdx + a_2 \int x^2 dx + a_3 \int x^3 dx,$$

it is equivalent to show that the formula gives exact results when $f(x)$ is $1, x, x^2$ and x^3.

Legendre Polynomials

- Tedious to extend the previous approach for higher-order cases.

- Relevant to our problem is the Legendre polynomials,

$$\{P_0(x), P_1(x), \dots, P_n(x), \dots\}$$

  with properties:

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

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

- The roots of the Legendre polynomials are distinct, lie in $(-1, 1)$, and have a symmetry with respect to the origin.

Legendre Polynomials (cont'd)

- The first few Legendre polynomials are

$$\begin{aligned} P_0(x) &= 1, \\ P_1(x) &= x, \\ P_2(x) &= x^2 - \frac{1}{3}, \\ P_3(x) &= x^3 - \frac{3}{5}x, \\ P_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35}. \end{aligned}$$

- 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.

Higher-Order Gaussian Quadrature

Theorem 8

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

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

Proof. Consider two cases.

(a) $P(x)$ of degree less than n

(b) $P(x)$ of degree at least n but less than $2n$.

Higher-Order Gaussian Quadrature (cont'd)

(a) $P(x)$ of degree less than n:

Rewrite $P(x)$ in terms of $(n-1)$th Lagrange coefficient polynomials with nodes at the roots of the nth Legendre polynomial $P_n(x)$. (The error term is 0):

$$P(x) = \sum_{i=1}^{n} P(x_i) L_i(x) = \sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i)$$

and

$$\int_{-1}^{1} P(x) dx = \int_{-1}^{1} \left[\sum_{i=1}^{n} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} P(x_i) \right] dx = \sum_{i=1}^{n} c_i P(x_i).$$

Higher-Order Gaussian Quadrature (cont'd)

(b) $P(x)$ of degree at least n but less than $2n$:

Divide $P(x)$ by the nth Legendre polynomial $P_n(x)$ as

$$P(x) = Q(x)P_n(x) + R(x)$$

where both $Q(x)$ and $R(x)$ are of degree less than n. We then have

$$\int_{-1}^{1} Q(x)P_n(x)dx = ?, \qquad \int_{-1}^{1} R(x)dx = ?$$

Since x_i is a root of $P_n(x)$ for each $i = 1, 2, \ldots, n$, we have

$$P(x_i) = ?$$

Putting all together, we have

$$\int_{-1}^{1} P(x)dx = \int_{-1}^{1} [Q(x)P_n(x) + R(x)]dx = \quad ? \quad = \sum_{i=1}^{n} c_i P(x_i)$$

$\square$

Higher-Order Gaussian Quadrature (cont'd)

- The constants c_i needed for quadrature can be generated from the formula, but 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

Higher-Order Gaussian Quadrature (cont'd)

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

Gaussian Quadrature on Arbitrary Intervals

- An integral $\int_a^b f(x)dx$ over an arbitrary $[a, b]$ can be transformed into an integral over $[-1, 1]$ by using the change of variables

$$t = \frac{2x - a - b}{b - a} \quad \Leftrightarrow \quad x = \frac{(b-a)t + a + b}{2}.$$

- We can then apply Gaussian Quadrature form to any interval $[a, b]$ as

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{(b-a)t + a + b}{2}\right)\frac{b-a}{2}dt.$$

Gaussian Quadrature on Arbitrary Intervals (cont'd)

Ex. Consider the integral $\int_1^3 x^6 - x^2 \sin(2x)\, dx = 317.3442466$. Compare the results for the closed Newton-Cotes formula with $n = 1$, the open Newton-Cotes formula with $n = 1$, and Gaussian Quadrature when $n = 2$.