Ch 04-4 Composite Numerical Integration

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Outline

- A Motivating Example
- The Composite Simpson's Rule
- The Composite Trapezoidal & Midpoint Rules
- Comparing the Composite Simpson & Trapezoidal Rules

Composite Numerical Integration: Motivating Example

Application of Simpson's Rule

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

$$\int_0^2 e^x \, dx \quad \text{and} \quad \int_2^4 e^x \, dx$$

and adding those for

$$\int_0^1 e^x \, dx, \quad \int_1^2 e^x \, dx, \quad \int_2^3 e^x \, dx \quad \text{and} \quad \int_3^4 e^x \, dx$$

Composite Numerical Integration: Motivating Example

Solution (1/3)

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

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

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.

Composite Numerical Integration: Motivating Example

Solution (2/3)

Applying Simpson's rule on each of the intervals $[0, 2]$ and $[2, 4]$ uses $h = 1$ and gives

$$\begin{aligned}
\int_0^4 e^x \, dx &= \int_0^2 e^x \, dx + \int_2^4 e^x \, dx \\
&\approx \frac{1}{3}\left(e^0 + 4e + e^2\right) + \frac{1}{3}\left(e^2 + 4e^3 + e^4\right) \\
&= \frac{1}{3}\left(e^0 + 4e + 2e^2 + 4e^3 + e^4\right) \\
&= 53.86385
\end{aligned}$$

The error has been reduced to -0.26570.

Composite Numerical Integration: Motivating Example

Solution (3/3)

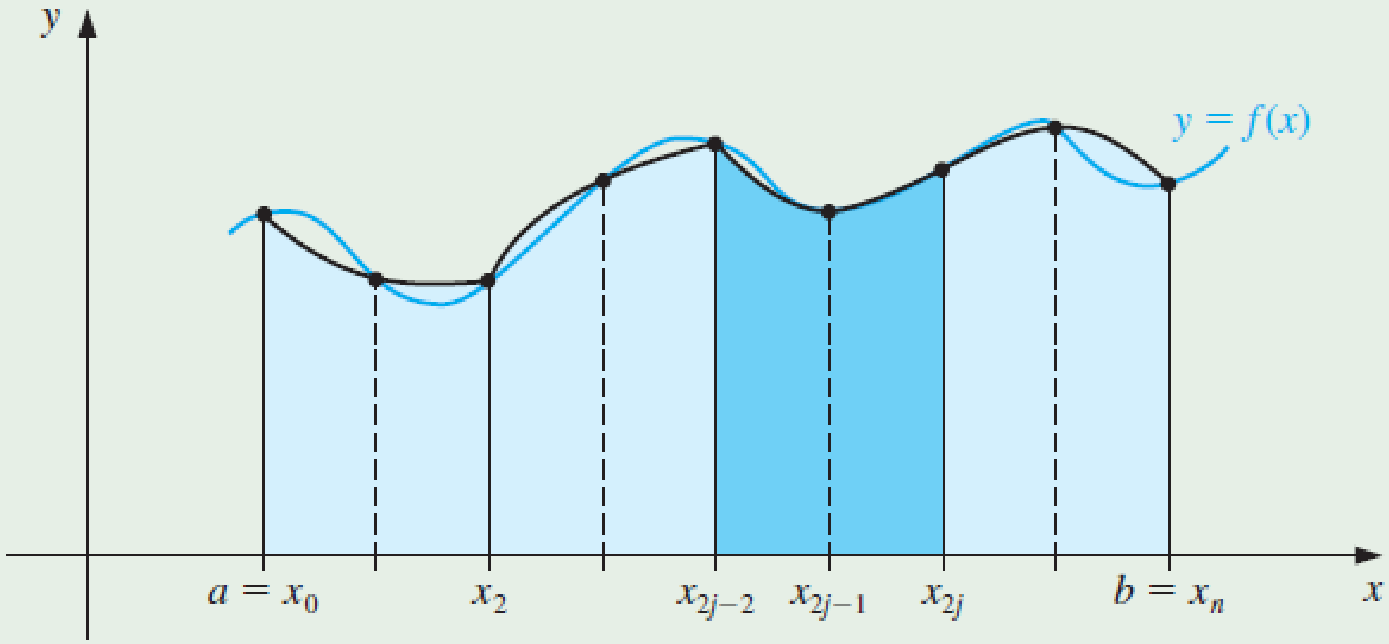
For the integrals on [0, 1],[1, 2],[3, 4], and [3, 4] we use Simpson's rule four times with $h = \frac{1}{2}$ giving

$$
\begin{aligned}
\int_0^4 e^x\,dx &= \int_0^1 e^x\,dx + \int_1^2 e^x\,dx + \int_2^3 e^x\,dx + \int_3^4 e^x\,dx \\
&\approx \frac{1}{6}\left(e_0 + 4e^{1/2} + e\right) + \frac{1}{6}\left(e + 4e^{3/2} + e^2\right) \\
&\quad + \frac{1}{6}\left(e^2 + 4e^{5/2} + e^3\right) + \frac{1}{6}\left(e^3 + 4e^{7/2} + e^4\right) \\
&= \frac{1}{6}\left(e^0 + 4e^{1/2} + 2e + 4e^{3/2} + 2e^2 + 4e^{5/2} + 2e^3 + 4e^{7/2} + e^4\right) \\
&= 53.61622.
\end{aligned}
$$

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

Composite Numerical Integration: Simpson's Rule

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.



Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term

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

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

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

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

Composite Numerical Integration: Simpson's Rule

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

Construct the Formula & Error Term (Cont'd)

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

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

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

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 See Theorem implies that $f^{(4)}$ assumes its maximum and minimum in $[a, b]$.

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

Since

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

we have

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

and

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

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

By the Intermediate Value Theorem ▸ See 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

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

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

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

Composite Numerical Integration: Simpson's Rule

These observations produce the following result.

Theorem: Composite Simpson's Rule

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

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

Composite Numerical Integration: Simpson's Rule

Comments on the Formula & Error Term

- Notice that the error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule.

Composite Numerical Integration: Simpson's Rule

Comments on the Formula & Error Term

- Notice that the error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule.
- However, these rates are not comparable because, for the standard Simpson's rule, we have h fixed at $h = (b - a)/2$, but for Composite Simpson's rule we have $h = (b - a)/n$, for n an even integer.
- This permits us to considerably reduce the value of h.
- The following algorithm uses the Composite Simpson's rule on n subintervals. It is the most frequently-used general-purpose quadrature algorithm.

Composite Integration: Simpson's Rule Algorithm

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

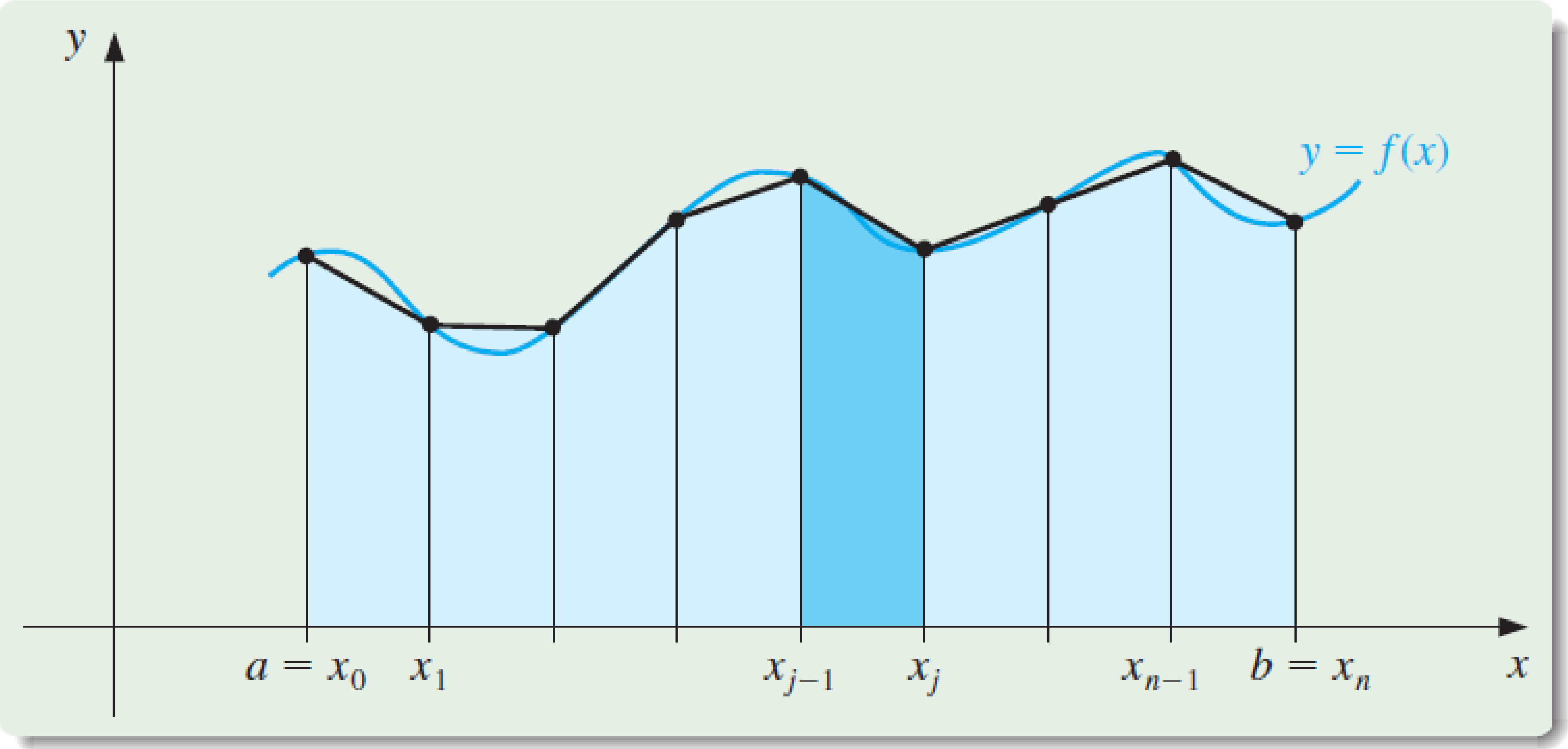
INPUT	endpoints a, b; even positive integer n
OUTPUT	approximation XI to I
Step 1	Set $h = (b - a)/n$
Step 2	Set $XI0 = f(a) + f(b)$
	$XI1 = 0;$ $\quad$ (*Summation of* $f(x_{2i-1})$)
	$XI2 = 0.$ $\quad$ (*Summation of* $f(x_{2i})$)
Step 3	For $i = 1, \ldots, n - 1$ do Steps 4 and 5:
	Step 4: Set $X = a + ih$
	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 Integration: Trapezoidal & Midpoint Rules

Preamble

- The subdivision approach can be applied to any of the Newton-Cotes formulas.
- The extensions of the Trapezoidal and Midpoint rules will be presented without proof.
- The Trapezoidal rule requires only one interval for each application, so the integer n can be either odd or even.
- For the Midpoint rule, however, the integer n must be even.

Numerical Integration: Composite Trapezoidal Rule



Note: The Trapezoidal rule requires only one interval for each application, so the integer n can be either odd or even.

Numerical Integration: Composite Trapezoidal Rule

Theorem: 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

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

Numerical Integration: Composite Midpoint Rule

Midpoint Rule (1-point open Newton-Cotes formula)

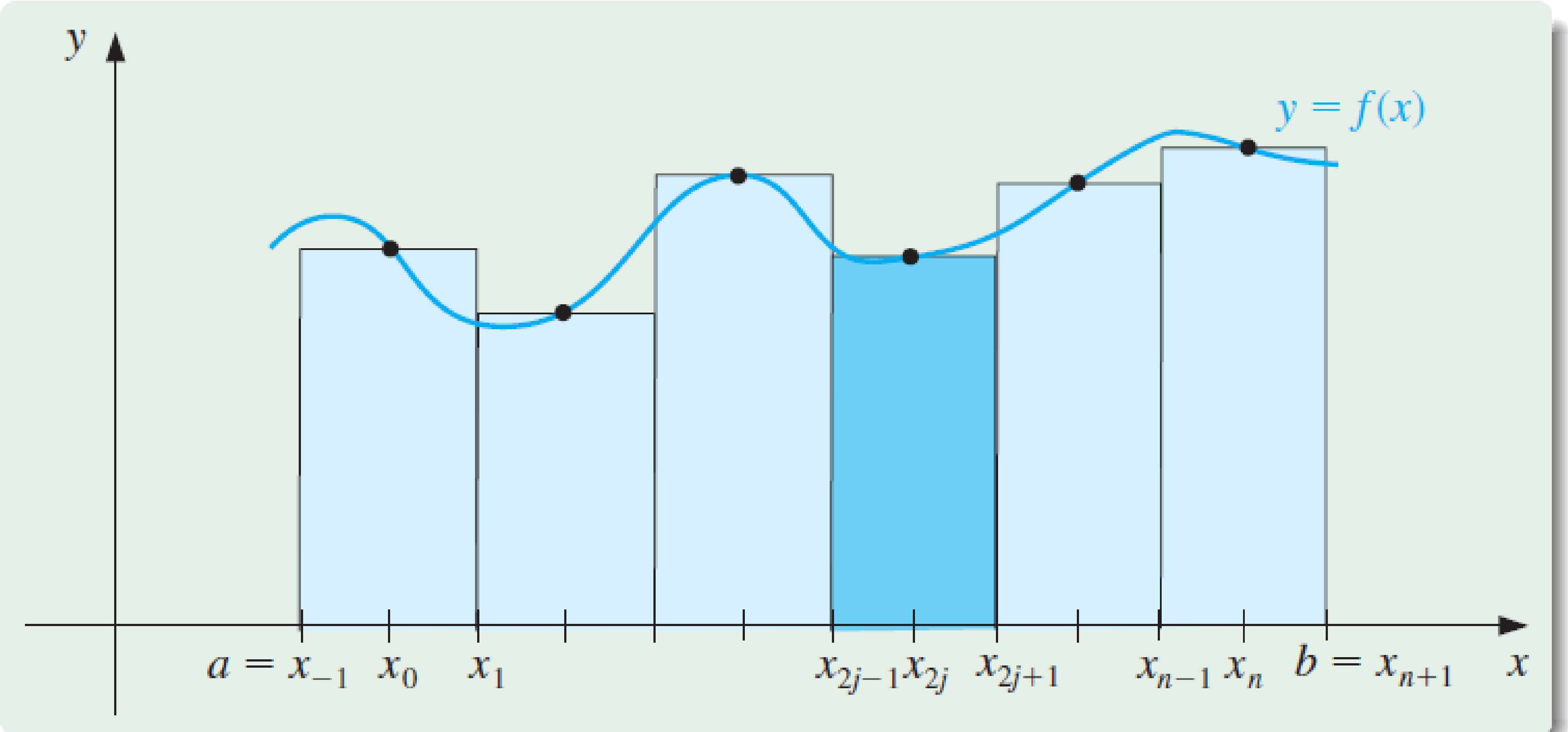
$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1$$

Theorem: 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

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

Numerical Integration: Composite Midpoint Rule



Note: The Midpoint Rule requires two intervals for each application, so the integer n must be even.

Composite Numerical Integration: Example

Example: Trapezoidal .v. Simpson's Rules

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.

Composite Numerical Integration: Example

Solution (1/5)

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

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

To ensure sufficient accuracy with this technique, we need to have

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

Composite Numerical Integration: Example

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

Solution (2/5)

Since $h = \pi/n$ implies that $n = \pi/h$, we need

$$\begin{aligned}\frac{\pi^3}{12n^2} &< 0.00002 \\ \Rightarrow \quad n &> \left(\frac{\pi^3}{12(0.00002)}\right)^{1/2} \approx 359.44\end{aligned}$$

and the Composite Trapezoidal rule requires $n \geq 360$.

Composite Numerical Integration: Example

Solution (3/5)

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

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

To ensure sufficient accuracy with this technique we need to have

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

Composite Numerical Integration: Example

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

Solution (4/5)

Using again the fact that $n = \pi/h$ gives

$$\frac{\pi^5}{180n^4} < 0.00002 \quad \Rightarrow \quad n > \left(\frac{\pi^5}{180(0.00002)}\right)^{1/4} \approx 17.07$$

So Composite Simpson's rule requires only $n \geq 18$.

Composite Numerical Integration: Example

Solution (5/5)

Composite Simpson's rule with $n = 18$ gives

$$\int_0^{\pi} \sin x \, dx \approx \frac{\pi}{54}\left[2\sum_{j=1}^{8} \sin\left(\frac{j\pi}{9}\right) + 4\sum_{j=1}^{9} \sin\left(\frac{(2j-1)\pi}{18}\right)\right]$$
$$= 2.0000104$$

This is accurate to within about 10^{-5} because the true value is $-\cos(\pi) - (-\cos(0)) = 2$.

Composite Numerical Integration: Conclusion

- Composite Simpson's rule is the clear choice if you wish to minimize computation.
- For comparison purposes, consider the Composite Trapezoidal rule using $h = \pi/18$ for the integral in the previous example.
- This approximation uses the same function evaluations as Composite Simpson's rule but the approximation in this case

$$\begin{aligned}\int_0^\pi \sin x \, dx &\approx \frac{\pi}{36}\left[2\sum_{j=1}^{17} \sin\left(\frac{j\pi}{18}\right) + \sin 0 + \sin \pi\right] \\ &= \frac{\pi}{36}\left[2\sum_{j=1}^{17} \sin\left(\frac{j\pi}{18}\right)\right] = 1.9949205\end{aligned}$$

is accurate only to about 5×10^{-3}.