Numerical Differentiation & Integration

Composite Numerical Integration I

Numerical Analysis (9th Edition)

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Beamer Presentation Slides
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Outline

1. A Motivating Example

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2 The Composite Simpson's Rule

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2. The Composite Simpson's Rule
3. The Composite Trapezoidal & Midpoint Rules

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4. Comparing the Composite Simpson & Trapezoidal Rules

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Composite Numerical Integration: Motivating Example

Application of Simpson's Rule

Use Simpson's rule to approximate

$$\int_0^4 e^x \, dx$$

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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)

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

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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.

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

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&\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)
\end{aligned}$$

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

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&= \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 $h = \frac{1}{2}$

Composite Numerical Integration: Motivating Example

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$$\int_0^4 e^x\, dx = \int_0^1 e^x\, dx + \int_1^2 e^x\, dx + \int_2^3 e^x\, dx + \int_3^4 e^x\, dx$$

$$\approx \frac{1}{6}\left(e_0 + 4e^{1/2} + e\right) + \frac{1}{6}\left(e + 4e^{3/2} + e^2\right)$$

$$+ \frac{1}{6}\left(e^2 + 4e^{5/2} + e^3\right) + \frac{1}{6}\left(e^3 + 4e^{7/2} + e^4\right)$$

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

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

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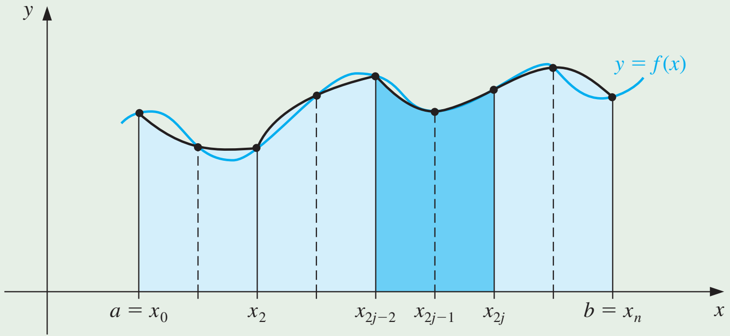
3 The Composite Trapezoidal & Midpoint Rules

4 Comparing the Composite Simpson & Trapezoidal Rules

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 $j = 0, 1, \ldots, n$,

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

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

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

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 $[x_{2j-2}, x_{2j}]$

Composite Numerical Integration: Simpson's Rule

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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 $[x_{2j}, x_{2j+2}]$,

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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

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

Composite Numerical Integration: Simpson's Rule

Construct the Formula & Error Term (Cont'd)

Since

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we have

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

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and

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

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

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

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

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

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

Composite Numerical Integration: Simpson's Rule

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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 $j = 0, 1, \ldots, n$.

Composite Numerical Integration: Simpson's Rule

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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

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- 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.

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- 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 $I = \int_a^b f(x)\, dx$:

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INPUT endpoints a, b; even positive integer n

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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 $XI0 = f(a) + f(b)$
	$XI1 = 0$; (*Summation of* $f(x_{2i-1})$)
	$XI2 = 0$. (*Summation of* $f(x_{2i})$)

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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 $XI1 = XI1 + f(X)$

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Step 4: Set $X = a + ih$
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else set $XI1 = XI1 + f(X)$

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

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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

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Composite Integration: Trapezoidal & Midpoint Rules

Preamble

- The subdivision approach can be applied to any of the Newton-Cotes formulas.

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Composite Integration: Trapezoidal & Midpoint Rules

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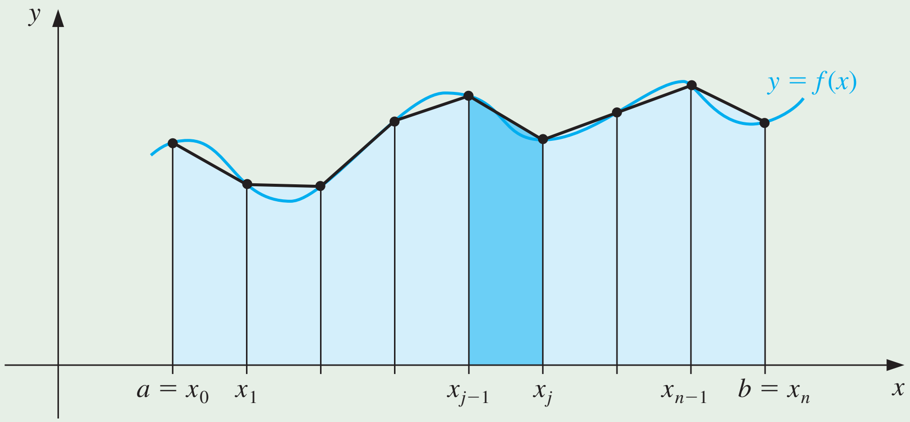
- The subdivision approach can be applied to any of the Newton-Cotes formulas.
- The extensions of the Trapezoidal and Midpoint rules will be presented without proof.
- The Trapezoidal rule requires only one interval for each application, so the integer n can be either odd or even.
- For the Midpoint 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 $j = 0, 1, \ldots, n$.

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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)

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

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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 $j = -1, 0, \ldots, n+1$.

Numerical Integration: Composite Midpoint Rule

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

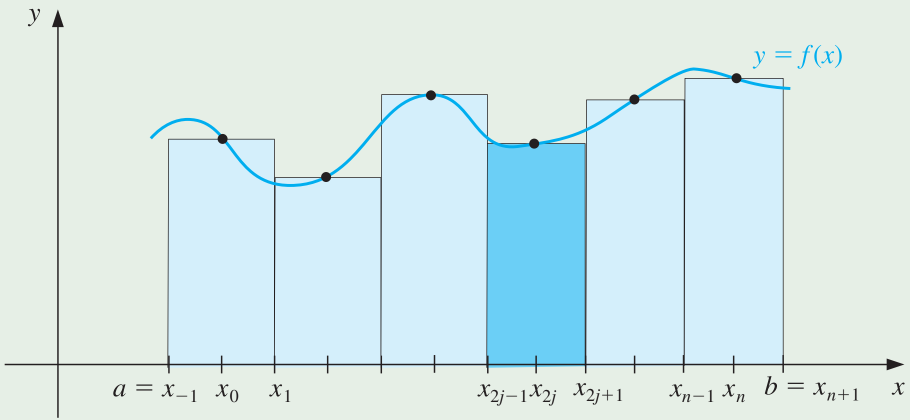
$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3}f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1$$

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.

Outline

1. A Motivating Example
2. The Composite Simpson's Rule
3. The Composite Trapezoidal & Midpoint Rules
4. Comparing the Composite Simpson & Trapezoidal Rules

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:

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Composite Numerical Integration: Example

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

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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

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

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

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

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

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

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$$= \frac{\pi}{36}\left[2\sum_{j=1}^{17}\sin\left(\frac{j\pi}{18}\right)\right] = 1.9949205$$

is accurate only to about 5×10^{-3}.

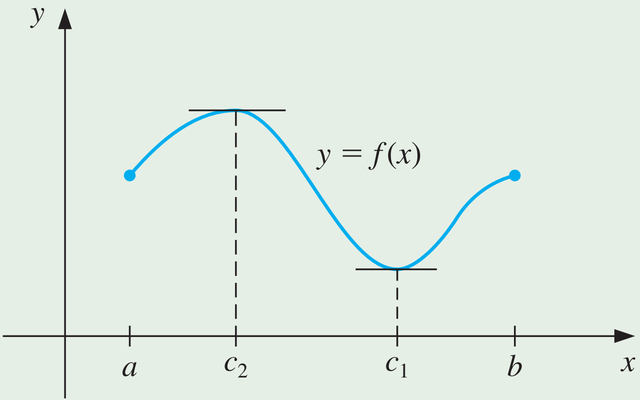
Questions?

Reference Material

The Extreme Value Theorem

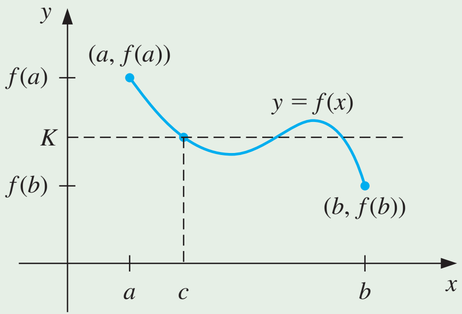
If $f \in C[a, b]$, then c_1, $c_2 \in [a, b]$ exist with $f(c_1) \leq f(x) \leq f(c_2)$, for all $x \in [a, b]$. In addition, if f is differentiable on (a, b), then the numbers c_1 and c_2 occur either at the endpoints of $[a, b]$ or where f' is zero.

◂ Return to Derivation of the Composite Simpson's Rule



Intermediate Value Theorem

If $f \in C[a,b]$ and K is any number between $f(a)$ and $f(b)$, then there exists a number $c \in (a,b)$ for which $f(c) = K$.



(The diagram shows one of 3 possibilities for this function and interval.)

Return to Derivation of the Composite Simpson's Rule