#### **Numerical Integration (Quadrature)**

IAM 550, Lec14, 2019-10-10, J. Raeder



From Wikipedia: Riemann was the second of six children, shy and suffering from numerous nervous breakdowns. Riemann exhibited exceptional mathematical skills, such as calculation abilities, from an early age but suffered from timidity and a fear of speaking in public.

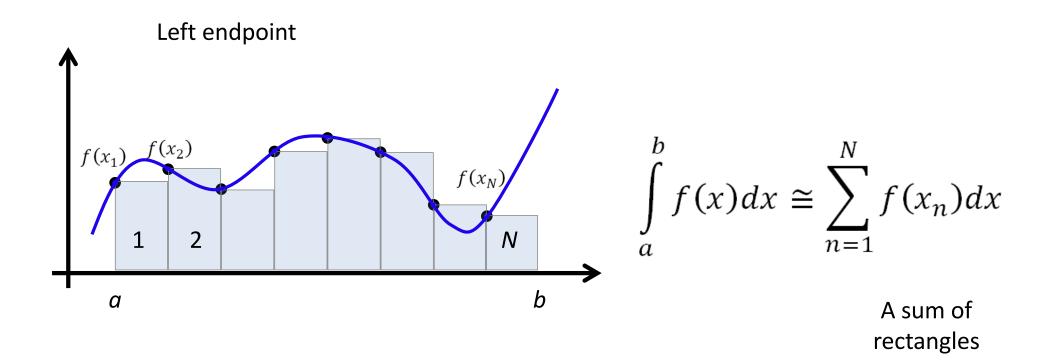
Bernhard Riemann, 1826-1866 (You should have met him in Calc II)

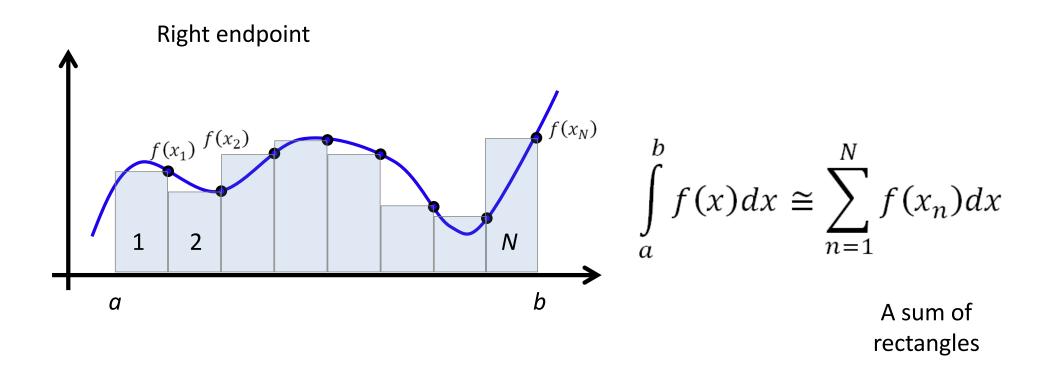
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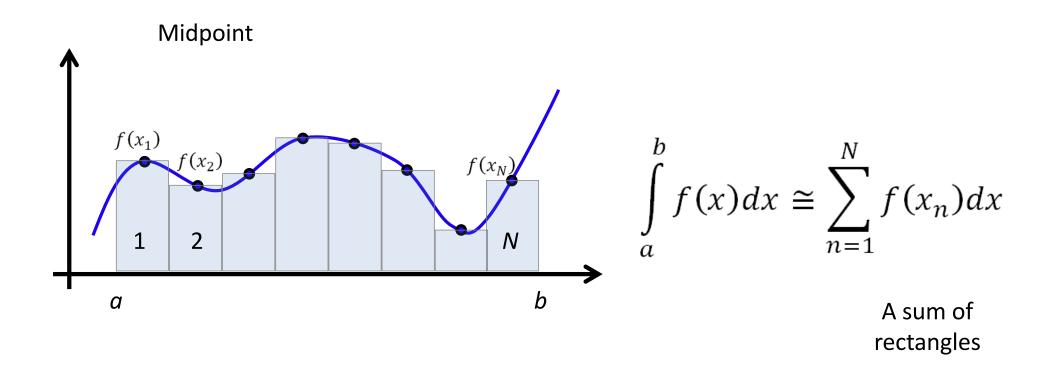
#### Announcements

#### Midterm exam:

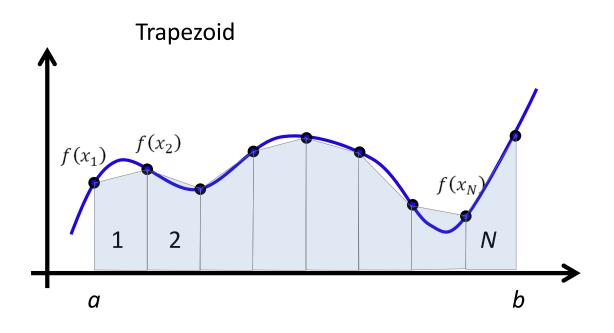
- 17 Oct, 2:10 3:20 (70 minutes)
- N108 (A-O) and W114 (P-Z)
- 115 points total, points over 100 carry over to final
- Material up to and including Lecture 13
- Students with SAS letter come see me
- Homework 2 will be on the web page by Friday COB.
   Due 2 weeks hence.





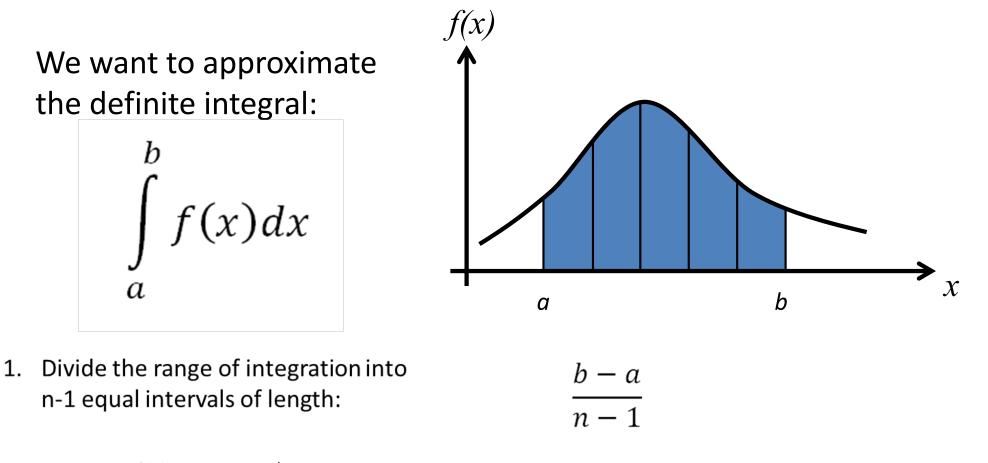


The simple Riemann sum. Will converge for N  $\rightarrow$  Inf, but maybe very slowly.



Probably a little better.

A more formal introduction to numerical integration



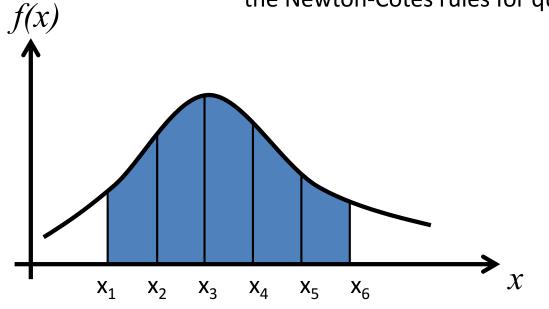
2. Replace f(x) with an  $n^{th}$  order polynomial that is easy to integrate:  $f(x) \cong f_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$ 

#### A more formal introduction to numerical integration

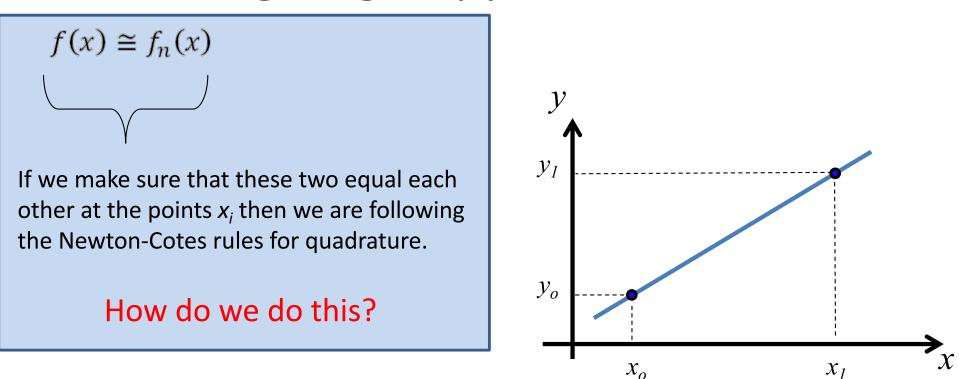
2. Replace f(x) with an  $n^{th}$  order polynomial that is easy to integrate

$$f(x) \cong f_n(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n$$

If we make sure that these two equal each other at the points  $x_i$  then we are following the Newton-Cotes rules for quadrature.



## Lagrange Approximation



What we learned way back when...

$$y = y_o + m(x - x_o)$$
  
 $m = \frac{(y_1 - y_o)}{(x_1 - x_o)}$ 

$$y = P(x) = y_o + (y_1 - y_o) \frac{(x - x_o)}{(x_1 - x_o)}$$

Or as Lagrange would have written:

$$y = P_1(x) = y_0 \frac{(x - x_1)}{(x_0 - x_1)} + y_1 \frac{(x - x_0)}{(x_1 - x_0)}$$
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## Lagrange Approximation

Or as Lagrange would have written:

So we can write in a type of shorthand:

$$P_1(x) = \sum_{k=0}^{1} y_k L_{1,k}(x)$$

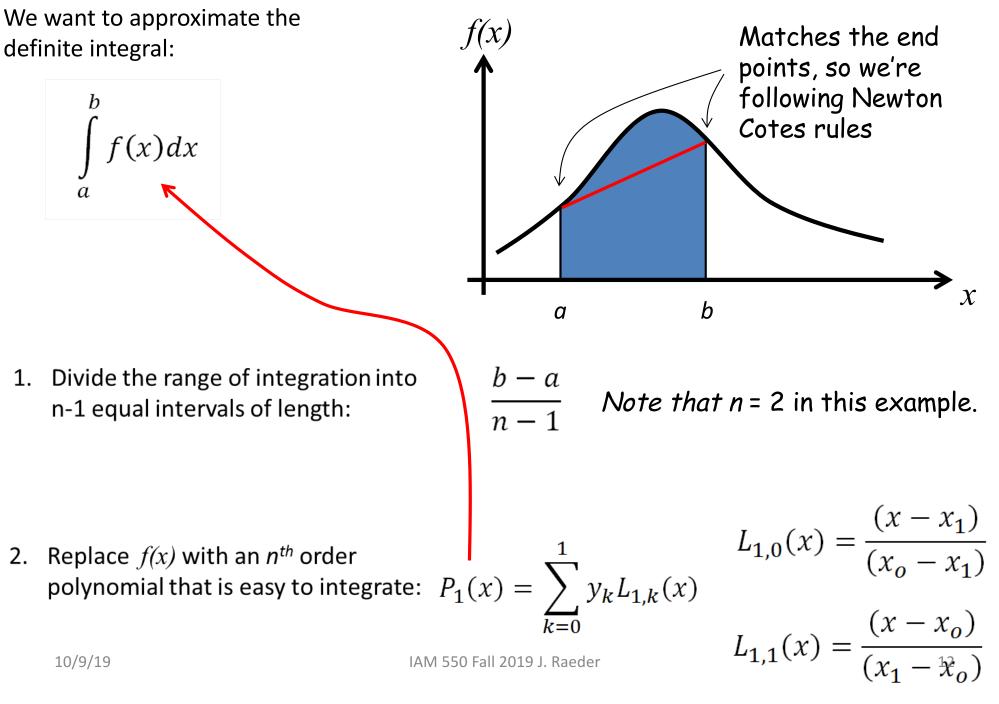
## Lagrange Approximation

For an  $N^{th}$  degree polynomial approximation that is exact at the points  $x_i$ :

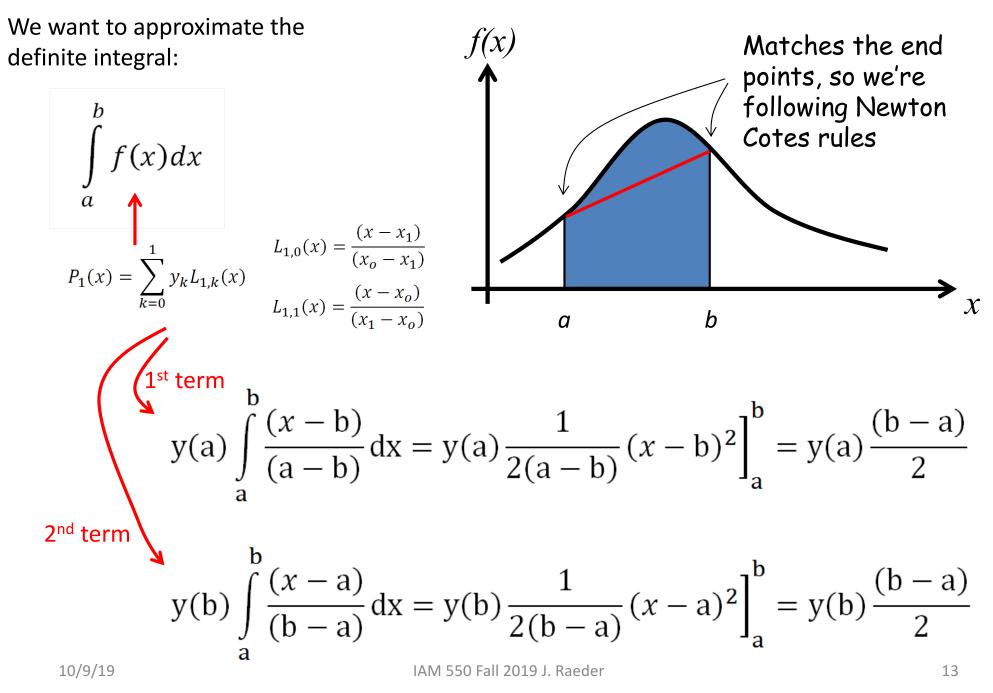
$$P_N(x) = \sum_{k=0}^N y_k L_{N,k}(x)$$

$$L_{N,k}(x) = \frac{(x - x_o) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_N)}{(x_k - x_o) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_N)}$$
Note that  $(x - x_k)$  and  $(x_k - x_k)$  are not present here.

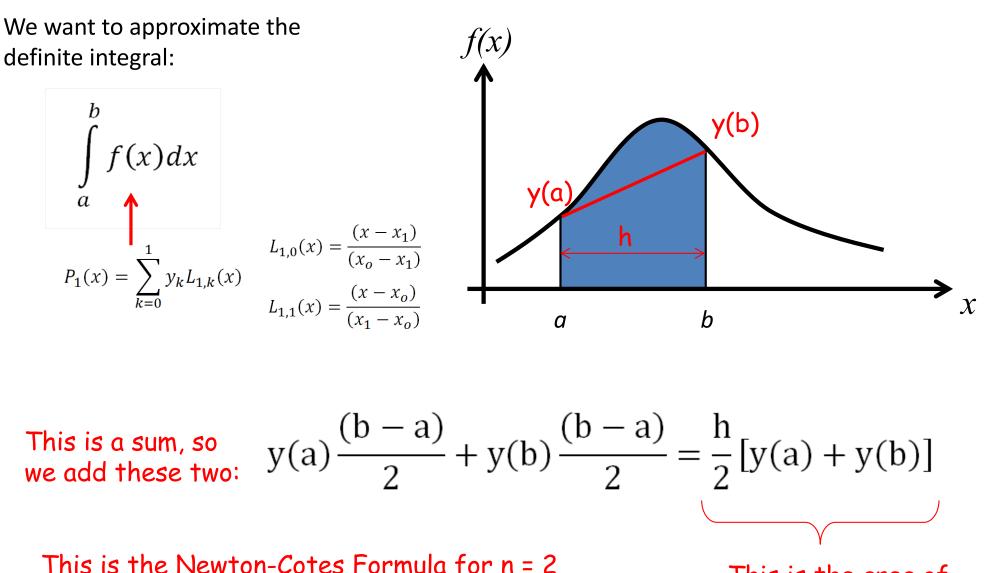
## So lets try it:



#### So lets try it:



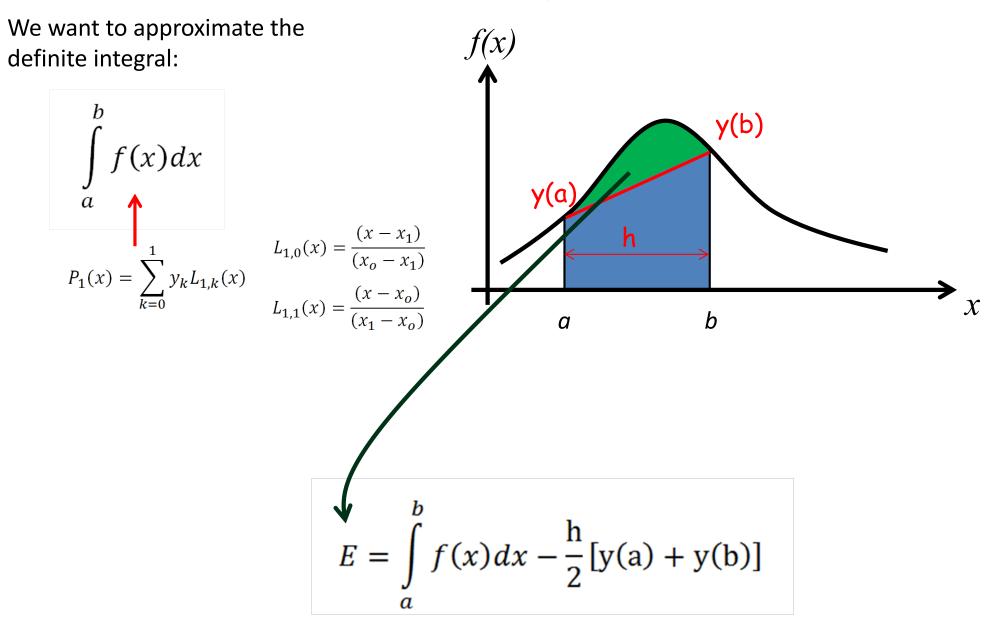
## So lets try it:



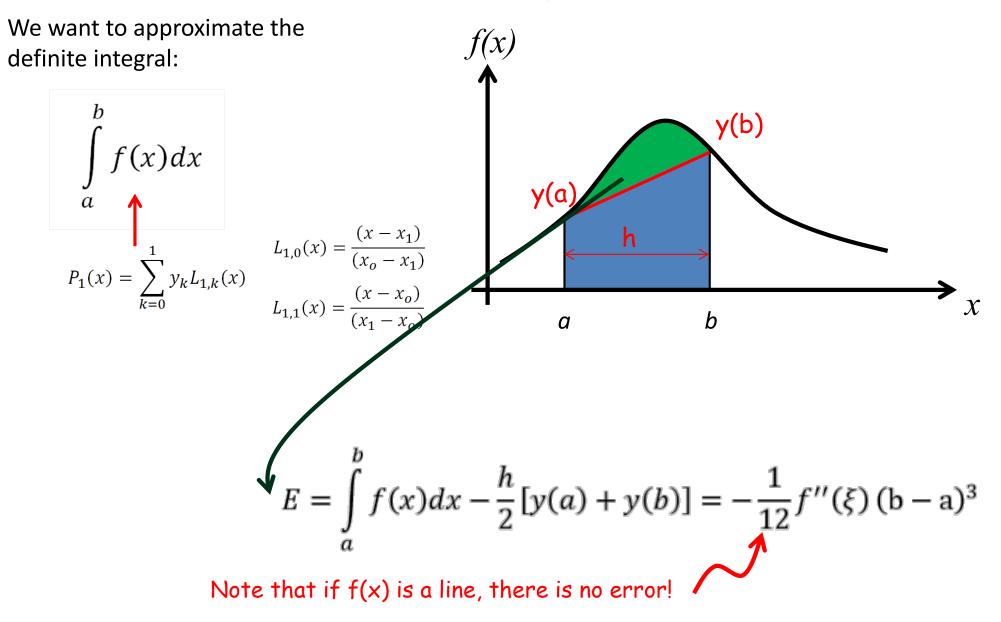
a.k.a trapezoidal rule.

This is the area of the trapezoid above.

## Error in the Trapezoidal Rule

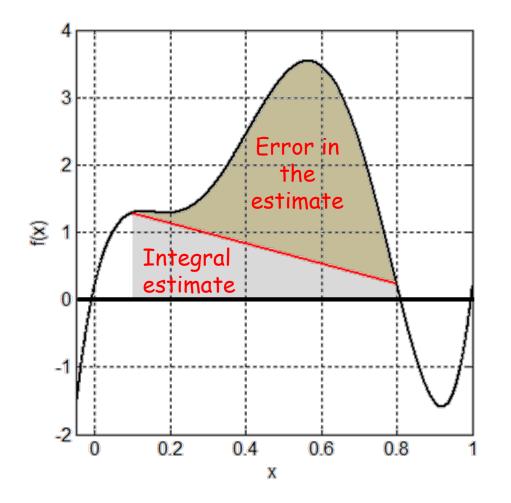


## Error in the Trapezoidal Rule



 $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ 

Integrate f(x) from a = 0.1 to b=0.8



True answer: 1.5471

f(0.1) = 1.289 f(0.8) = 0.232 h = 0.7

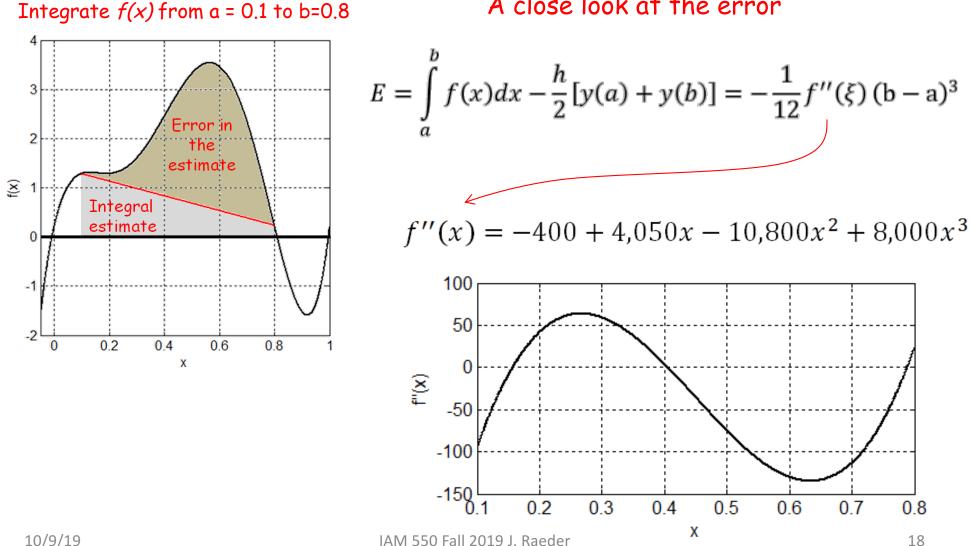
Trapezoid rule estimate: h/2\*[f(0.1) + f(0.8)] = 0.5324

E = 1.5471-0.5324 = 1.015 Percent error = 65.6%

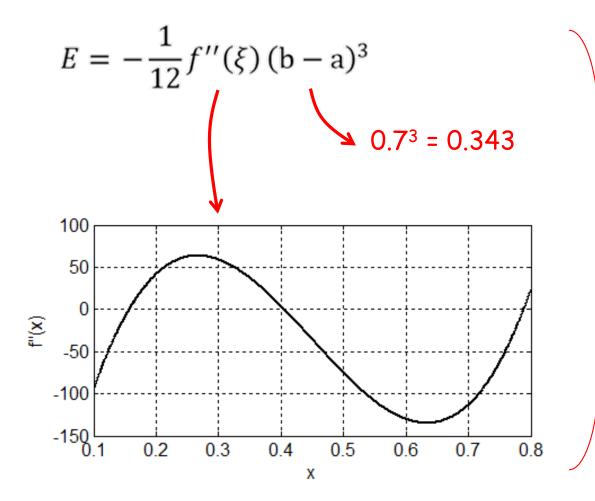
Note that we don't always know this error!

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

A close look at the error



$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

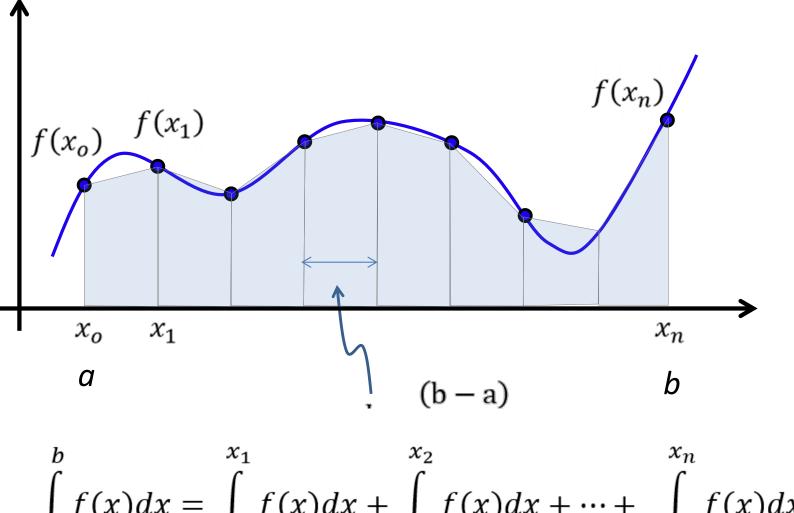


This suggests the error should be somewhere between -1.7 to 3.7.

If we looked at a much smaller interval (i.e., b-a << 0.7) we'd have a much more accurate answer.

Question: what would the range of errors be if we were using a step size of 0.1 and were integrating from 0.2 to 0.3? What if we were integrating from 0.4 to 0.5, or 0.6 to 0.7?

#### Composite Trapezoidal Rule



$$\int_{a} f(x)ax = \int_{x_0} f(x)ax + \int_{x_1} f(x)ax + \dots + \int_{x_{n-1}} f(x)ax$$

This is exact! But to numerically solve this we could use the trapezoidal rule on each piece.

# Composite Trapezoidal Rule $f(x_0)$ $f(x_1)$ $f(x_n)$ $f(x_n)$

This is the exact solution:

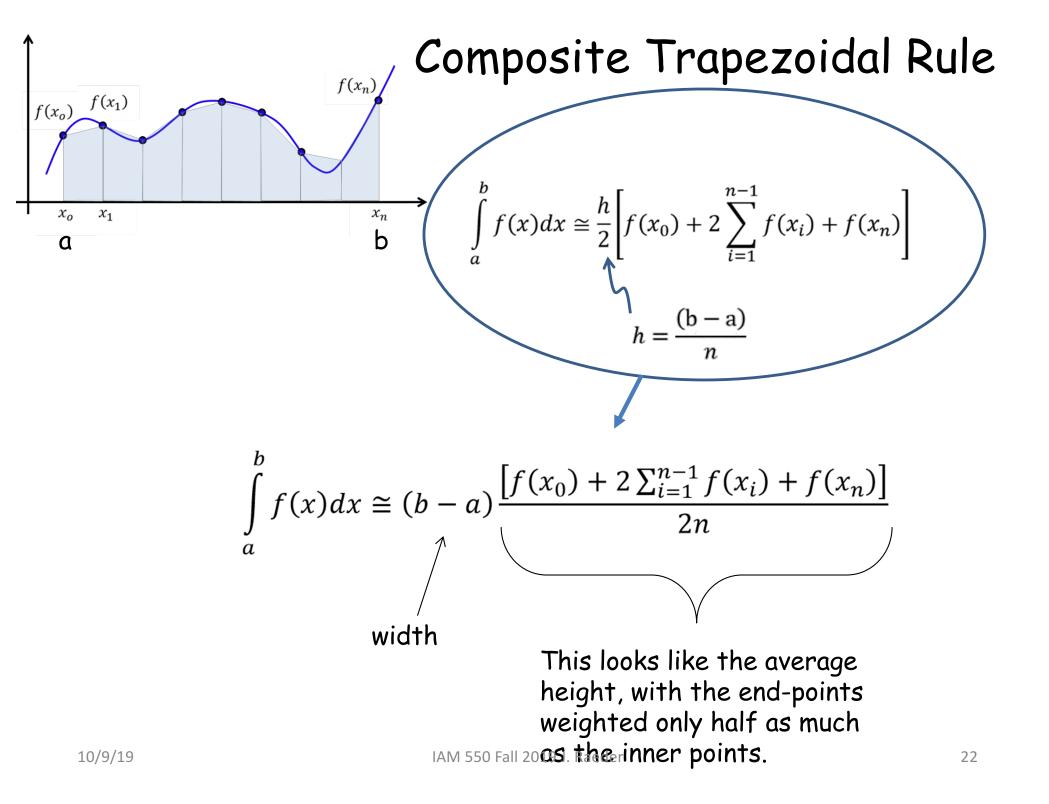
$$\int_{a}^{b} f(x)dx = \int_{x_{0}}^{x_{1}} f(x)dx + \int_{x_{1}}^{x_{2}} f(x)dx + \dots + \int_{x_{n-1}}^{x_{n}} f(x)dx$$

This is the composite trapezoidal rule:

$$\int_{a}^{b} f(x)dx \cong \frac{h}{2}[f(x_{0}) + f(x_{1})] + \frac{h}{2}[f(x_{1}) + f(x_{2})] + \dots + \frac{h}{2}[f(x_{n-1}) + f(x_{n})]$$

This is the composite trapezoidal rule stated a little more compactly (and easier to program, perhaps):

$$\int_{a}^{b} f(x)dx \cong \frac{h}{2} \left[ f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$$

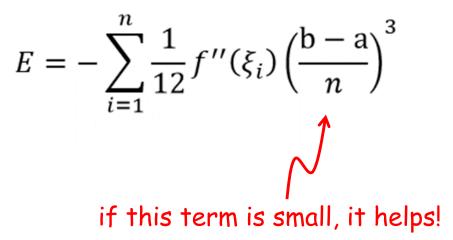


#### Error in the Composite Trapezoidal Rule

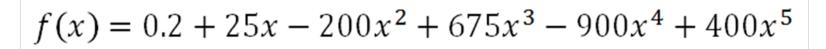
Recall the error when we used only one trapezoid:

$$E = -\frac{1}{12}f''(\xi)(b-a)^3$$

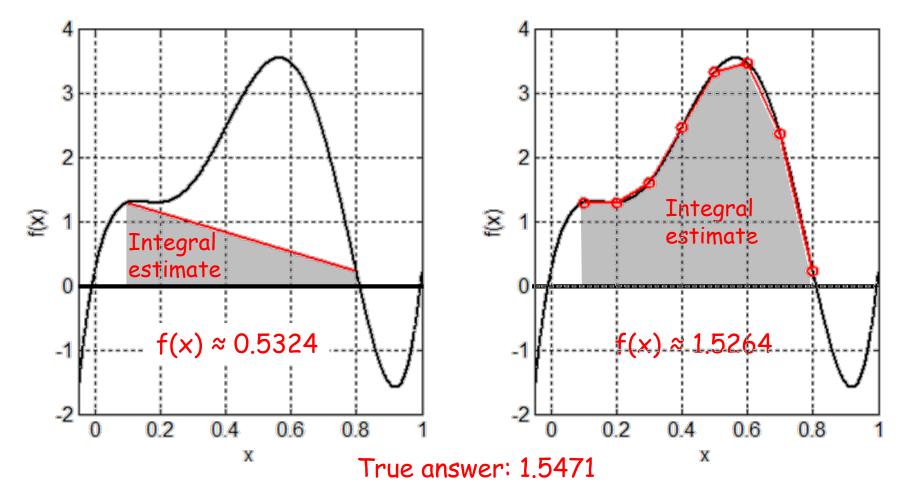
If we divide the integral up into *n* pieces, we sum the individual errors:



#### Return to the previous example



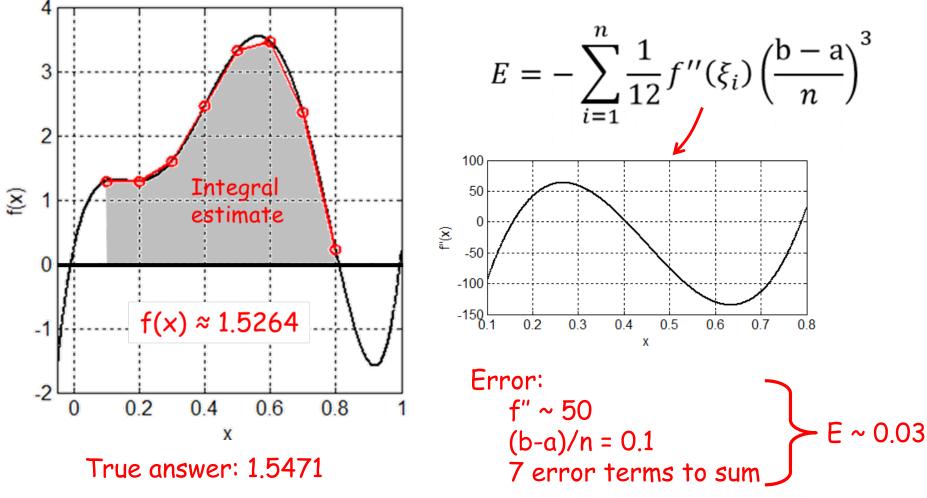
#### Integrate f(x) from a = 0.1 to b=0.8



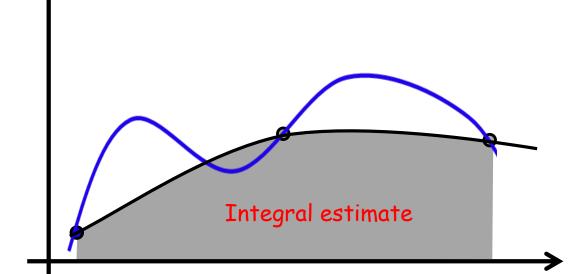
#### Return to the previous example

 $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ 

Integrate f(x) from a = 0.1 to b=0.8

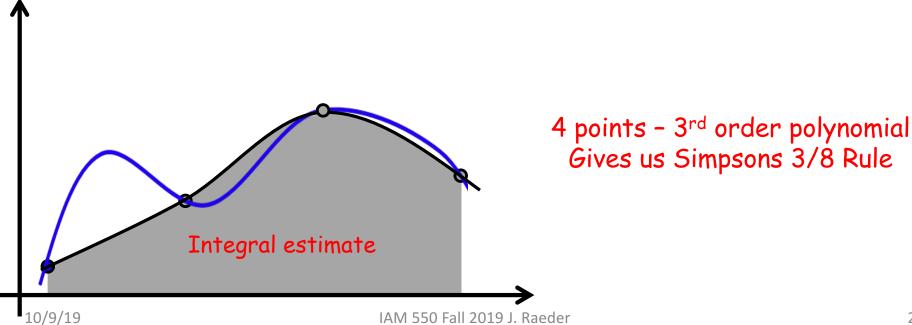


#### Simpson's 1/3 Rule



If we add a midpoint to the trapezoidal rule, we can fit a higher-order polynomial.

3 points – Parabola Gives us Simpsons 1/3 Rule



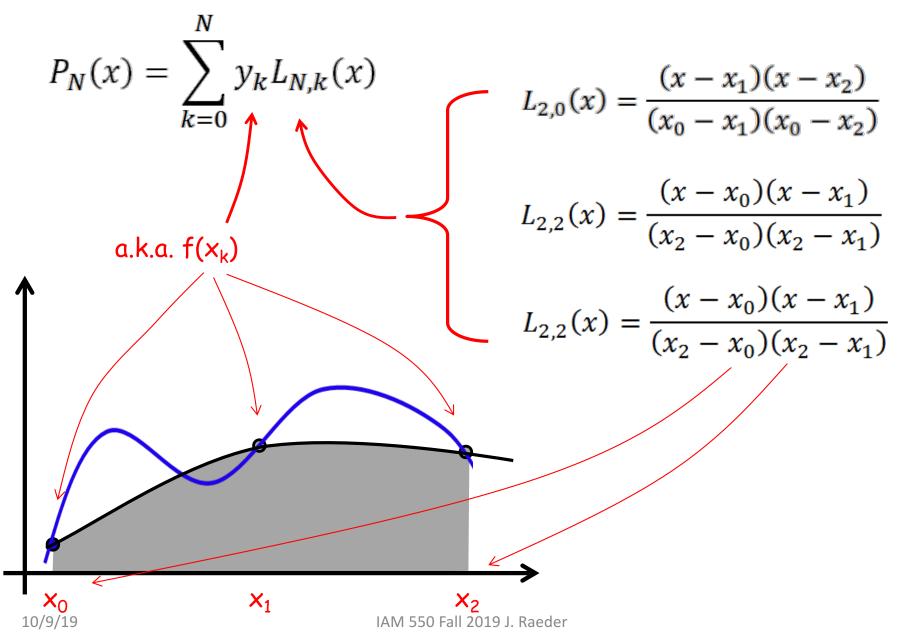
#### Recall Lagrange's Approximation

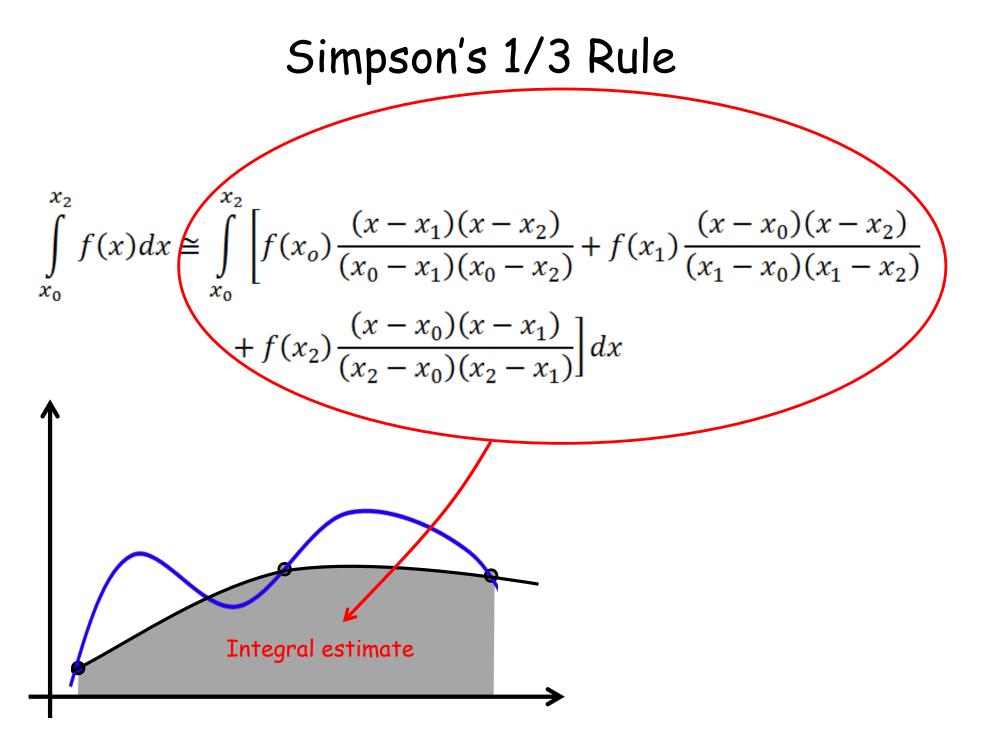
$$P_N(x) = \sum_{k=0}^{N} y_k L_{N,k}(x)$$
For Simpsons 1/3 rule,  
there will be 3 terms in  
this summation.  

$$L_{N,k}(x) = \frac{(x - x_0) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_N)}{(x_k - x_0) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_N)}$$
Note that  $(x - x_k)$  and  $(x_k - x_k)$  are  
not present here.

After we figure out the correct form for Lagrange's approximation, we'll integrate it.

#### Recall Lagrange's Approximation

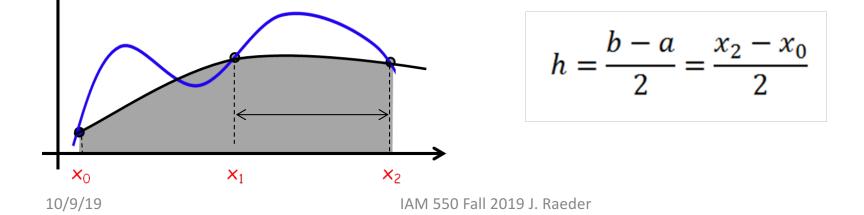




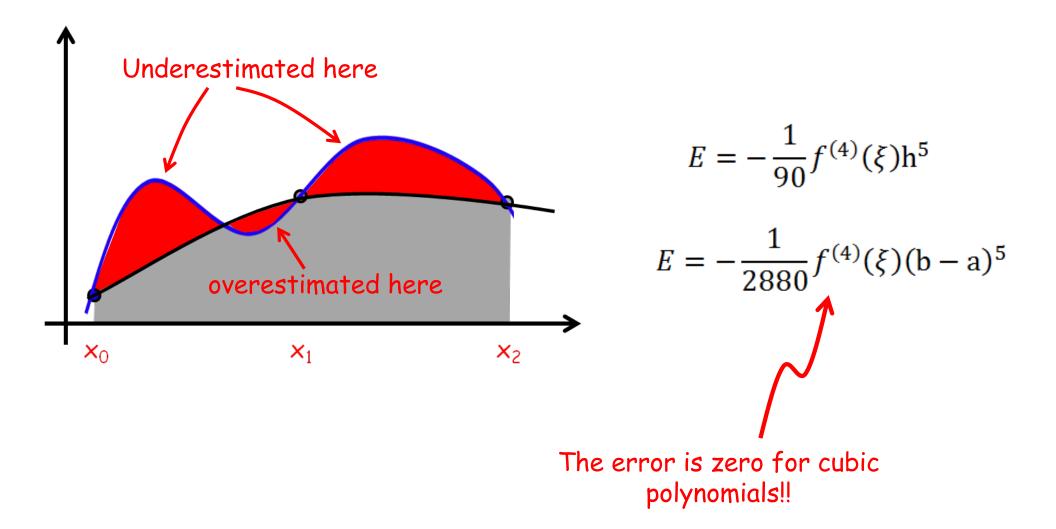
#### Simpson's 1/3 Rule

$$\int_{x_0}^{x_2} f(x)dx \cong \int_{x_0}^{x_2} \left[ f(x_0) \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1) \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2) \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \right] dx$$

$$= \frac{h}{3} [f(x_o) + 4f(x_1) + f(x_2)] \qquad \text{Note the } 1/3 \rightarrow \text{rule name}$$



#### Error in Simpson's 1/3 Rule

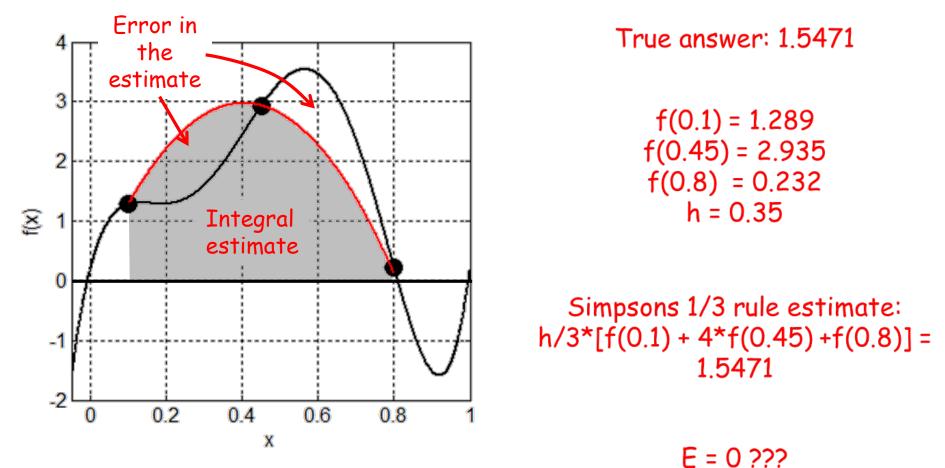


Caution: as before when developed the trapezoidal rule, this error only applies to singlesegment applications of Simpson's 1/3 Rule

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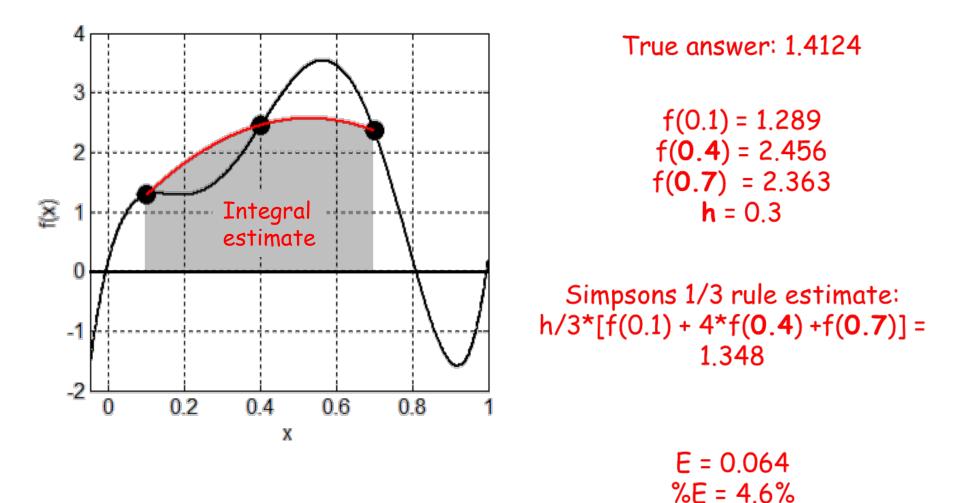
 $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ 

Integrate f(x) from a = 0.1 to b=0.8



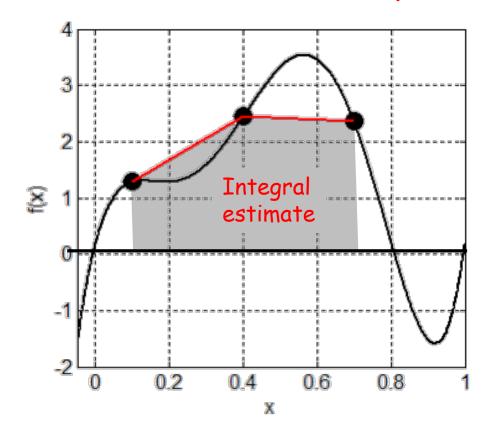
 $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ 

Integrate f(x) from a = 0.1 to b=0.7



 $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ 

Integrate *f(x)* from a = 0.1 to b=0.7 but use the trapezoidal rule for comparison



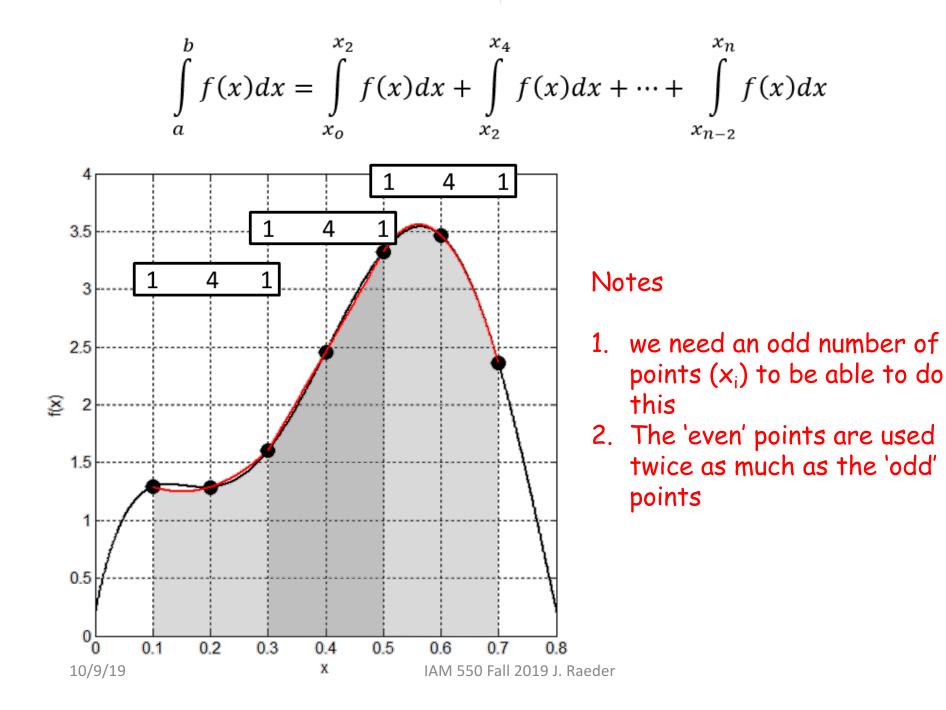
True answer: 1.4124

f(0.1) = 1.289 f(0.4) = 2.456 f(0.7) = 2.363 h = 0.3

**Trapezoidal rule estimate**: h/2\*[f(0.1) + 2\*f(0.4) +f(0.7)] = 1.285

> E = 0.127 %E = 9.0%

#### Composite Simpson's 1/3 Rule



#### Composite Simpson's 1/3 Rule

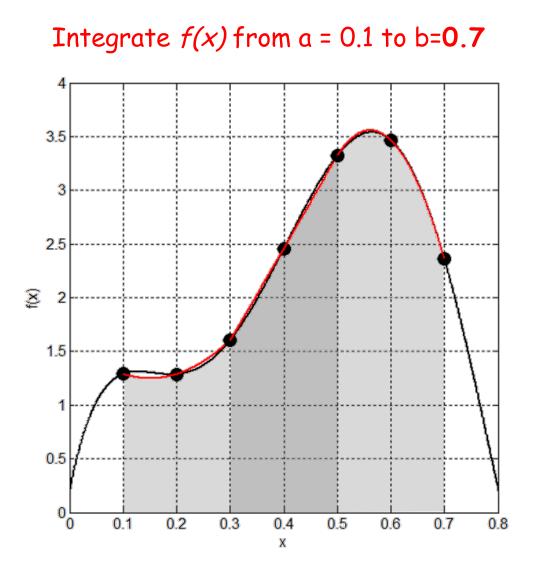
$$\int_{a}^{b} f(x)dx = \int_{x_{0}}^{x_{2}} f(x)dx + \int_{x_{2}}^{x_{4}} f(x)dx + \dots + \int_{x_{n-2}}^{x_{n}} f(x)dx$$

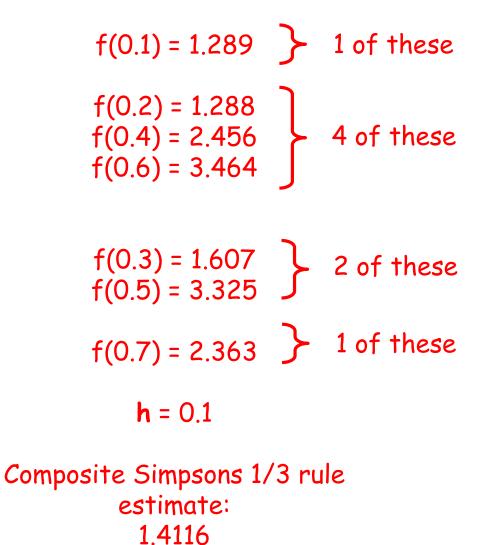
$$\int_{a}^{b} f(x)dx \approx 2h \frac{[f(x_{o}) + 4f(x_{1}) + f(x_{2})]}{6} + 2h \frac{[f(x_{2}) + 4f(x_{3}) + f(x_{4})]}{6} + \cdots + 2h \frac{[f(x_{n-2}) + 4f(x_{n-1}) + f(x_{n})]}{6}$$

$$= \frac{h}{3} \left[ f(x_0) + 4 \sum_{i=1,3,5}^{n-1} f(x_i) + 2 \sum_{i=2,4,6}^{n-2} f(x_i) + f(x_n) \right]$$

## Return to Our Example



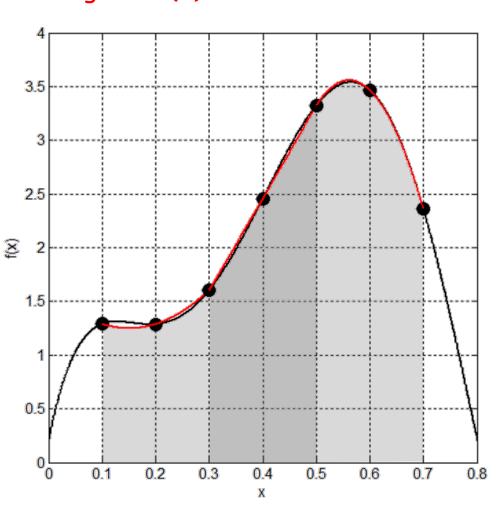




E = 0.0008 %E = 0.06%

## Return to Our Example

True answer: 1.4124



Integrate f(x) from a = 0.1 to b=0.7

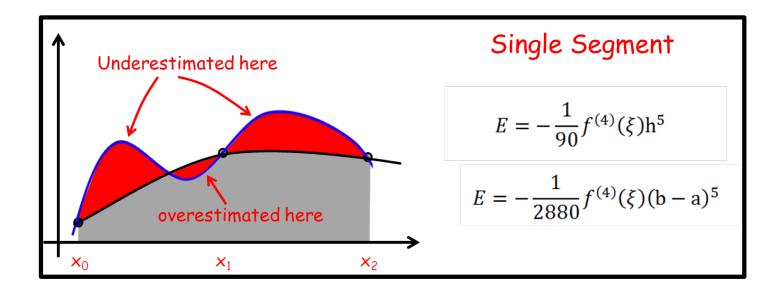
Composite Simpsons 1/3 rule estimate: 1.4116

E = 0.0008 %E = 0.06%

Trapezoidal Rule estimate with same points: 1.3966 E = 0.0158 %E = 1.12%

Note! If we wanted to integrate to from 0.1 to 0.8, we can't use steps of 0.1 with Simpsons 1/3 rule.

## Error in the Composite Simpson's 1/3 Rule



If we divide the integral up into *m* segments, we sum the individual errors:

$$E = -\sum_{i=1}^{m} \frac{1}{2880} f^{(4)}(\xi_i) \left(\frac{b-a}{2m}\right)^5$$

If there are n points, then there are m = (n-1)/2 segments

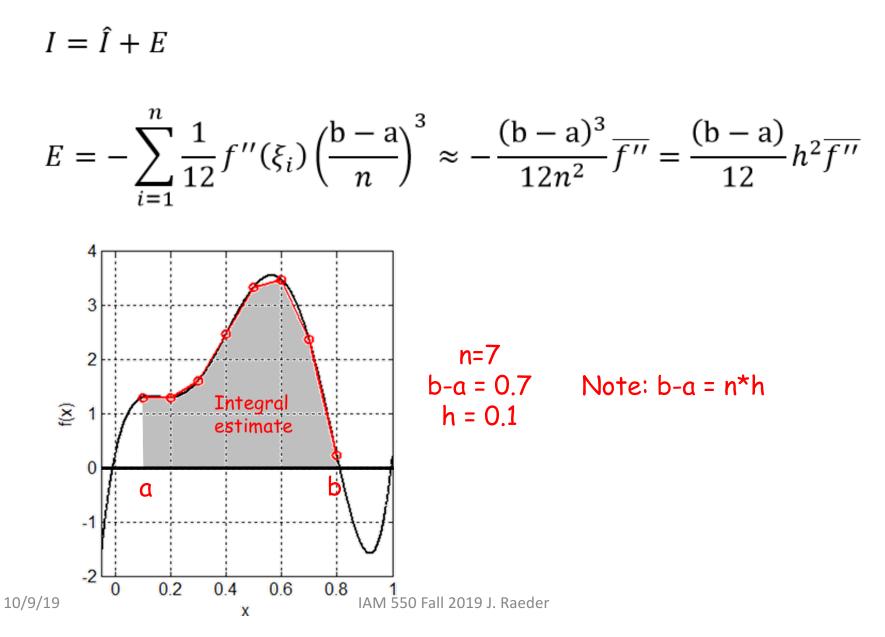
#### Newton-Cotes Integration Formulas

We've done 1<sup>st</sup> order Lagrange polynomials (trapezoidal rule) and 2<sup>nd</sup> order Lagrange polynomials (Simpsons 1/3 rule), and can keep going.

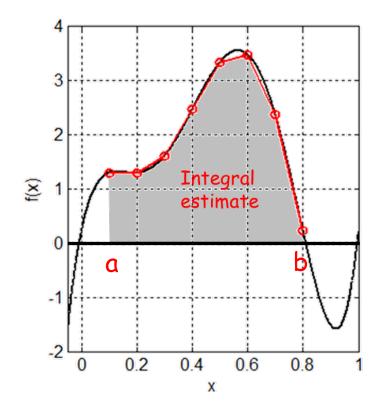
From Chapra, Applied Numerical Methods with MATLAB, 3rd Ed. p. 481

**TABLE 19.2** Newton-Cotes closed integration formulas. The formulas are presented in the format of Eq. (19.13) so that the weighting of the data points to estimate the average height is apparent. The step size is given by h = (b - a)/n.

Segments (n)	Points	Name	Formula	Truncation Error
١	2	Trapezoidal rule	$(b-a)\frac{f(x_0) + f(x_1)}{2}$	$-(1/12)h^3f''(\xi)$
2	3	Simpson's 1/3 rule	$(b-a)\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$	$-(1/90)h^5f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b-a)\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$	$-[3/80]h^5f^{(4)}(\xi)$
4	5	Boole's rule	$(b-a)\frac{7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)}{90}$	$-[8/945]h^7 f^{(6)}(\xi)$
5	6		$(b-a)\frac{19f(x_0) + 75f(x_1) + 50f(x_2) + 50f(x_3) + 75f(x_4) + 19f(x_5)}{288}$	$-(275/12,096)h^7f^{(6)}(\xi)$
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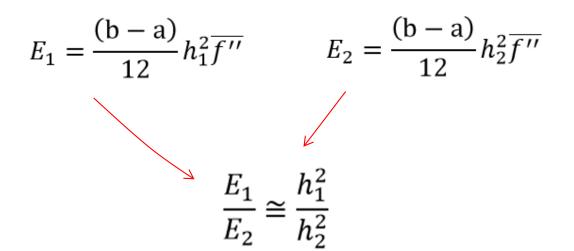
What if I made two separate estimates, with different step sizes (recall Richardson extrapolation)?



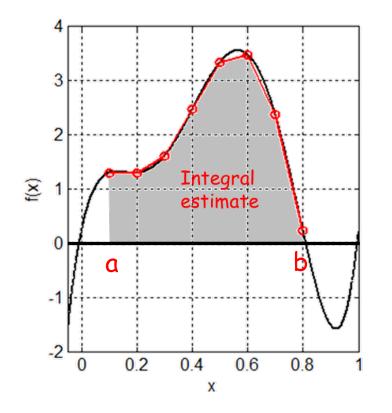
Estimate 1, with<br/>step size h1:Estimate 2, with<br/>step size h2: $I = \hat{I}(h_1) + E(h_1)$  $I = \hat{I}(h_2) + E(h_2)$ 

$$\hat{I}(h_1) + E(h_1) = \hat{I}(h_2) + E(h_2)$$

Each estimate will have an error that depends similarly on the 2<sup>nd</sup> derivative but with different step sizes:



What if I made two separate estimates, with different step sizes (known as Richardson extrapolation)



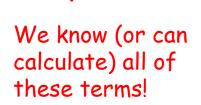
Solve for E2 and	$E_1 \sim$	$h_{1}^{2}$
substitute:	$\overline{E_2} =$	$\overline{h_2^2}$

$$\hat{I}(h_1) + E(h_2)\frac{h_1^2}{h_2^2} = \hat{I}(h_2) + E(h_2)$$

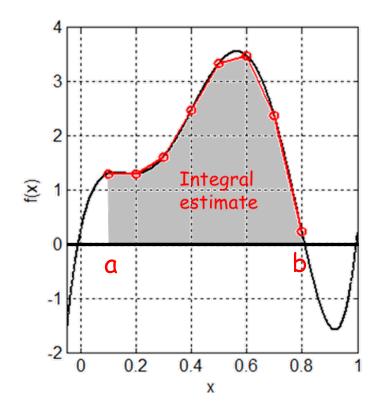
 $E(h_2) = \frac{\hat{I}(h_1) - \hat{I}(h_2)}{(1 - h_1^2)}$ 

Solve for E2





What if I made two separate estimates, with different step sizes (Richardson extrapolation)



We can now use our estimate of the *error* to improve our estimate of the integral:

$$I = \hat{I}(h_2) + E(h_2) = \hat{I}(h_2) + \frac{\hat{I}(h_1) - \hat{I}(h_2)}{\left(1 - \frac{h_1^2}{h_2^2}\right)}$$
$$\hat{I}(1 - \frac{h_1^2}{h_2^2})$$
$$E(h_2) = \frac{\hat{I}(h_1) - \hat{I}(h_2)}{\left(1 - \frac{h_1^2}{h_2^2}\right)}$$

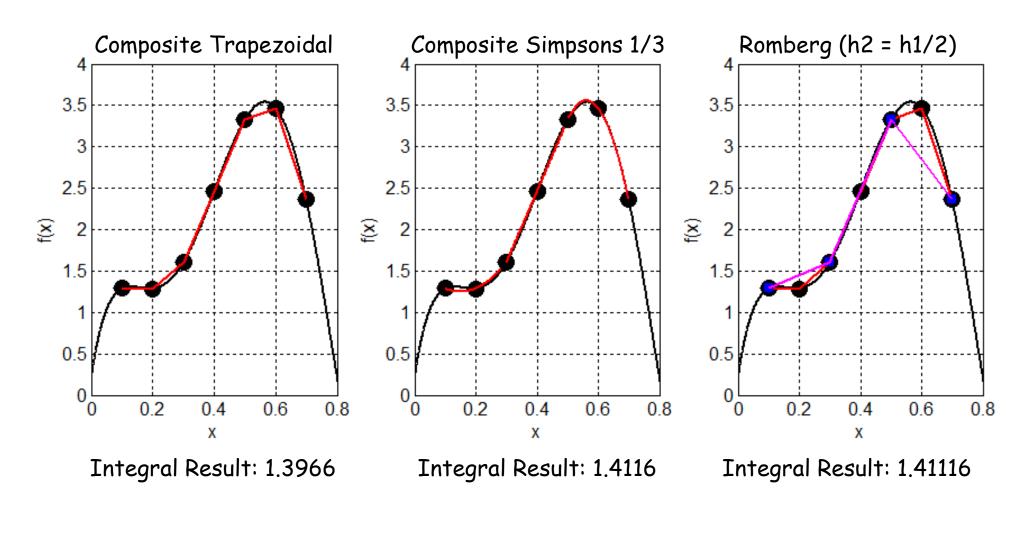
If h2 = h1/2:

$$I = \frac{4}{3}\hat{I}(h_1) - \frac{1}{3}\hat{I}(h_2)$$

This turns out to be  $O(h^4)$ .

With h2=h1/2 you can reuse the  $f(x_i)$  from  $I_2$  to save computation time. IAM 550 Fall 2019 J. Raeder

#### Comparison: Trapezoidal, Simpsons 1/3, Romberg



True Answer: 1.4124

#### The Typical Romberg Integration Scheme Uses Iterations:

Trap for step size:  $(b-a) \longrightarrow$ Trap for step size:  $(b-a)/2 \longrightarrow$  Result of iteration 1

Trap for step size: (b-a) Trap for step size: (b-a)/2 Trap for step size: (b-a)/4 🜌

Result of iteration 1  $\longrightarrow$  Result of iteration 2  $\rightarrow$ 

Trap for step size: (b-a) Result of iteration 1 Trap for step size: (b-a)/2 Intermediate iteration 2 Intermediate iteration 3 Result of iteration 2 Intermediate iteration 3 Ans. Trap for step size: (b-a)/4 🤍 Intermediate iteration 3 Trap for step size: (b-a)/8 🌙

Overkill for us, but MATLAB does something like this with the integrate() function. Romberg has the advantage that it provides an error estimate without knowing the true integral. You can specify a precision and stop the iterations when it is reached.

## Take-home messages

- We have several methods for doing numerical integration
  - Left/right-end rule
  - Trapezoidal Rule
  - Simpsons 1/3 Rule
  - Romberg
  - Other extended methods (lots of them, Gauss-Legendre)
- In all cases: small step size helps!
- If you have f() given by data, trapezoidal is good enough, because your data have errors to begin with.
- You should spend time with these notes, working through the examples and making sure you understand the different methods.