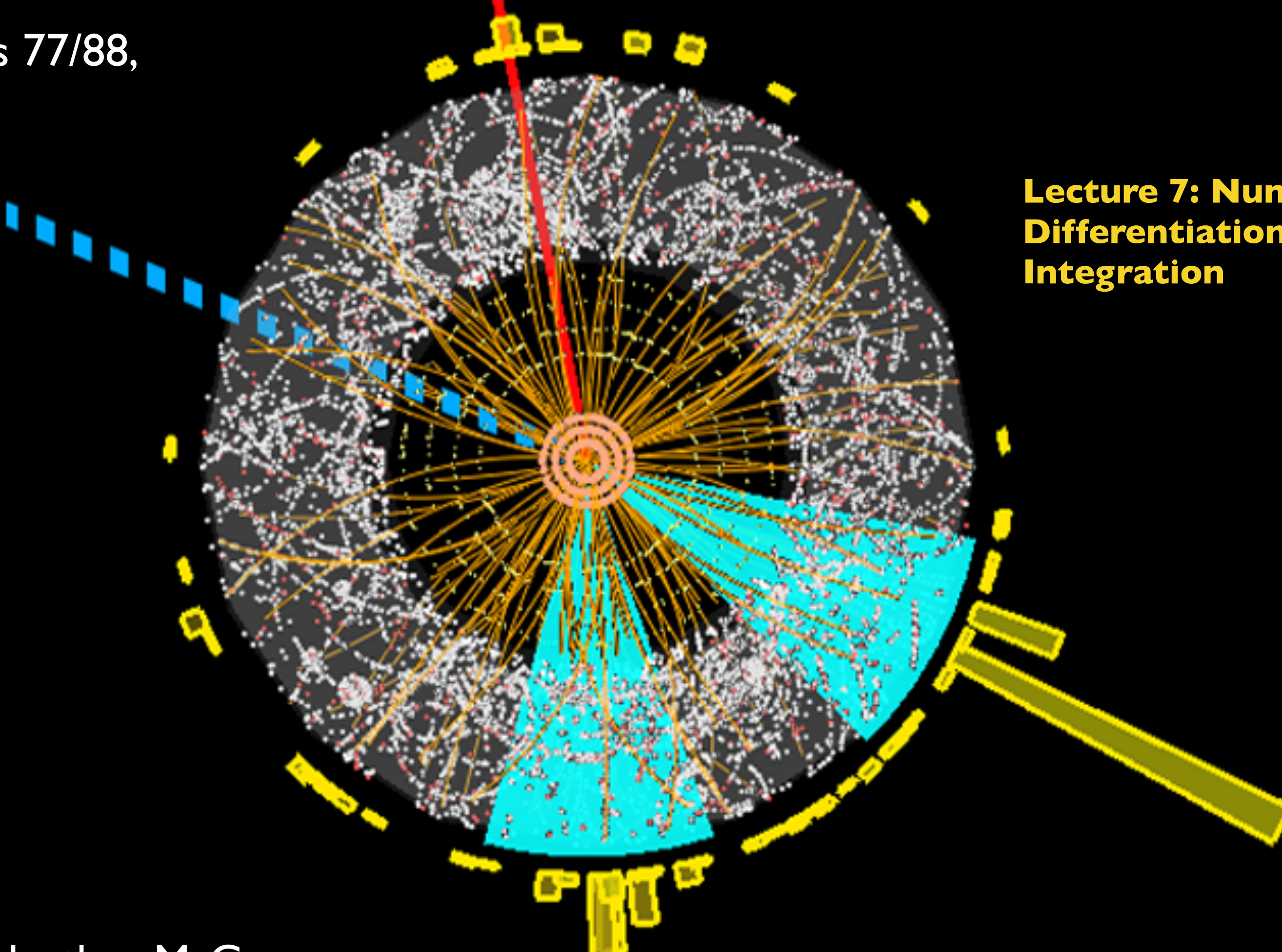
Introduction to Computational Techniques in Physics/Data Science Applications in Physics

Physics 77/88,



Lecture 7: Numerical Differentiation and Integration

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Numerical Differentiation

- Definition
  - $$\frac{df(x)}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$
- Approximation
  - $$\frac{df(x)}{dx} = \frac{\Delta f(x)}{\Delta x}$$
- Similarly
  - $$\Delta^n f(x) = \Delta\left(\Delta^{n-1} f(x)\right)$$

Numerical Differentiation

- The nth difference of a polynomial of degree n is a constant, $a_n n! h^n$, and the $(n+1)$ difference is zero
- Let's take $f(x) = x^2$ as an example

x_i	$f(x_i)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
2	$f(2) =$ 4			
		$\Delta f(2) =$ 5		
3	$f(3) =$ 9		$\Delta^2 f(2) =$ 2	
		$\Delta f(3) =$ 7		$\Delta^3 f(2) =$ 0
4	$f(4) =$ 16		$\Delta^2 f(3) =$ 2	
		$\Delta f(4) =$ 9		$\Delta^3 f(3) =$ 0
5	$f(5) =$ 25		$\Delta^2 f(4) =$ 2	
		$\Delta f(5) =$ 11		
6	$f(6) =$ 36			

Taylor Series

- Expand any function $f(x)$
  - $f(x_0 + kh) = f(x_0) + kh f'(x_0) + \frac{(kh)^2 f''(x_0)}{2!} + \dots + \frac{(kh)^n f^n(x_0)}{n!}$
- Rearrange to solve for $f'(x)$
- $$\frac{f(x_0 + kh) - f(x_0)}{kh} = f'(x_0) + \frac{(kh)''(x_0)}{2!} + \dots + \frac{(kh)^{n-1} f^n(x_0)}{n!}$$
- Backward difference ($k = -1$)

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

- Forward difference ($k = 1$)
- $$\frac{f(x_0 + h) - f(x_0)}{h} = f'(x_0) + O(h)$$

Taylor Series: Central Difference

- $f(x_0 + kh) = f(x_0) + khf'(x_0) + \frac{(kh)^2 h''(x_0)}{2!} + \ldots + \frac{(kh^{n})f^n(x_0)}{n!}$
- $f(x_0 - kh) = f(x_0) - khf'(x_0) + \frac{(kh^2)h''(x_0)}{2!} + \cdots + (-1)^2 \frac{(kh)^n f^n(x_0)}{n!}$
- Subtract the two and set k = 1:
- $\frac{f(x_0+h) - f(x_0-h)}{2h} = f'(x_0) + O(h^2)$

central difference

Higher Order Approximations

- 1st order $f'(x) =$ $\dfrac{f(x_0+h) - f(x_0)}{h}$
- 2nd order $f'(x) =$ $\dfrac{f(x_0+h) - f(x_0-h)}{2h}$
- 1st order $f''(x) =$ $\dfrac{f(x_0+h) + f(x_0-h) - 2f(x)}{(2h)^2}$
- 2nd order $f''(x) =$ $\dfrac{-f(x_0+3h) + 4f(x+2h) - 5f(x+h) + 2f(x)}{h^2}$

Numerical Integration

- Consider the definite integral
    - $I = \int_a^b f(x)\,dx$
- The integral can be approximated by a weighted sum
    - $I \approx \sum_{i=1}^{n} \omega_i f(x_i) \Delta x_i$
- The ω_i are weights , and the x_i are abscissas
- Assuming that f is finite and continuous on the interval [a , b] numerical integration leads to a unique solution
- The goal of any numerical integration method is to choose abscissa and weights such that errors are minimized for the smallest n possible for a given function

Numerical Integration

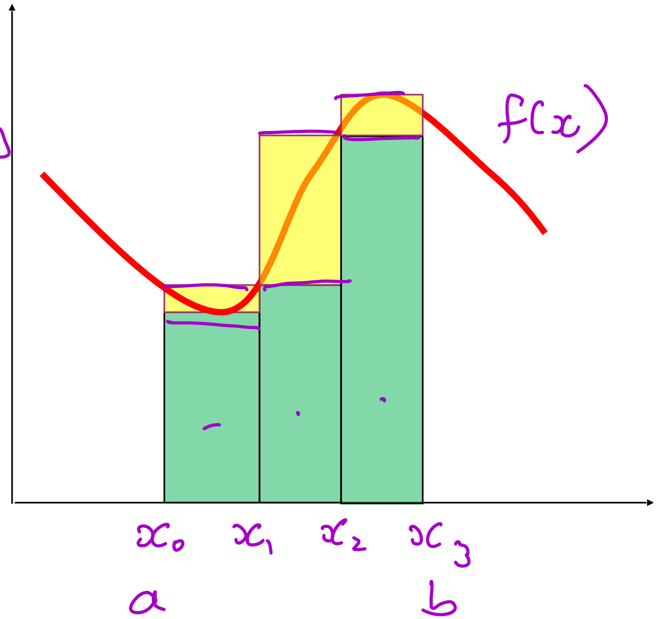
- How can we choose the evaluation points, x_i's, and the weights, w_i's, such that
- $$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i) \Delta x_i$$
- In general, there are two sets of degrees of freedom
  - The spacing of the evaluation points
  - The weighted importance of each point

Numerical Integration Methods

- Upper and Lower Sums
- Newton-Cotes Methods:
  - a) Trapezoid Rule
  - b) Simpson Rules
- Romberg Method
- Gauss Quadrature

Upper and Lower Sums

- Partition the interval into subintervals
  - $P = \{ a = x_0 \leq x_1 \leq x_2 \leq \ldots \leq x_n = b \}$
- Define
  - Minimum: $m_i = \{ f(x) : x_i \leq x \leq x_{i+1} \}$
  - Maximum: $M_i = \{ f(x) : x_i \leq x \leq x_{i+1} \}$
- Lower Sum
  - $\underline{L}(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$
- Upper Sum
  - $\underline{U}(f, P) = \sum_{i=1}^{n-1} M_i (x_{i+1} - x_i)$
- Estimate of the integral = $\dfrac{L + U}{2}$
- Error $\leq$ $\dfrac{U - L}{2}$



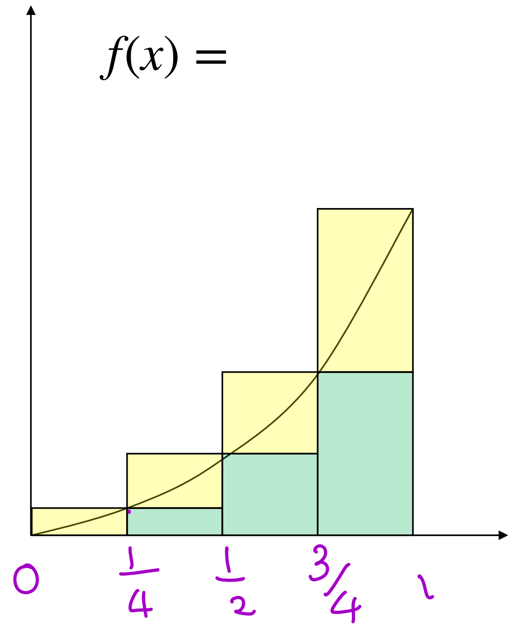
Example

- $\int_0^1 x^2 dx =$ 1/3 (true value)
- Partition P = $\{0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1\}$
- n = 4 four equal intervals

i	0	1	2	3
m_i	0	1/16	$\frac{1}{4}$	$\frac{9}{16}$
M_i	1/16	$\frac{1}{4}$	$\frac{9}{16}$	1

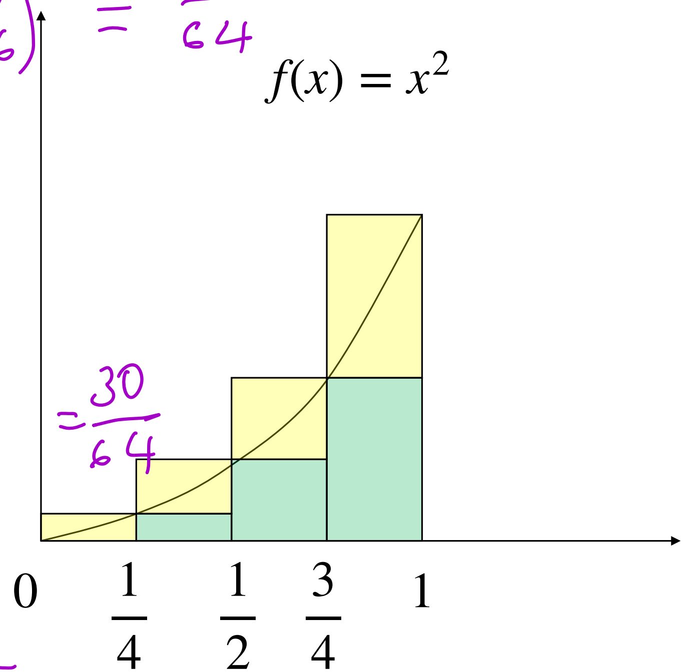
- $x_{i+1} - x_i =$ 1/4

$f(x) =$



Example (cont)

- Lower Sum
  - $L(f,P) = \sum_{i=0}^{n-1} m_i(\underline{x_{i+1} - x_i})$
  - $= \frac{1}{4}\left\{0 + \frac{1}{16} + \frac{1}{4} + \frac{9}{16}\right) = \frac{14}{64}$
  - $= 14/64$
- Upper Sum
  - $U(f,P) = \sum_{i=0}^{n-1} M_i(x_{i+1} - x_i)$
  - $= \frac{1}{4}\left\{\frac{1}{16} + \frac{1}{4} + \frac{9}{16} + 1\right) = \frac{30}{64}$
  - $= 30/64$



- I $= \frac{L+U}{2} = \frac{1}{2}\left(\frac{30}{64} + \frac{14}{64}\right) = \frac{11}{32}$
- Error $\leq \frac{U-L}{2} = \frac{1}{2}\left(\frac{30}{64} - \frac{14}{64}\right) = 1/8$

Upper and Lower Sums

- Estimates based on upper and lower sums are easy to obtain for monotonic functions
  - functions that are always increasing or decreasing
- For non-monotonic functions, finding the maxima and minima of the function can be difficult and other methods are better

Newton-Cotes Methods

- In Newton-Cotes, the function is approximated by a polynomial of order n
- Computing the integral of a polynomial is
   - $\int_a^b f(x)d(x) \approx \int_a^b (a_0 + a_1 x + \cdots + a_n x^n)\, dx$
   - $\approx a_0(b-a) + a_1 \frac{(b^2-a^2)}{2} + \ldots + a_n \frac{(b^{n+1}-a^{n+1})}{n+1}$

Newton-Cotes Methods

- Trapezoid Method
  - Uses first order polynomials
  - $\int_a^b f(x)dx \approx \int_a^b a_0 + a_1 x \, dx$
- Simpson's 1/3 Rule
  - Uses second order polynomials
  - $\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1 x + a_2 x^2) \, dx$

Trapezoid Method

- $I = \int_a^b f(x)dx \approx \int_a^b \left(f(a) + \frac{f(b)-f(a)}{b-a}(x-a) \right) dx$
- $\approx \int_a^b f(a) - a\frac{f(b)-f(a)}{b-a} + \frac{f(b)-f(a)}{b-a}\,x \; dx$

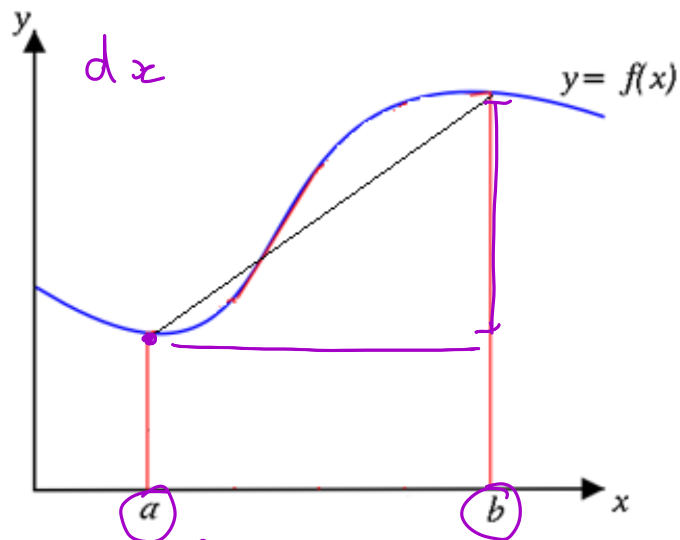
$$= \left[f(a) - a\frac{f(b)-f(a)}{b-a} \right] x \Big|_a^b$$

$$+ \frac{f(b)-f(a)}{b-a}\frac{x^2}{2}\Big|_a^b$$

$$= \left[f(a) - a\frac{f(b)-f(a)}{b-a} \right](b-a) + \frac{f(b)-f(a)}{2(b-a)}(b^2-a^2)$$

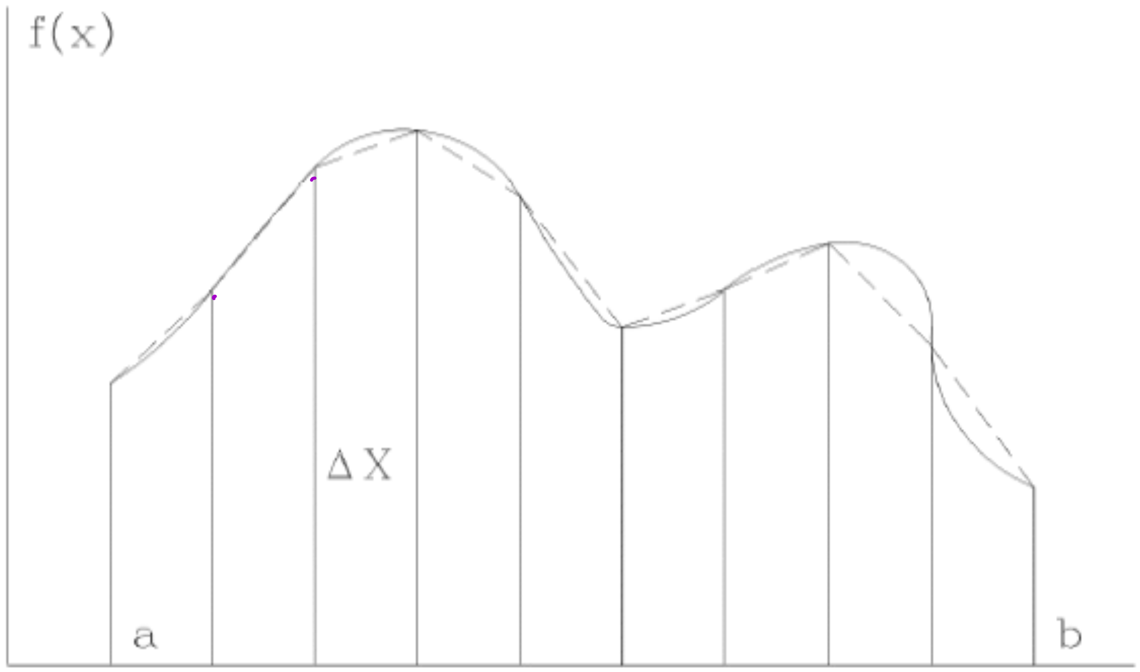
$$= [b-a]\frac{[f(a)+f(b)]}{2} - a(f(b)-f(a)) \quad \frac{(f(b)-f(a))(b+a)}{2}$$

$$\frac{f(b)-f(a)}{2}(b-a)$$



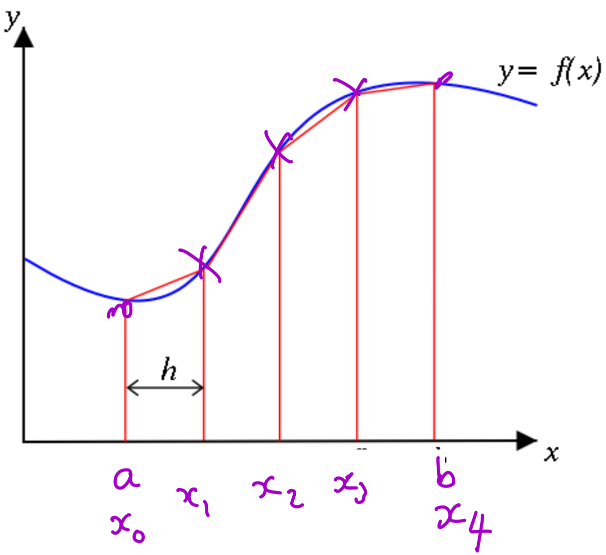
Numerical Integration

- Composite Trapezoid Rule



Trapezoid Rule

- Approximate integrals using the areas of the trapezoids



$$\int_a^b f(x)dx \approx \sum \text{area of trapezoids}$$

$$= h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + h\frac{f(x_2)+f(x_3)}{2} + h\frac{f(x_3)+f(x_4)}{2}$$

$$= \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + 2f(x_3) + f(x_4)\right]$$

For n intervals this generalizes to

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

Numerical Integration

- Trapezoid Rule
  - $\int_a^b f(x)dx = \sum_{i=1}^{n-1} \frac{f(x_{i+1}) + f(x_i)}{2} \Delta x_i$
  - $\Delta x_i =$ $(b-a)/n-1$
- So the weights are
  - $w_i = \begin{cases} 0.5 & i = 0, N \\ 1 & \text{otherwise} \end{cases}$

Simpson's Rule

- Trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating over interval
- Simpson's 1/3 rule is an extension of the trapezoidal rule where the integrand is approximated by a second-order polynomial
- $I = \int_a^b f(x)dx \approx \int_a^b f_2(x)\,dx$
- Here, $f_2(x)$ is a second order polynomial
  - $f_2(x) = a_0 + a_1 x + a_2 x^2$

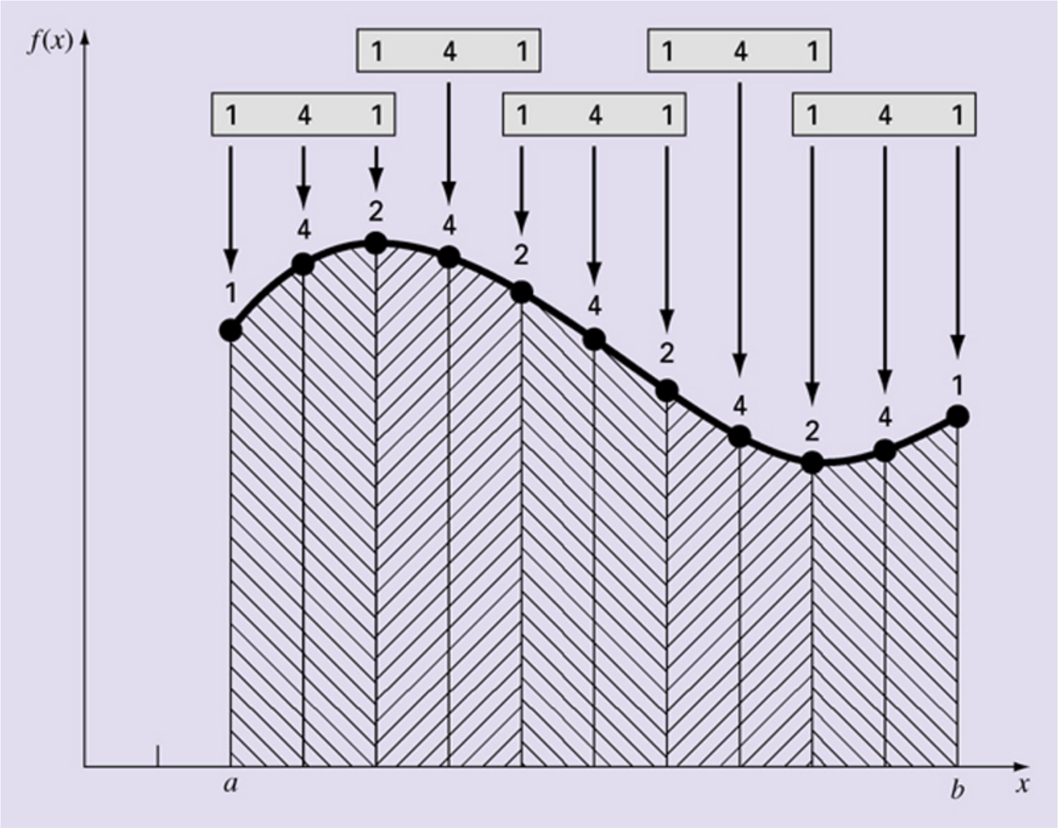
Simpson's Rule

- Simpson's rule:
  - $\int_a^b f(x)dx = \frac{\Delta x}{3}[f(a) + \underline{4}f(a+\Delta x) + f(b)]$
    - where $\Delta x = \frac{b-a}{2}$
- Simpson's rule can only be applied when there are an even number of subintervals
  - $\int_{x_1}^{x_n} f(x)dx \approx \sum_{i=1,3,5}^{n-2} \frac{x_{i+1} - x_i}{3}[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})]$

Composite Simpson's Rule

- Simpson's rule for x_0, x_1, x_2 is given as:
- $$\int_{x_0}^{x_2} p_1(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$
- We can do the same on x_2, x_3, x_4 to get
- $$\int_{x_2}^{x_4} p_1(x)dx = \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$
- Hence on the entire region
- $$\int_{x_0}^{x_4} f(x)dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)\right]$$
- In general for an even number of intervals
- $$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(a) + f(b)\right] + \frac{4h}{3}\sum_{i=1}^{n/2} f(x_{2i-1}) + \frac{2h}{3}\sum_{i=1}^{n/2-1} f(x_{2i})$$

Composite Simpson's Rule



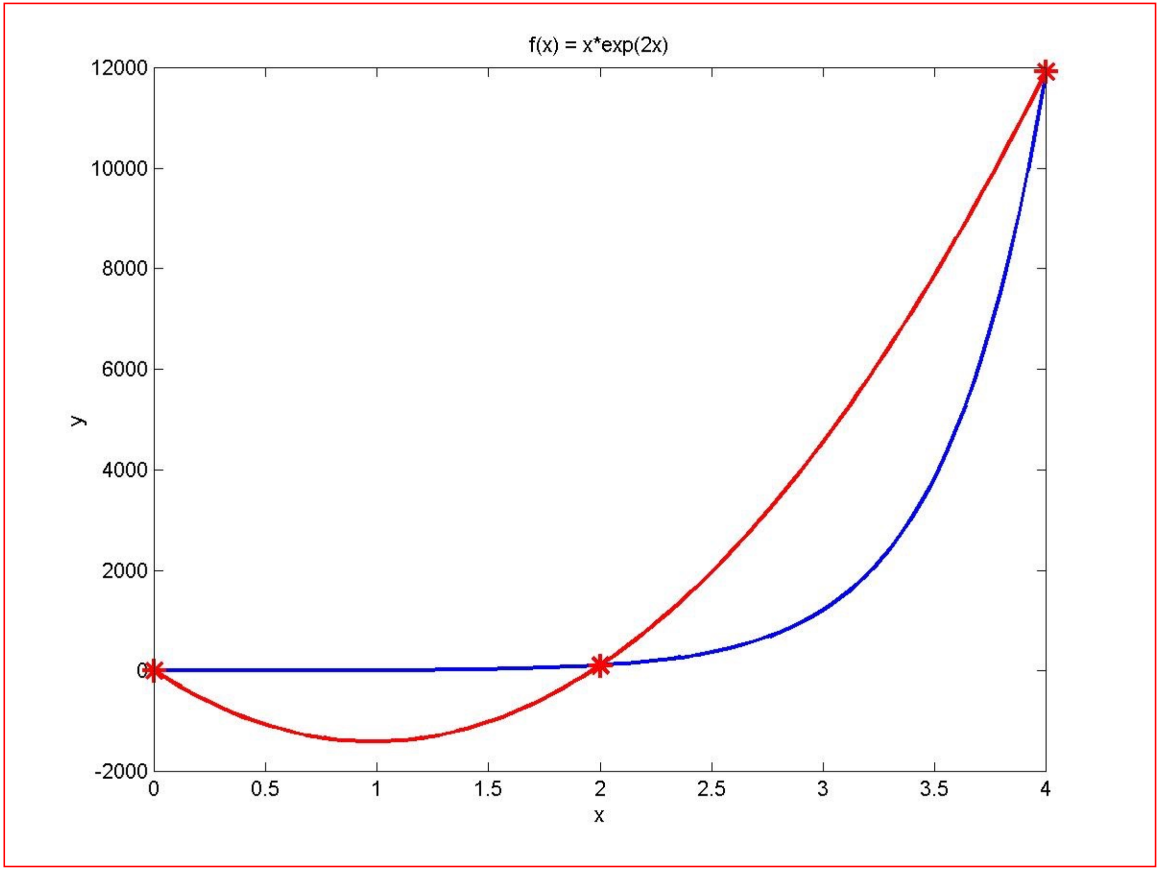
Applicable only if the number of segments is even

Weights in Simpson's Rule

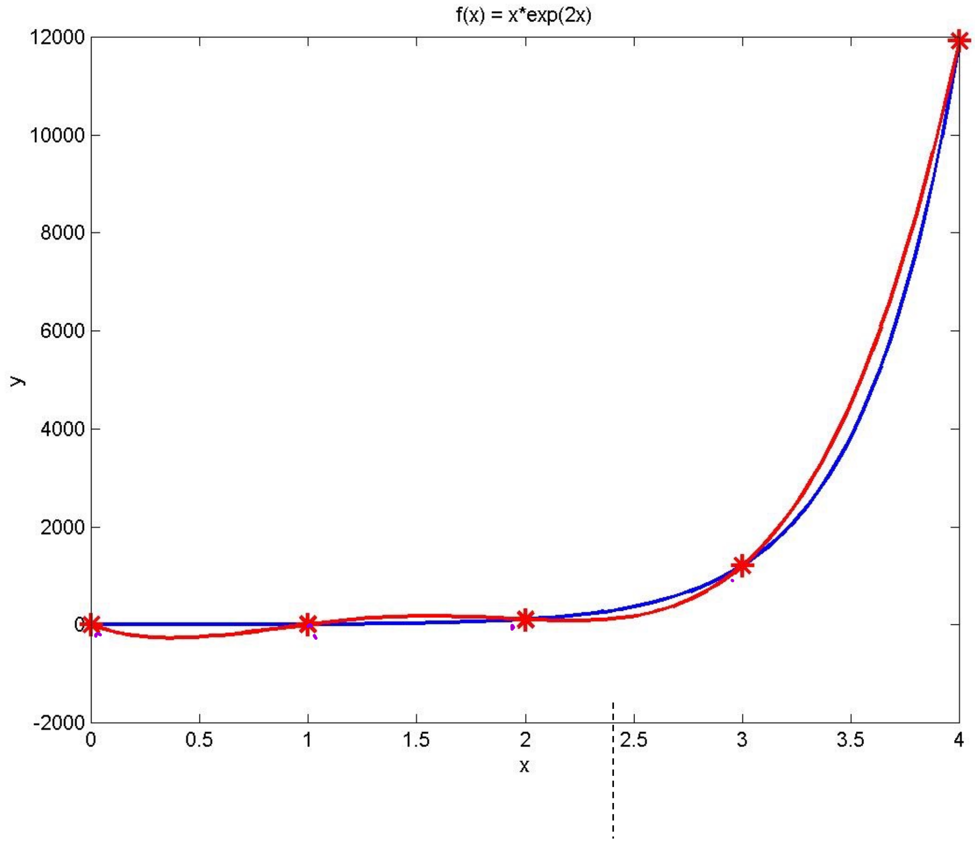
- For 1/3 Simpson' Rule the weights are:

- $w_i = \begin{cases} 1/3 & \text{end points} \\ 4/3 & \text{odd points} \\ 2/3 & \text{even points} \end{cases}$

Simpson's Rule



Composite Simpson's 1/3 Rule



Higher order fits

- Can increase the order of the fit to cubic, quartic etc.
- For a cubic fit over x_0,x_1,x_2,x_3 we find

$$\int_{x_0}^{x_3} f(x)dx \cong \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right]$$

- For a quartic fit over x_0,x_1,x_2,x_3,x_4

Simpson's 3/8th Rule

$$\int_{x_0}^{x_4} f(x)dx \cong \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right]$$

Boole's Rule

- In practice these higher order formulas are not that useful, we can devise better methods if we first consider the errors involved

Error in the Trapezoid Rule

- Consider a Taylor expansion of f(x) about a

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \ldots$$

- The integral of f(x) written in this form is then

$$\int_a^b f(x)dx = \left[af(a) + \frac{(x-a)^2}{2!}f'(a) + \frac{(x-a)^3}{3!}f''(a) + \frac{(x-a)^4}{4!}f'''(a) + \frac{(x-a)^5}{5!}f''''(a) \right]_a^b$$

$$= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \frac{h^4}{24}f'''(a) + \ldots$$

$$h = b - a$$

Error in the Trapezoid Rule

- Perform the same expansion about b

$$\int_a^b f(x)dx = hf(b) - \frac{h^2}{2}f'(b) + \frac{h^3}{6}f''(b) - \frac{h^4}{24}f'''(b)$$

- If we take an average of (1) and (2) then

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + f(b)\right] + \frac{h^2}{4}\left[f'(a) - f'(b)\right] + \frac{h^3}{12}\left[f''(a) + f''(b)\right] + \frac{h^4}{48}\left[f'''(a) - f'''(b)\right)$$

- Notice that odd derivatives are differenced while even derivatives are added

Error in the Trapezoid Rule

- We also make Taylor expansions of f' and f'' around both a & b which allow us to substitute for terms in f'' and f'''' and to derive

$$\int_a^b f(x)dx = \frac{h}{2}\left[f(a) + f(b)\right] + \frac{h^2}{12}\left[f'(a) - f'(b)\right] + \frac{h^4}{720}\left[f'''(a) - f'''(b)\right] \cdots$$

- It takes *quite a bit of work* to get to this point, but the key issue is that we have now created correction terms which are all differences
- If we now use this formula in the composite trapezoid rule there will be a large number of cancellations

Error in the Composite Trapzoid

- We now sum over a series of trapezoids to get

$$\int_a^b f(x)dx = \frac{h}{2}\Big[\big(f(a)+f(x_1)\big)+\big(f(x_1)+f(x_2)\big)+\ldots+\big(f(x_{n-2})+f(x_{n-1})\big)+\big(f(x_{n-1})+f(b)\big)\Big]$$

$$+\frac{h^2}{12}\Big[\big(f'(a)-f'(x_1)\big)+\big(f'(x_1)-f'(x_2)\big)+\ldots+\big(f'(x_{n-2})-f'(x_{n-1})\big)+\big(f'(x_{n-1})-f'(b)\big)\Big]$$

$$+\frac{h^4}{720}\Big[\big(f'''(a)-f'''(x_1)\big)+\big(f'''(x_1)-f'''(x_2)\big)+\ldots+\big(f'''(x_{n-2})-f'''(x_{n-1})\big)+\big(f'''(x_{n-1})-f'''(b)\big)\Big]$$

$$+\ldots$$

$$=\frac{h}{2}\big[f(a)+f(b)\big]+h\sum_{i=1}^{n-1}f(a+ih)+\frac{h^2}{12}\big[f'(a)-f'(b)\big]+\frac{h^4}{720}\big[f'''(a)-f'''(b)\big]+\ldots \quad (11)$$

- Note now $h = \frac{b-a}{n}$
- The expansion is in powers of h^{2i}

Error in estimating the integral

Assumption : $f'(x)$ is continuous on $[a,b]$

Equal intervals (width = h)

Theorem : If Trapezoid Method is used to

approximate $\int_a^b f(x)dx$ then

$$Error = \frac{b-a}{12} h^2 \left(f'(b) - f'(a) \right)$$

$$|Error| \le \frac{b-a}{12} h^2 \max_{x \in [a,b]} |f'(x)|$$

Estimating error for trapezoid rule

$$\int_0^{\pi} \sin(x)dx, \quad \textit{find } h \textit{ so that } |\text{error}| \le \frac{1}{2}\times 10^{-5}$$

$$|Error| \le \frac{b-a}{12} h^2 \max_{x\in[a,b]} |f'(x)|$$

$$b = \pi \quad a = 0 \quad f'(x) = \cos(x)$$

$$|f'(x)| \le 1 \Rightarrow |Error| \le \frac{\pi}{12} h^2 \le \frac{1}{2}\times 10^{-5}$$

$$\Rightarrow \qquad h^2 \le \frac{6}{\pi} 10^{-5} = 1.91\times 10^{-5} \Rightarrow h \le 0.004$$

~ 750 equally spaced points

Gaussian Quadrature

- So far, we've considered regularly spaced abscissa
- We've also only looked at solely at closed int. formulae
- Gaussian quadrature achieves high accuracy and efficiency by the optimal choice of abscissa
- We generally apply a change of variables to make the integral map [-1, 1]
- There are a number of number of families of Gaussian quadrature, we'll look at Gauss-Legendre
- Slides were adapted from http://numericalmethods.eng.usf.edu/topics/gauss_quadrature.html

See here for further details

Theory of Gaussian Quadrature

- Recall the trapezoid method
  - $\int_a^b f(x)dx =$ $h\left[\sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}\left(f(x_0) + f(x_n)\right)\right]$
- Let's express it as
  - $\int_a^b f(x)dx = \sum_{i=0}^{n} c_i f(x_i)$
  - where $c_i = \begin{cases} h & i = 1, 2, \dots, n-1 \\ 0.5 & i = 0 \text{ and } n \end{cases}$

Basis of Gaussian Quadrature Rule

- Previously we discussed how the trapezoid rule was developed using the method of undetermined coefficients
  - $\int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$

$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

- The two-point Gaussian Quadrature Rule is an extension of the Trapezoidal Rule approximation
  - where the arguments of the function are not predetermined as a and b, but as unknowns x_1 and x_2
  - $I = \int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$

Basis of the Gaussian Quadrature Rule

- We can find our four unknowns x_1, x_2, c_1 and c_2 by assuming that the formula gives exact results for integrating a general 3rd order polynomial
  - $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$
- Then we find that
  - $$\int_a^b f(x)dx = \int_a^b (a_0 + a_1 x + a_2 x^2 + a_3 x^3)dx$$
  - $$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4}\right]_a^b$$
  - $$= a_0(b-a) + a_1\left(\frac{b^2-a^2}{2}\right) + a_2\left(\frac{b^3-a^3}{3}\right) + a_3\left(\frac{b^4-a^4}{4}\right)$$
- Recalling that $I \approx c_1 f(x_1) + c_2 f(x_2)$
- $$\Rightarrow I = c_1(a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3) + c_2(a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3)$$

Basis of the Gaussian Quadrature Rule

- Equating the two expressions yields
  - $a_0(b-2) + a_1(\frac{b^2-a^2}{2}) + a_2(\frac{b^3-a^3}{3}) + a_3\frac{b^4-a^4}{4})$

=

- As the constants a_0, a_1, a_2, a_3 are arbitrary
- $b - a = c_1 + c_2$ $\quad \frac{b^2-a^2}{2} = c_1 x_1 + c_2 x_2$
- $\frac{b^3-a^3}{3} = c_1 x_1^2 + c_2 x_2^2$ $\quad \frac{b^4-a^4}{4} = c_1 x_1^3 + c_2 x_2^3$
- Only one solution to the four equations
- $x_1 = \frac{(b-a)}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$; $x_2 = \frac{(b-a)}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$
- $c_1 = \frac{b-a}{2}$; $c_2 = \frac{b-a}{2}$

Gaussian Quadrature

- In conclusion, the two-point Gaussian Quadrature Rule is
   - $\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$
   - $= \frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)$

$$+ \frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)$$

Higher Point Gaussian Quadrature Formulae

- $$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$
- is called the three-point Gaussian Quadrature Rule
- As for the two-point rule, one can calculate the coefficients $c_1 c_2 + c_3$ and the functional arguments x, x_2 and x_3 by assuming that the formula gives exact expressions for integrating a fifth order polynomial
  - $$\int_a^b (a_0 + a_1 + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5)dx$$
- General n-point rules would approximate the integral
  - $$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + \dots \; c_n f_n(x)$$

Arguments and Weighing Factors

- In handbooks, the coefficients and arguments are given for Gaussian quadrature rules for integrals of the form

$$\int_{-1}^{+1} g(x)dx \approx \sum_{i=1}^{n} c_i \, g(x_i)$$

Weighting factors c and function arguments x used in Gaussian Quadrature Formulae.

Points	Weighting Factors	Function Arguments
2	c_1 = 1.000000000 c_2 = 1.000000000	x_1 = -0.577350269 x_2 = 0.577350269
3	c_1 = 0.555555556 c_2 = 0.888888889 c_3 = 0.555555556	x_1 = -0.774596669 x_2 = 0.000000000 x_3 = 0.774596669
4	c_1 = 0.347854845 c_2 = 0.652145155 c_3 = 0.652145155 c_4 = 0.347854845	x_1 = -0.861136312 x_2 = -0.339981044 x_3 = 0.339981044 x_4 = 0.861136312

Arguments and Weighing Factors

- Now that we have a table for $\int_{-1}^{1} g(x)dx$ integrals,
  - how can we use it for $\int_a^b f(x)\,dx$ integrals:
- Recall that any integral with limits [a,b] can be converted into an integral with limits [-1,1]
- Let $x =$ $mt + c$
  - If $x = a \Rightarrow$ $t = -1$
  - If $x = b \Rightarrow$ $t = 1$
- $\Rightarrow m =$ $\frac{b-a}{2}$ and $c =$ $\frac{a+b}{2}$
- i.e. $x =$ $\frac{b-a}{2}t + \frac{a+b}{2}$; $dx =$ $\frac{b-a}{2}$
- Substituting x and dx yields