

# Numerical Methods Lecture 4 - Numerical Integration / Differentiation

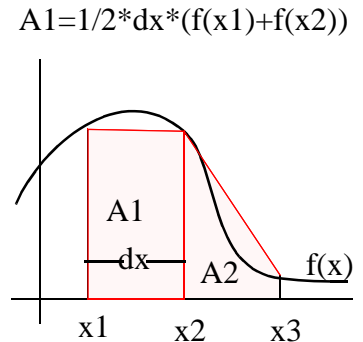
## Numerical Integration - approximating the area under a function

We will consider 3 methods: Trapezoidal rule, Simpson's rule, Gauss Quadrature

The basic concept is to break the area up into smaller pieces with simple shapes fitted to approximate the function over short lengths. The area under these simple shapes are then added up to approximate the total.

### Trapezoidal rule - piece-wise linear approximation to curve f(x)

- chop area into N smaller pieces (sample of two pieces on the right)
- connect areas with straight lines, creating trapezoids
- find the area under each trapezoid  $A = 1/2 * dx * (f(x) + f(x+dx))$
- add up the trapezoids



Example, the figure at the bottom of the page chops a function into 4 trapezoids over the range [a, b]. The trapezoidal rule adds up the area of each of the 4 trapezoids to represent the area under the function f(x).

$$dx = (b-a)/N \quad (a, b \text{ are limits, } N \text{ is number of pieces we divide the area into})$$

$$A1 = 1/2 * dx * (f(x1) + f(x2))$$

$$A2 = 1/2 * dx * (f(x2) + f(x3))$$

$$A3 = 1/2 * dx * (f(x3) + f(x4))$$

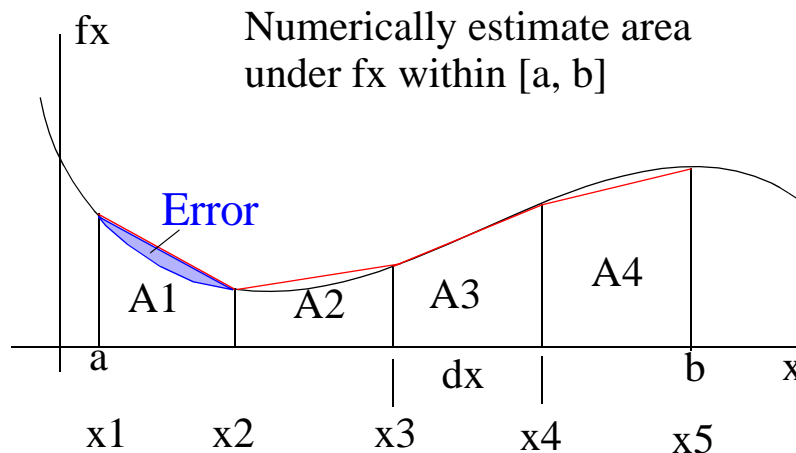
$$A4 = 1/2 * dx * (f(x4) + f(x5))$$

$$\text{Area} = \frac{1}{2} * dx * (f(x1) + 2*f(x2) + 2*f(x3) + 2*f(x4) + f(x5))$$

The generalized equation expressing trapezoidal rule is then  $\implies \text{Area} \cong \frac{1}{2} dx \left[ f(x_1) + 2 \sum_{i=2}^N f(x_i) + f(x_{N+1}) \right]$

**Error:** The error (in blue) between the area of the trapezoid and the curve it represents builds up

**Error reduction:** We can reduce error if we can shorten the straight lines used to estimate curves. Increasing the number (increase N) of trapezoids used over the same range [a,b] will reduce error in the area estimate.



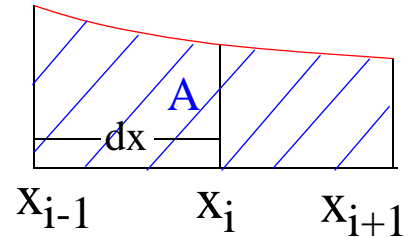
**We can also get a little more sophisticated than straight line estimates**

The error using trapezoidal rule comes from using a series of straight lines to represent a curve. To reduce this error, we'll now look at using a series of second order curves to repress the function.

**Simpson's Rule** - piece-wise second order approximation of f(x).

$$A = dx/3 * [f(x_{i-1}) + 4*f(x_i) + f(x_{i+1})]$$

- chop area into N smaller pieces
- connect every **3** points with **second order** curve fit, this gives us N/2 smaller areas representing the curve in the range [a,b]
- Find the area under each second order polynomial estimate.  
 $A = dx/3 * [f(x_1) + 4*f(x_2) + f(x_3)]$
- Add up the smaller areas to estimate area under the curve



Example, the figure at the bottom of the page chops a function into 8 pieces over the range [a, b]. Every two adjacent pieces are joined to form a sub-area. The Simpson's rule adds up the 4 sub-areas to represent the area under the function f(x).

$$A_1 = dx/3 * (f(x_1) + 4f(x_2) + f(x_3))$$

$$A_2 = dx/3 * (f(x_3) + 4f(x_4) + f(x_5))$$

$$A_3 = dx/3 * (f(x_5) + 4f(x_6) + f(x_7))$$

$$A_4 = dx/3 * (f(x_7) + 4f(x_8) + f(x_9))$$

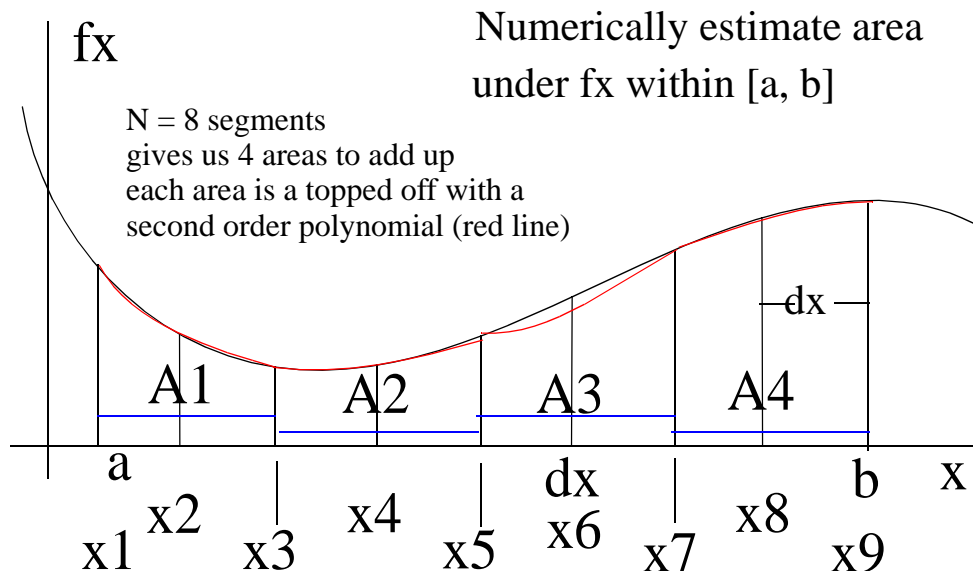
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$$Area = A_1 + A_2 + A_3 + A_4$$

$$= dx/3 * (f(x_1) + 4f(x_2) + 2f(x_3) + 4f(x_4) + 2f(x_5) + 4f(x_6) + 2f(x_7) + 4f(x_8) + f(x_9))$$

$$Simpson's rule is ==> Area \cong \frac{1}{3} dx \left[ f(x_1) + \left[ 4 * \sum_{j=2, even}^N f(x_j) \right] + \left[ 2 * \sum_{k=3, odd}^{N-1} f(x_k) \right] + f(x_{N+1}) \right]$$

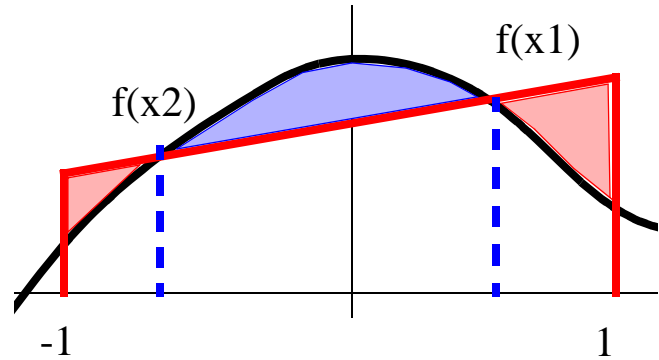
- Reduce error by increasing N
- This method requires N to be even, since we need 3 points per sub-area



## Gauss Quadrature Integration

Rather than cutting the range up into small pieces, we can try to find a single trapezoid that represents the function over the given range. The trapezoid is defined by the range  $[-1, 1]$  and the evaluation of the function at  $f(x_1)$  and  $f(x_2)$ . See figure ==>

If we pick  $x_1$  and  $x_2$  correctly, the blue area (under estimate) will balance out the red area (overestimate), and the total area under the trapezoid will be the same as the function.



The trick is then to find the correct values for  $x_1$  and  $x_2$ , and to weight the function evaluations. Our integral estimate becomes:

$$\int_{-1}^1 f(x) dx = c_0 f(x_0) + c_1 f(x_1)$$

We need to solve for 4 unknown values ( $c_0, c_1, x_0, x_1$ ). We'll need four equations. We'll get these by assuming that the above estimate is exact for constant through 3rd order functions:

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^1 1 dx = 2 \qquad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^1 x dx = 0$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^1 x^2 dx = \frac{2}{3} \qquad c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^1 x^3 dx = 0$$

solving these four equations simultaneously gives us the following solutions:

$$c_0 = c_1 = 1 \qquad x_0 = \frac{-1}{\sqrt{3}} \qquad x_1 = \frac{1}{\sqrt{3}}$$

### The result:

- This says that we can estimate the area under any function between  $[-1, 1]$  Just by evaluating the function at two carefully chosen spots!!

$$\int_{-1}^1 f(x) dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \qquad (1)$$

- Also, the derivation provides that the answer is exact if the function being integrated is a polynomial up to third order!!

The extension:

What if the range of integration is not  $[-1, 1]$  ??

Let's say  $x = \bar{x}$  when the range is  $[-1, 1]$ .

Let's also say the range of interest is  $[a, b]$

Skipping the derivation...

We reduce the integration to an equivalent over the range  $[-1, 1]$  by applying the following change of variables

$$x = \frac{(b+a) + (b-a)\bar{x}}{2} \quad (2) \quad dx = \frac{b-a}{2}d\bar{x} \quad (3)$$

To apply this change of variables, we re-write equation (1) now as:

$$\int_a^b f(x)dx = \left[ f\left(\frac{(b+a) + (b-a)\left(-\frac{1}{\sqrt{3}}\right)}{2}\right) + f\left(\frac{(b+a) + (b-a)\left(\frac{1}{\sqrt{3}}\right)}{2}\right) \right] * \left(\frac{b-a}{2}\right) \quad (4)$$

**Example:** Integrate the following function over the range [ 0 , 0.8 ]

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)dx$$

Re-writing Eq. 4 above gives the general solution:

$$\int_a^b f(x)dx = (f(x_0) + f(x_1))\left(\frac{b-a}{2}\right) \quad (5)$$

$$\text{where } x_0 = \frac{(b+a) + (b-a)\left(-\frac{1}{\sqrt{3}}\right)}{2} \text{ and } x_1 = \frac{(b+a) + (b-a)\left(\frac{1}{\sqrt{3}}\right)}{2} \quad (6)$$

For this example,  $a = 0$  and  $b = 0.8$ . Plugging these values into (6), then plugging  $x_0, x_1$  into (5), we get

$$\text{Gauss Quadrature Area estimate} = f(0.169) + f(0.631) = 0.516741 + 1.305837 = 1.822577$$

$$\text{Exact Answer} = 1.640533$$

Note, if we truncated the function being integrated after the  $x^3$  term, then the area we estimate using (5) and (6) will be exact, since Gauss quadrature is exact for up to third order polynomial equations.

### Extension

Gauss quadrature can be extended to higher orders, involving more evaluation points, for example

$$\int_{-1}^1 f(x)dx = c_0f(x_0) + c_1f(x_1) + c_2f(x_2) + \dots + c_{n-1}f(x_{n-1})$$

## Numerical Differentiation

Read section 23.1

Derivative represents the slope of a function  $f(x)$  at a particular value  $x$

slope is  $\frac{\text{rise}}{\text{run}} = \text{change in } f(x) / \text{change in } x$

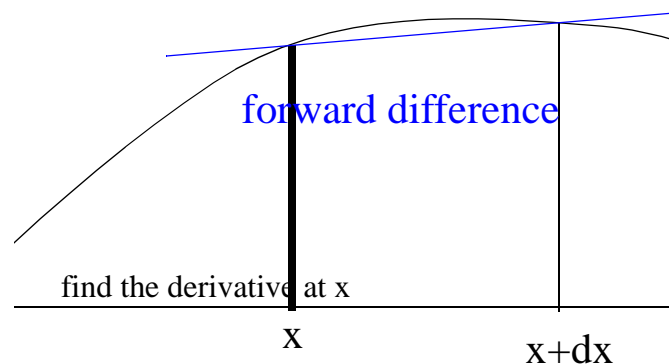
formally the definition of the derivative is:

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}$$

Here we will approximate the limit by taking some small  $\Delta x$  rather than mathematically letting it go to 0.

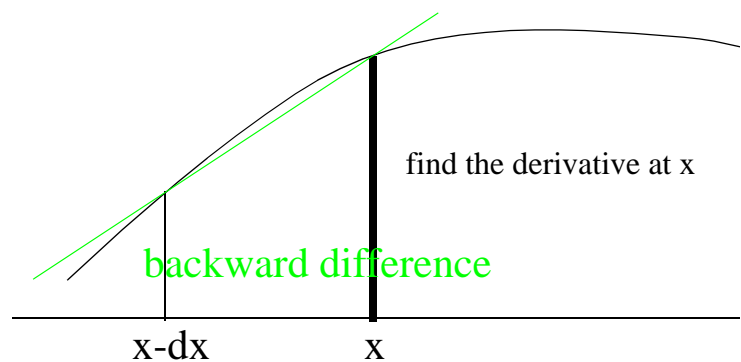
### Forward difference method

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$



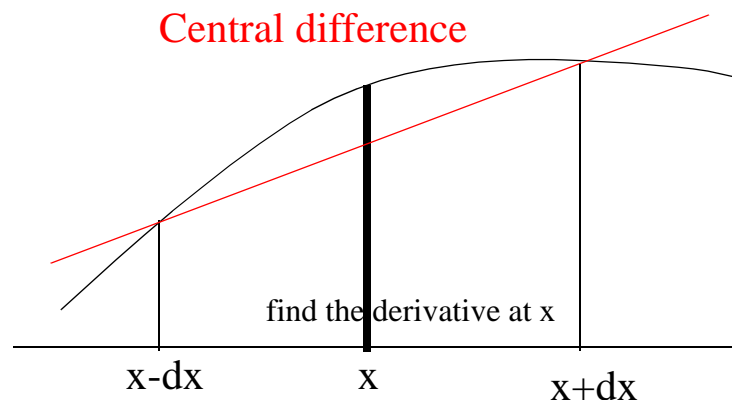
### Backward difference method

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x) - f(x - \Delta x)}{\Delta x}$$

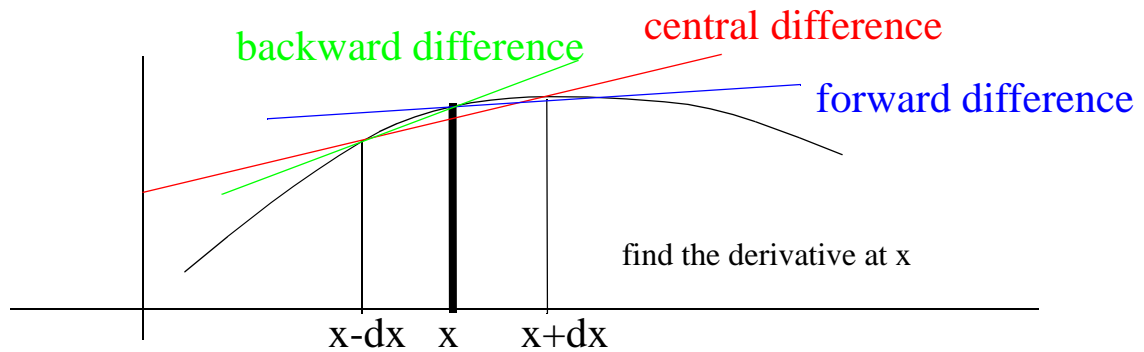


### Central difference method

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}$$



## Comparison of all three methods



Typically, central difference is the most accurate method since forward and backward biases are averaged out. In fact, just like Simpson's rule is one order higher accuracy than Trapezoidal rule, the central difference method has one order higher accuracy than forward or backward difference.

- User supplies location  $x$  at which to estimate derivative
- User supplies the  $dx$  value  $\Delta x$
- Apply one of the three equations to estimate derivative

## Mixing and Matching Numerical Methods:

Consider the Newton Raphson root finding method from NM Lecture 3. This requires the function and its derivative to iteratively solve for a root. Suppose I have a complicated looking function and I don't have the time, skill, or inclination to find its derivative analytically to use in the Newton Raphson routine. How might I combine the central difference method with Newton Raphson?