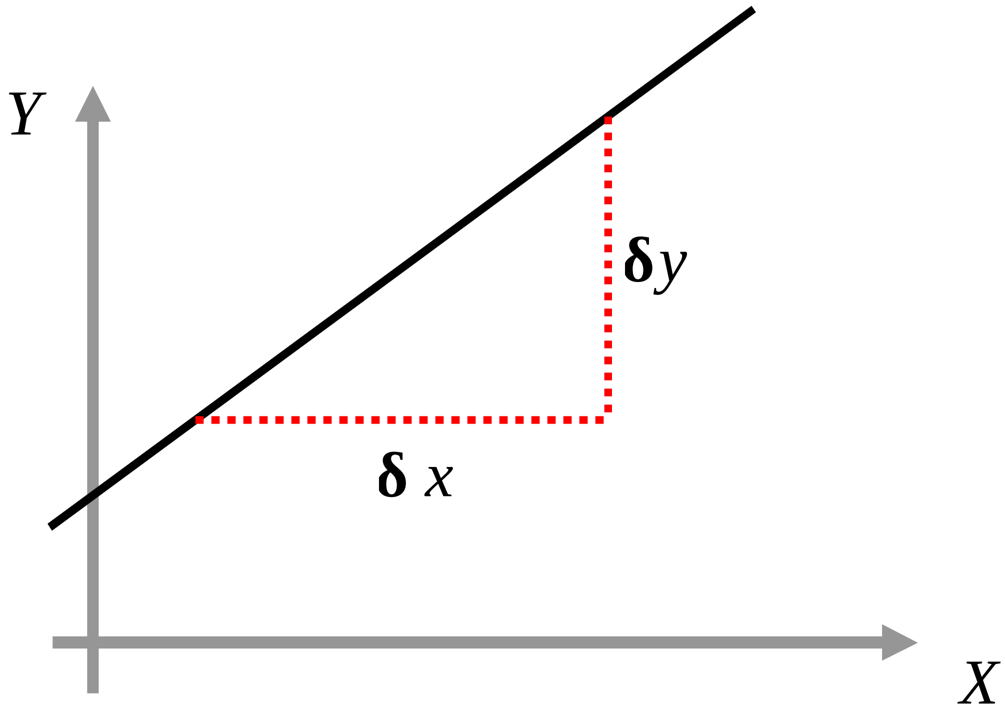
NUMERICAL DIFFERENTIATION AND INTEGRATION

Numerical Differentiation

Methods of finding a derivative

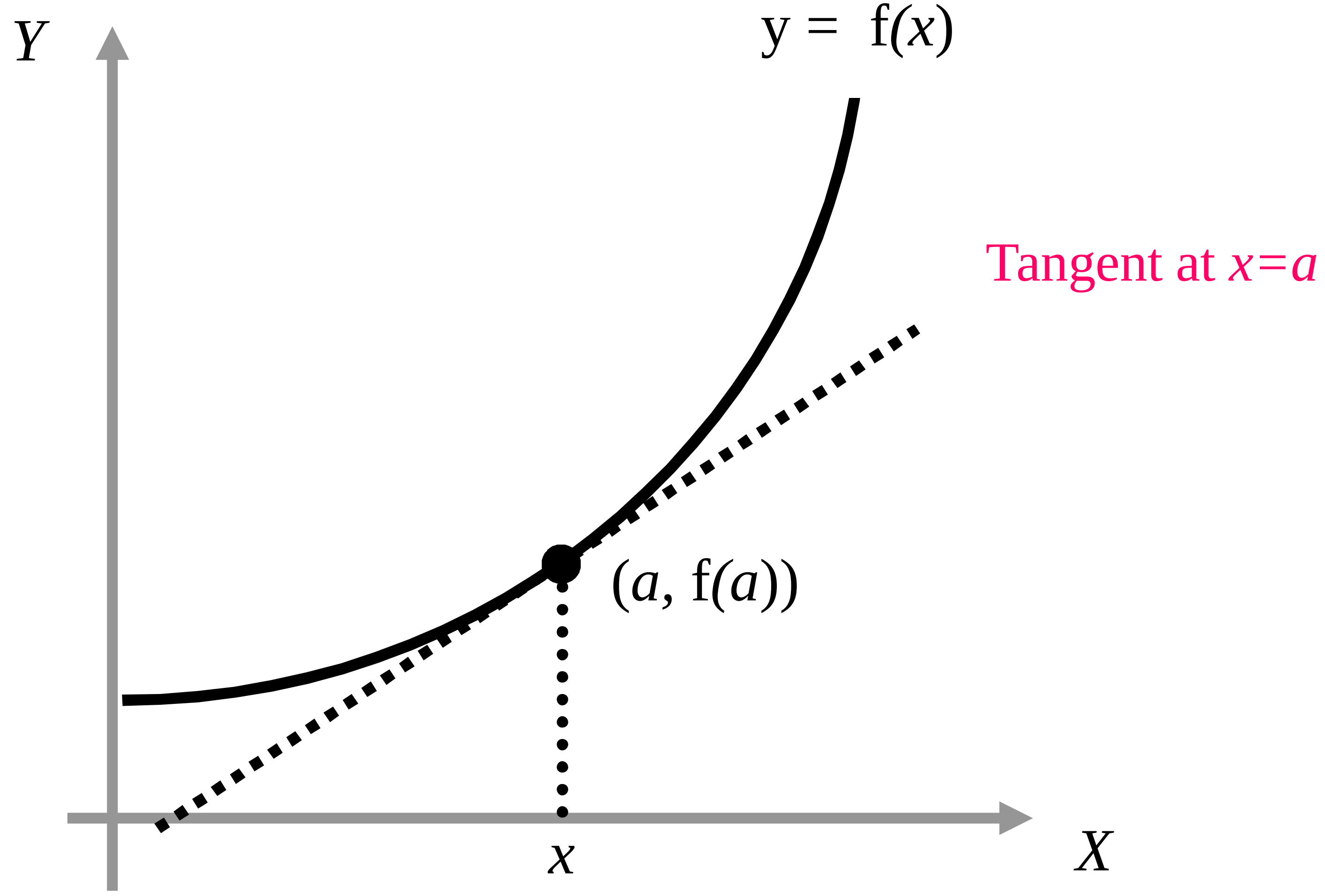
- Analytic methods
  - requires hard work
  - produces exact answer
  - not always possible
- Symbolic methods
  - computer does hard work
  - produces exact answer
  - not always possible
- Numerical methods
  - computer does the hard work
  - produces approximate answer
  - always possible

Gradient



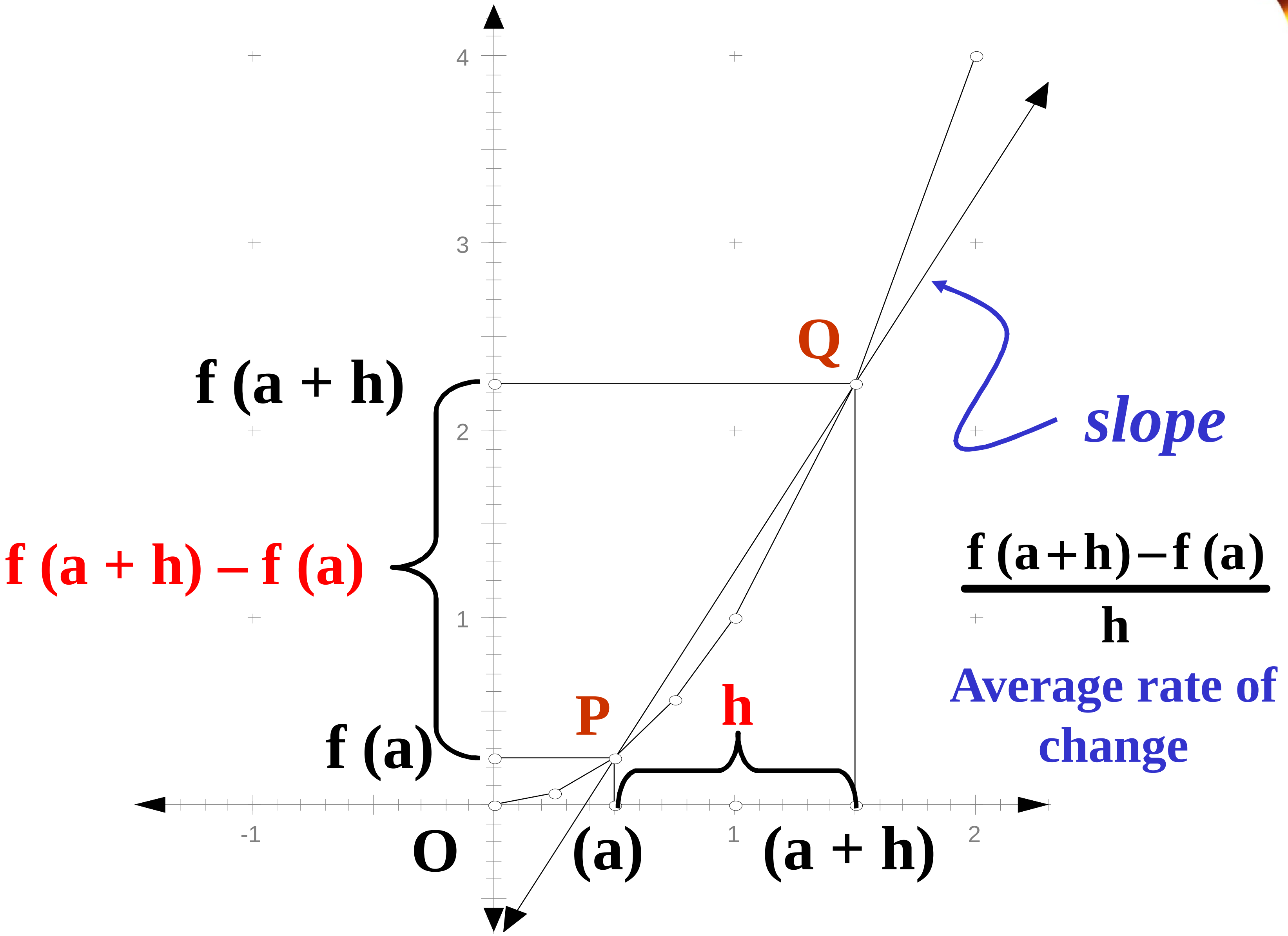
$$\text{Gradient} = \frac{\text{change in } y}{\text{change in } x} = \frac{\delta y}{\delta x}$$

Gradient at a Point



f′(a) = the gradient (slope) at the point *x*.

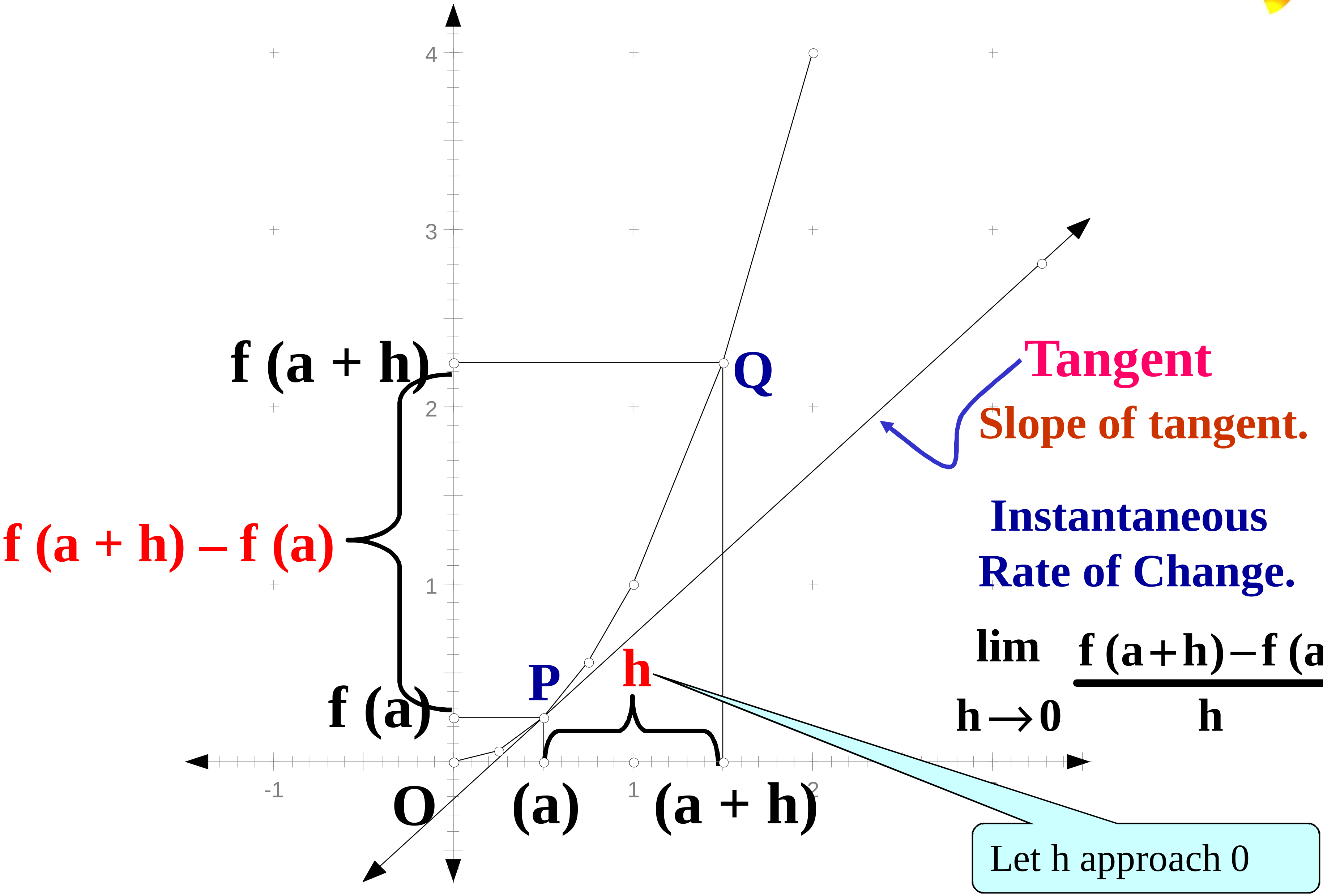
Gradient at a Point-cont.



$$\frac{f(a+h)-f(a)}{h}$$

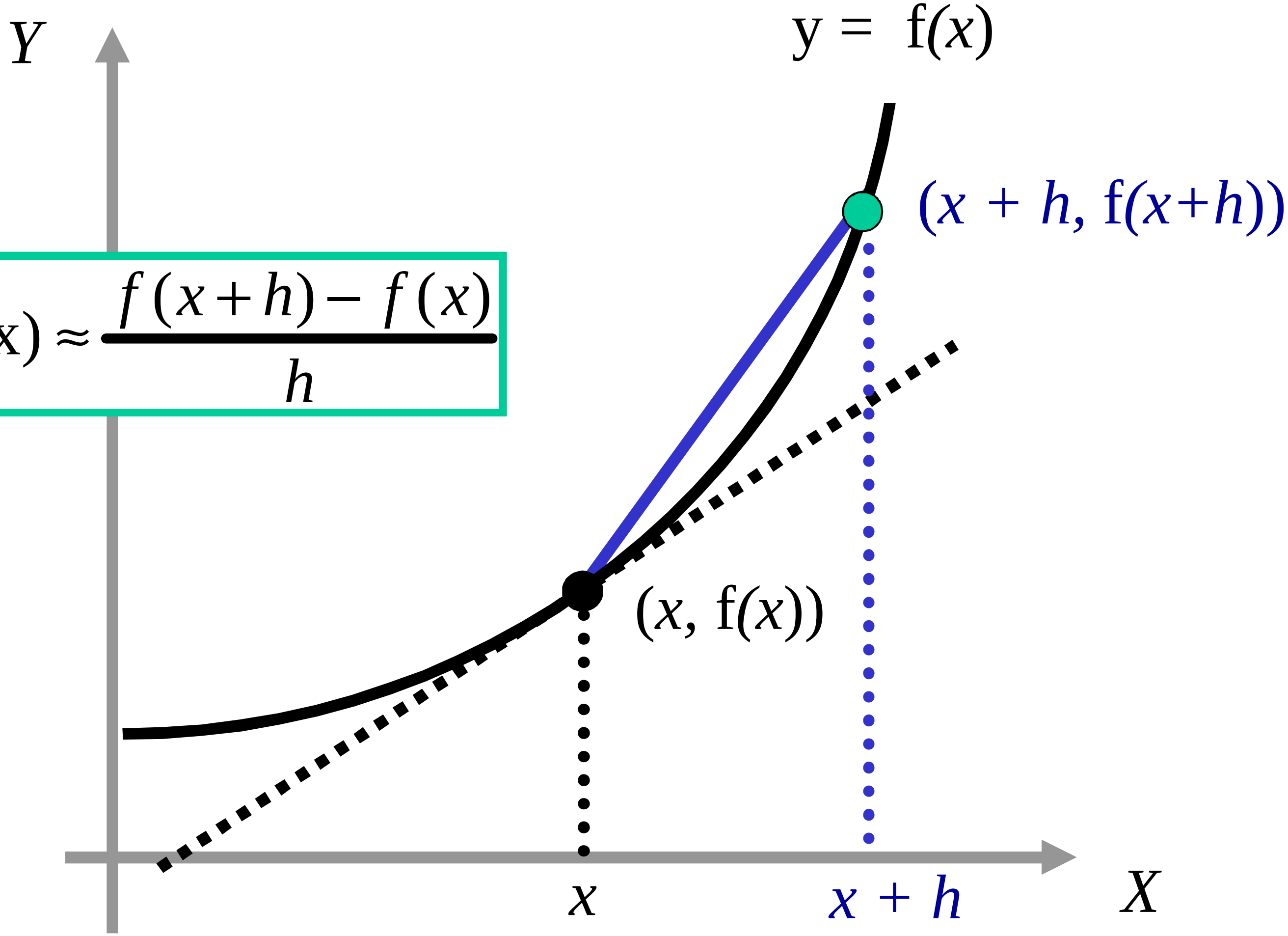
Average rate of change

Instantaneous Rate of Change



$$\lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

Forward Approximation

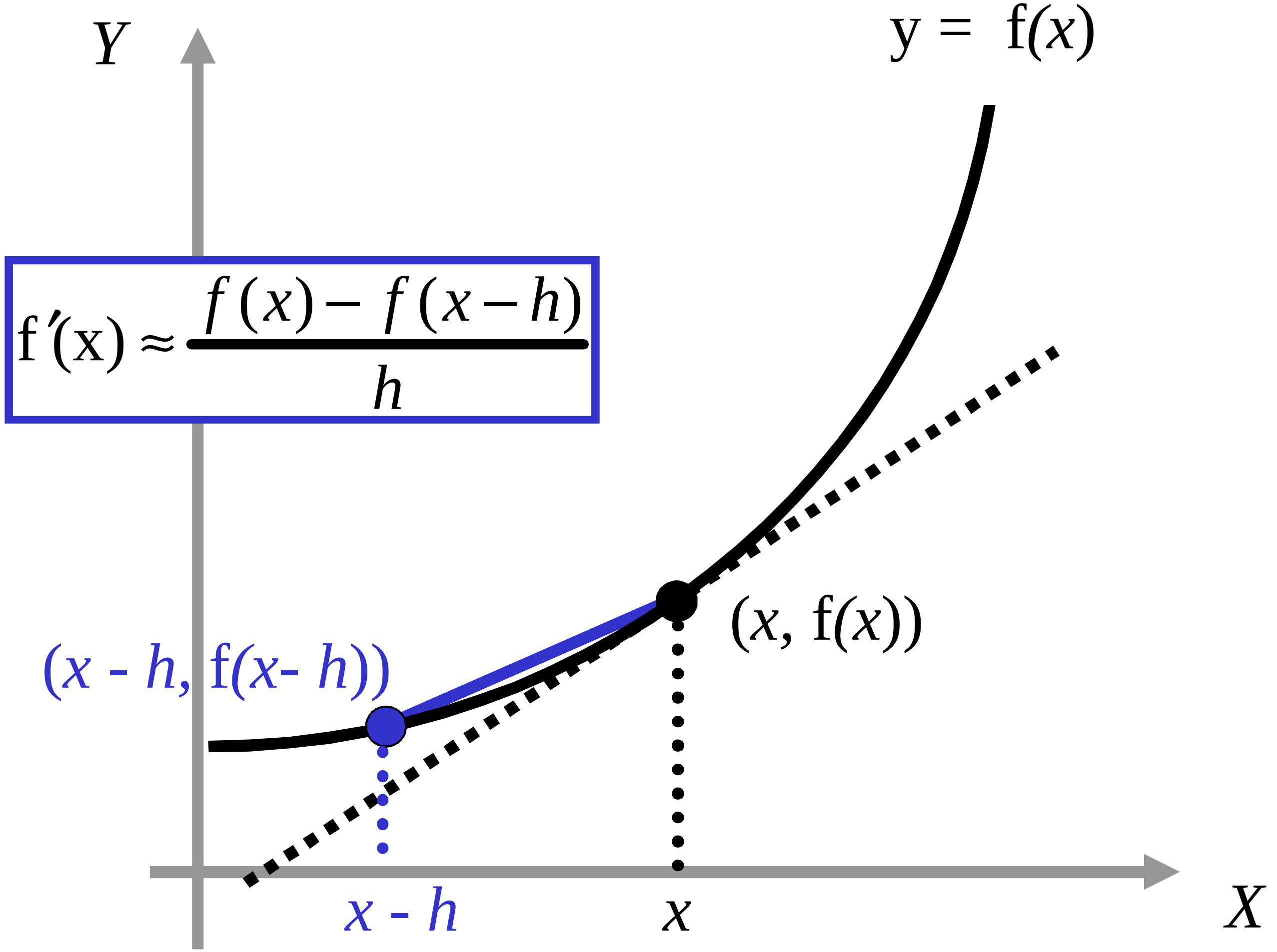


$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Approximate f′(x) *by* using ***forward differences***

Use chord joining x to (*x* + *h*, f(*x*+*h*)) , *h* should be very small

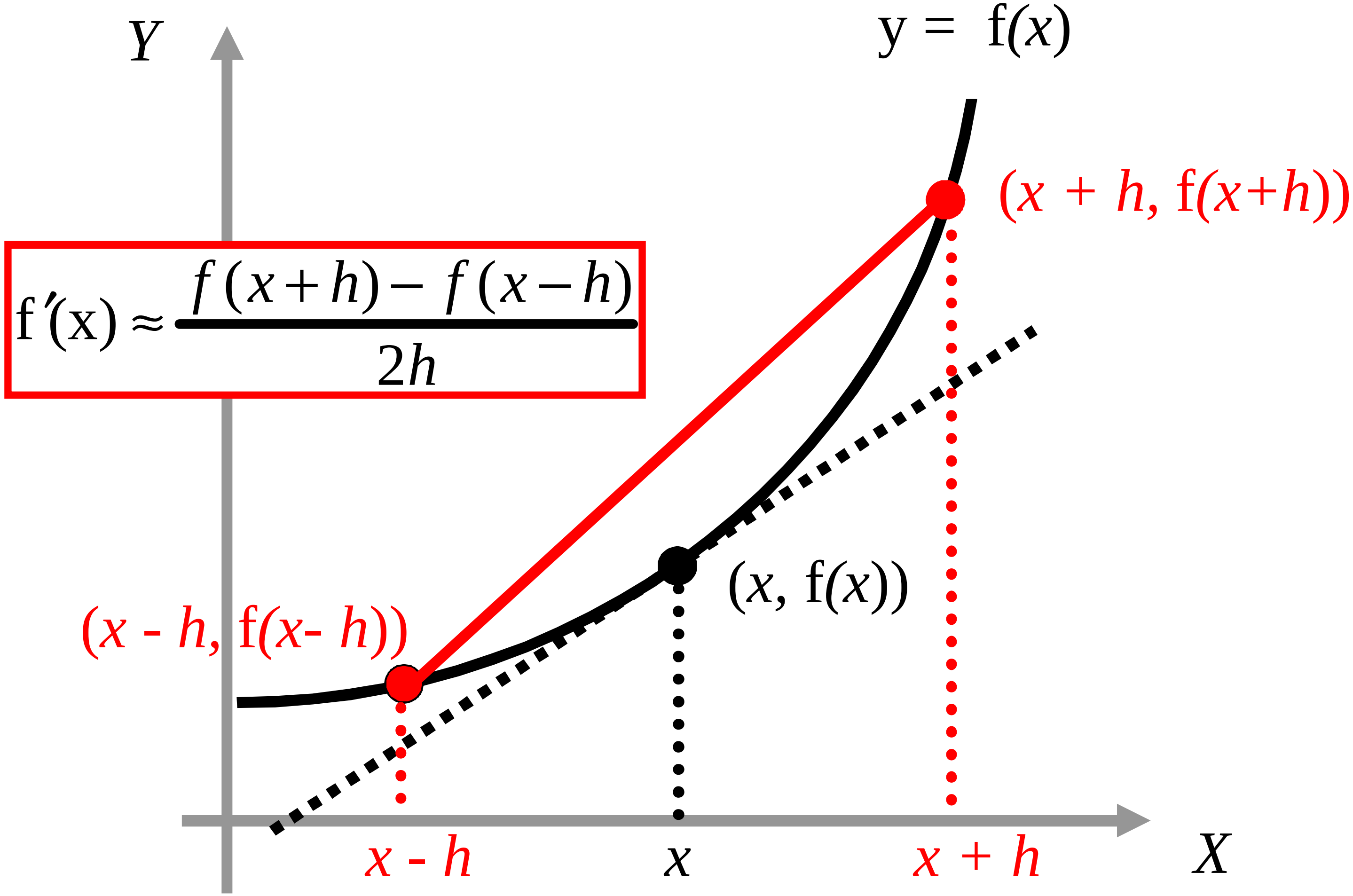
Backward Approximation



Approximate f′(x) *by* using ***backward differences***

Use chord joining (*x* - *h*, f(*x*-*h*)) to *x* , *h* should be very small

Central Approximation



Approximate f′(x) *by* using ***central differences***

Use chord joining (x - h, f(x-h)) to (x + h, f(x+h)) ,h should be very small

Summary

Forward Approximation

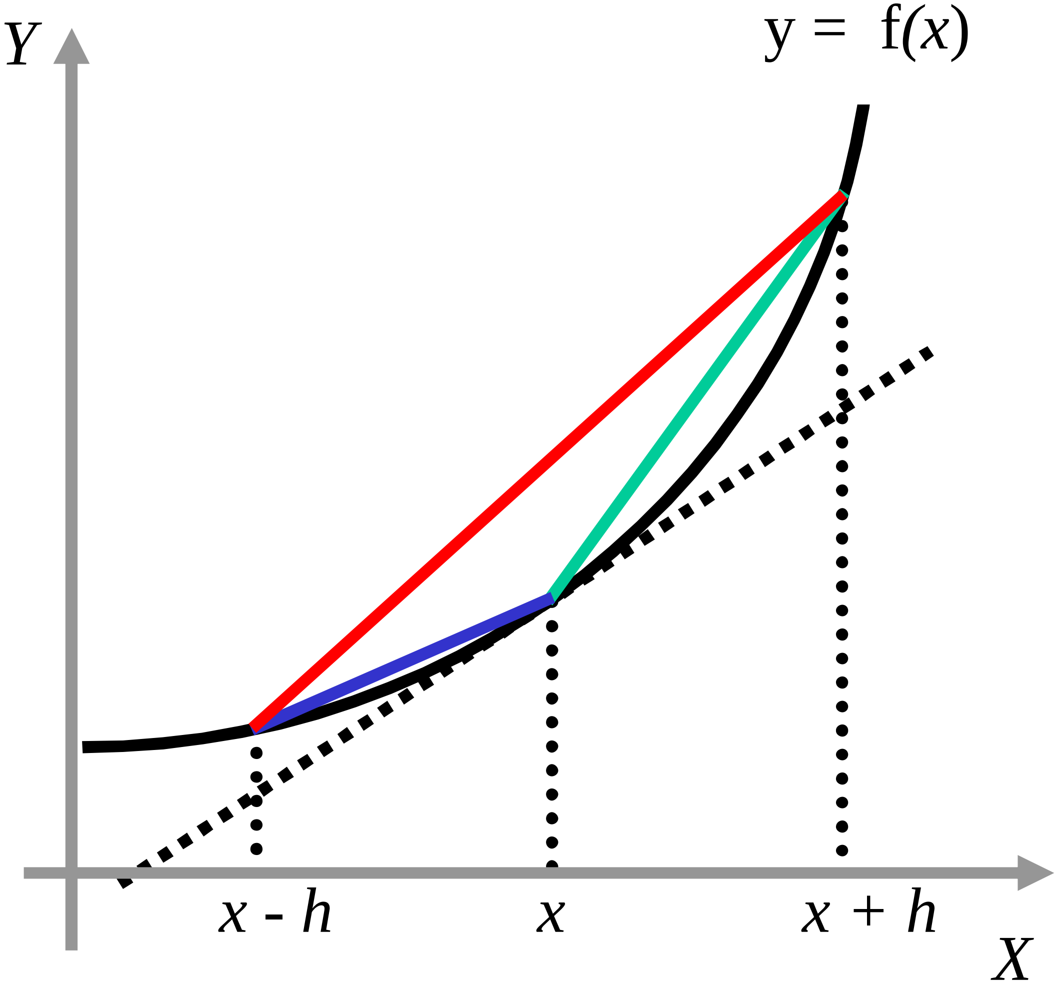
$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Backward Approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

Central Approximation

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$



Which Approximation is Best to Use?

Taylor Series

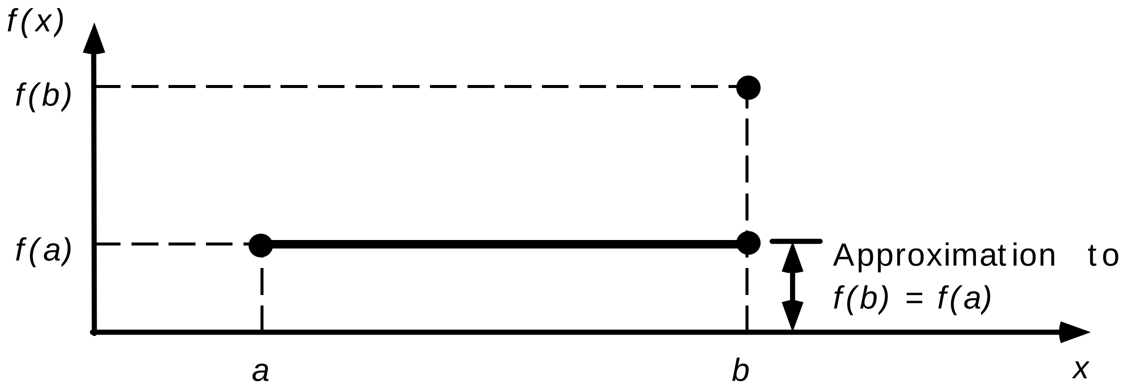
Taylor series expansion of a function *f(x)* at point *x* close to point *a*

$$f(x) = f(a) + (x-a) f'(a) + \frac{(x-a)^2}{2!} f''(a) + \frac{(x-a)^3}{3!} f'''(a) + \cdots + \frac{(x-a)^n}{n!} f^n(a) + \cdots$$

Taylor Series

Find *f(b)* given *f(a)*

$f(b) = f(a)$ Using just one term



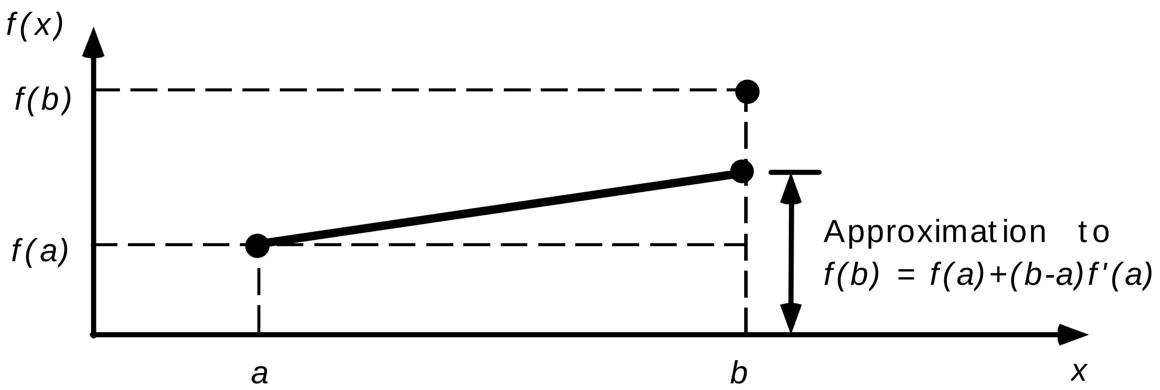
(a) one term

Taylor Series

Find *f(b)*

$$f(b) = f(a) + (b-a)\,f'(a)$$

Using two terms

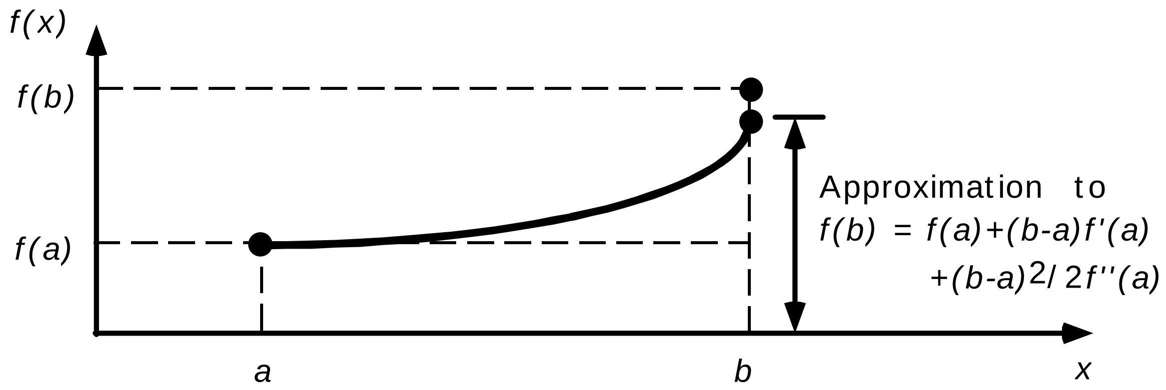


(b) two terms

Taylor Series

Find *f(b)*

$$f(b) = f(a) + (b-a)f'(a) + \frac{(b-a)^2}{2!} f''(a)$$ Using three terms



(c) three terms

Error in Truncating Taylor Series

$$f(b) = f(a)+(b\text{-}a)f'(a)+\frac{(b\text{-}a)^2}{2!}f''(a)+\frac{(b\text{-}a)^3}{3!}f'''(a)+ \mathrm{L} +\frac{(b\text{-}a)^n}{n!}f^n(a)+ \mathrm{L}$$

- If we truncate the series after the *n*th term, the error will be

$$error < \frac{(x\text{-}a)^{n+1}}{(n+1)!}\left|f^{n+1}(x)\right|_{\max} \qquad \vartheta(x\text{-}a)^{n+1}$$

- For example, if we truncate after the 3rd term

$$f(x) = f(a)+(x\text{-}a)f'(a)+\frac{(x\text{-}a)^2}{2!}f''(a)+\vartheta(x\text{-}a)^3$$

Forward First Derivative

Consider the Taylor series expansion of *f(x)* near a point '*x*'

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \cdots$$

Solve for $f'(x)$

$$f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) + \cdots = \frac{f(x+h)-f(x)}{h} + \vartheta(h)$$

Truncate here

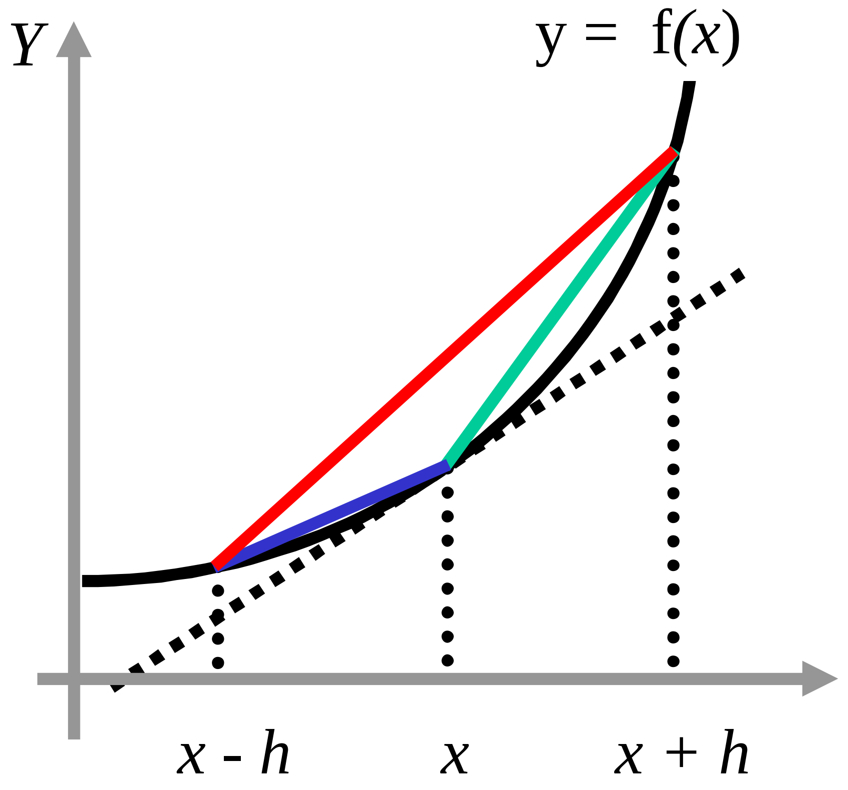
First order approximation of first derivative

$$f'(x) \approx \frac{f(x+h)-f(x)}{h} \qquad Error = \vartheta(h) = -\frac{h}{2}f''(x) + \cdots$$

Backward & Central First Derivative

Instead of *f(x+h)*, now expand *f(x-h)* to get the backward difference formula

Subtract *f(x-h)* expansion from *f(x+h)* expansion to get the central difference formula



The central approximation should always be best….

Why?

Error of the order of h^2

The Second Derivative

$$f''(x) \approx \frac{f'(x+h) - f'(x-h)}{2h}$$

$$f'(x+h) \approx \frac{f(x+2h) - f(x)}{2h} \qquad f'(x-h) \approx \frac{f(x) - f(x-2h)}{2h}$$

$$f'(x+h) - f'(x-h) \approx \frac{[f(x+2h) - f(x)] - [f(x) - f(x-2h)]}{2h}$$

$$= \frac{f(x+2h) - 2f(x) + f(x-2h)}{2h}$$

$$\boxed{f''(x) \approx \frac{f(x+2h) - 2f(x) + f(x-2h)}{4h^2}}$$

Another Way of Writing these Formulae *(the first derivatives)*

- **Forward difference formula**

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

- **Backward difference formula**

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{y_i - y_{i-1}}{x_i - x_{i-1}}$$

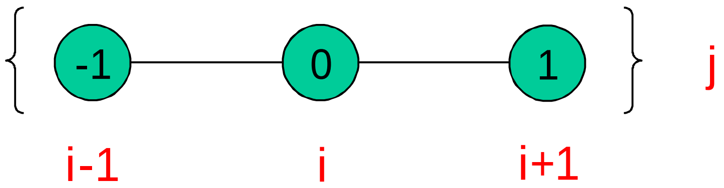
- **Central difference formula**

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$$

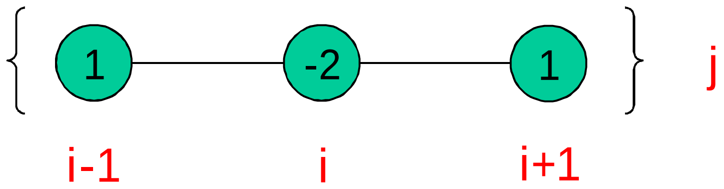
The Partial Derivatives

- Partial derivative of a function of two variables
  - General point as (x_i, y_j)
  - The value of the function $u(x, y)$ at that point as $u_{i,j}$
  - The spacing in the x and y directions is the same, h
  - Using subscripts to indicate partial differentiation

$$u_x \approx \frac{1}{2h}[-u_{i-1,j} + u_{i+1,j}] \approx \frac{1}{2h}$$



$$u_{xx} \approx \frac{1}{h^2}[u_{i-1,j} - 2u_{i,j} + u_{i+1,j}] \approx \frac{1}{h^2}$$



The Partial Derivatives

- For the mixed second partial derivative and higher derivatives, the schematic form is especially convenient.
- The Laplacian operator $\nabla^2 u = u_{xx} + u_{yy}$
- The bi-harmonic operator $\nabla^4 u = u_{xxxx} + 2u_{xxyy} + u_{yyyy}$

$$u_{xy} \approx \frac{1}{4h^2} \begin{array}{c} \left\{ \begin{array}{ccc} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{array} \right\} \\ \begin{array}{ccc} i-1 & i & i+1 \end{array} \end{array} \begin{array}{c} j+1 \\ j \\ j-1 \\ \end{array}$$

$$\nabla^2 u \approx \frac{1}{h^2} \begin{array}{c} \left\{ \begin{array}{ccc} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{array} \right\} \\ \begin{array}{ccc} i-1 & i & i+1 \end{array} \end{array} \begin{array}{c} j+1 \\ j \\ j-1 \\ \end{array}$$

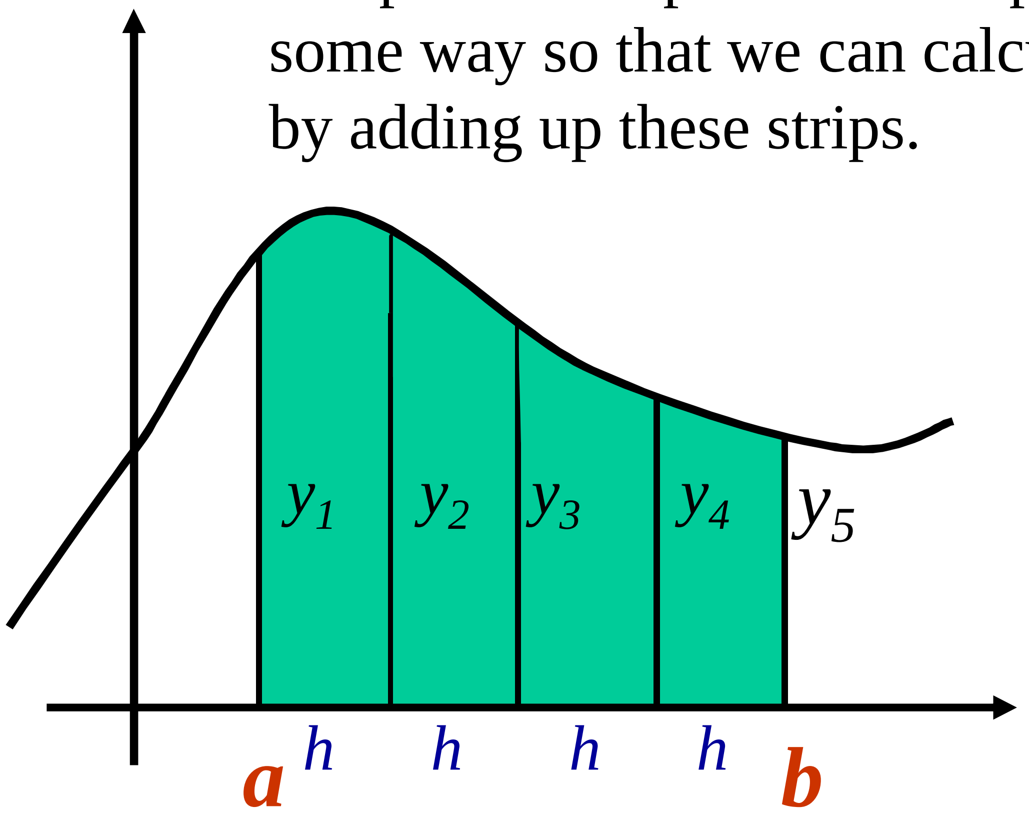
$$\nabla^4 u \approx \frac{1}{h^4} \left\{ \begin{array}{ccccc} & & 1 & & \\ & 2 & -8 & 2 & \\ 1 & -8 & 20 & -8 & 1 \\ & 2 & -8 & 2 & \\ & & 1 & & \end{array} \right\}$$

Numerical Integration

Finding Areas Numerically

Finding Areas Numerically

The basic idea is to divide the x-axis into *equally spaced divisions* as shown and to complete the top of these strips of area in some way so that we can calculate the area by adding up these strips.



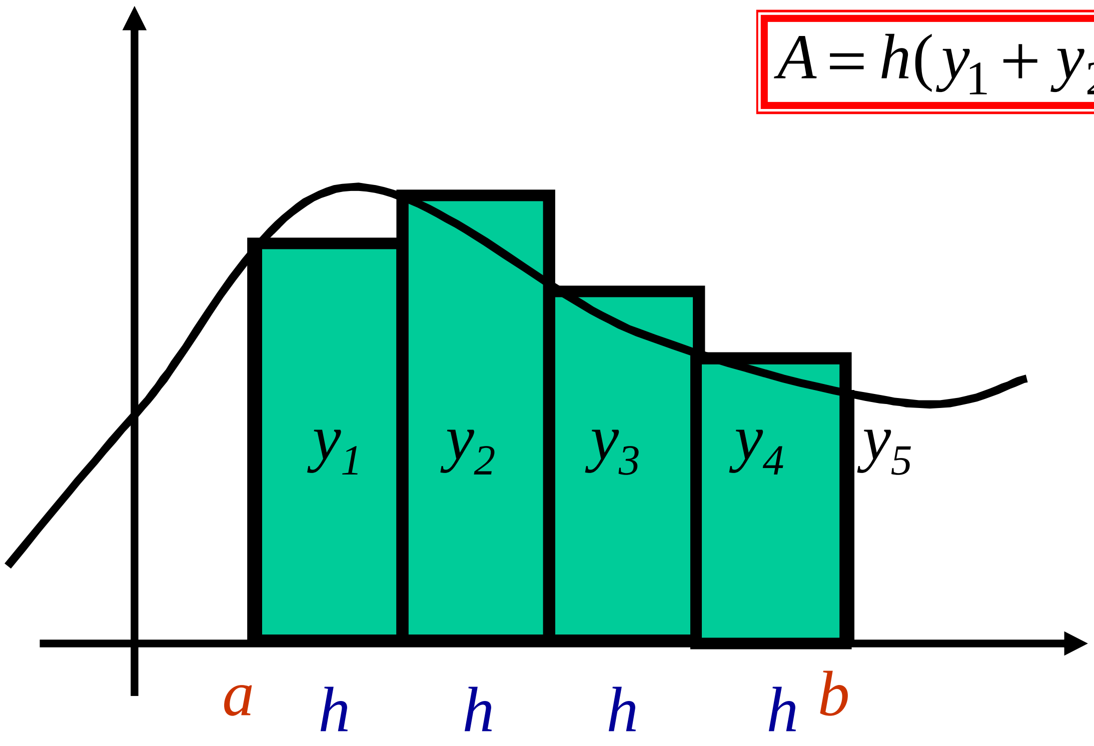
Finding Areas Numerically

The first way is to complete the strips as shown. We are then adding up rectangles of height and width .

In this case the area is à $A = h(y_1 + y_2 + y_3 + y_4)$

Note that the last y-value is not used.

$$\boxed{A = h(y_1 + y_2 + ...y_{n-1})}$$



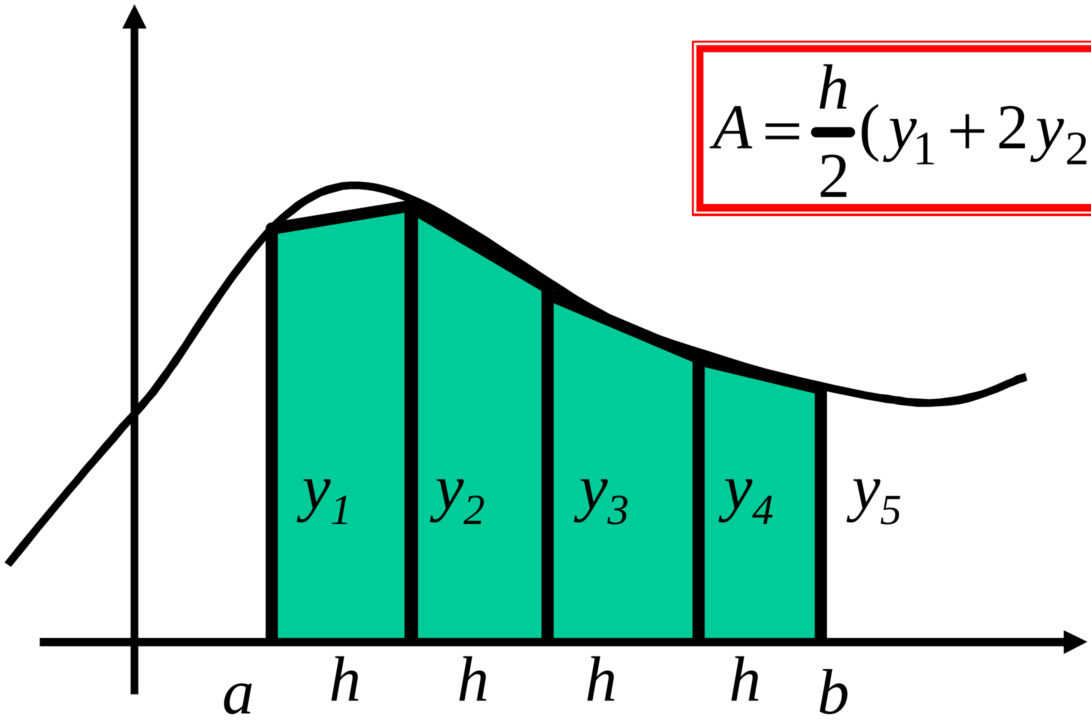
Finding Areas Numerically

The Trapezium (Trapezoidal) rule:

Complete the strips to get trapezia. Add up areas of the form

$$\frac{h}{2}(y_1+y_2) \ +\frac{h}{2}(y_2+y_3) \ +\frac{h}{2}(y_3+y_4) \ +\frac{h}{2}(y_4+y_5)$$

$$\boxed{A=\frac{h}{2}(y_1+2y_2+2y_3+...+y_n)}$$

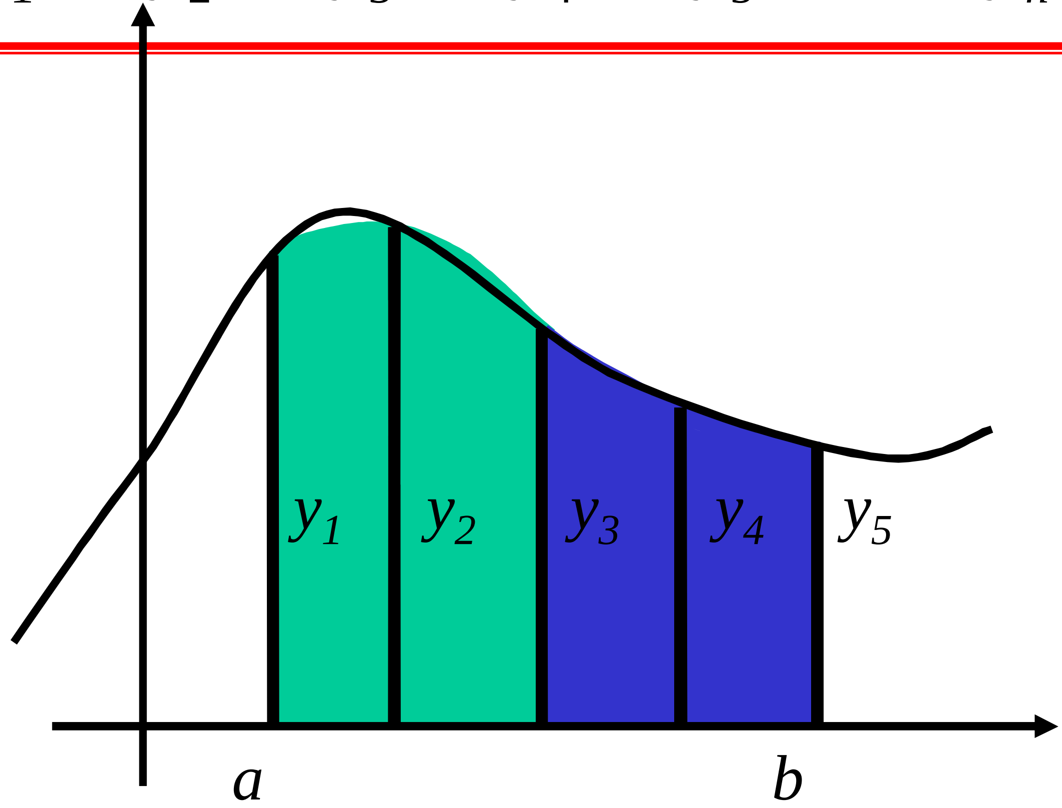


Finding Areas Numerically

Simpson's Rule:

We complete the tops of the strips as shown with parabolas.

$$\boxed{A = \frac{h}{3}(y_1 + 4y_2 + 2y_3 + 4y_4 + 2y_5 + \ldots + 4y_{n-1} + y_n)}$$



Examples

Estimate $\int_0^6 f(x)dx$ given $f(x)$ is defined by

x	0	1	2	3	4	5	6
y	-1	-0.5	0	1	3	1	0

Rectangle $A = h(y_1 + y_2 + \ldots . y_{n-1}) \quad = 1(-1 - 0.5 + 0 + 1 + 3 + 1) \; \boxed{= 3.5}$

Trapezium $A = \frac{h}{2}(y_1 + 2y_2 + 2y_3 + \ldots + y_n)$

$= 0.5(-1 + 2(-0.5 + 0 + 1 + 3 + 1) + 0) \; \boxed{= 4}$

Simpson $A = \frac{h}{3}(y_1 + 4y_2 + 2y_3 + 4y_4 + 2y_5 + \ldots + 4y_{n-1} + y_n)$

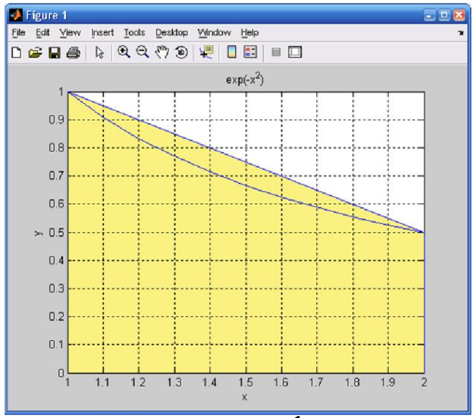
$= \frac{1}{3}(-1 + 4 \times -0.5 + 2 \times 0 + 4 \times 1 + 2 \times 3 + 4 \times 1 + 0) \; \boxed{= 3.67}$

Choosing the Step Size ‘h’

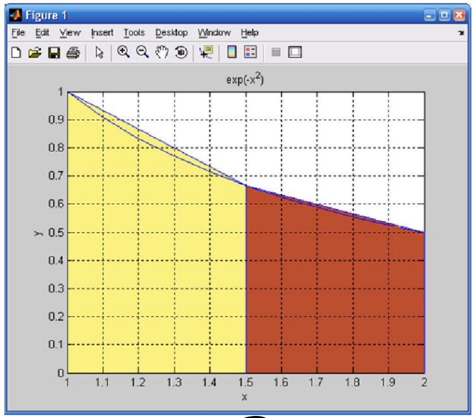
h=(a-b)/n

Choose large ‘n’ to reduce errors

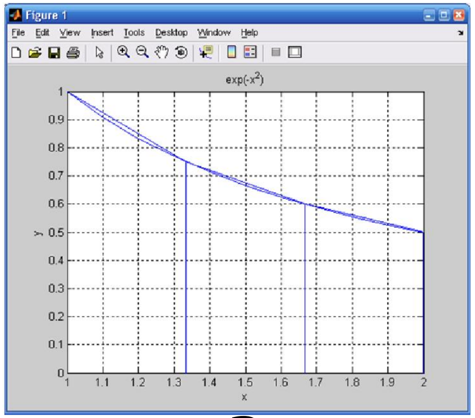
Trapezoidal Rule



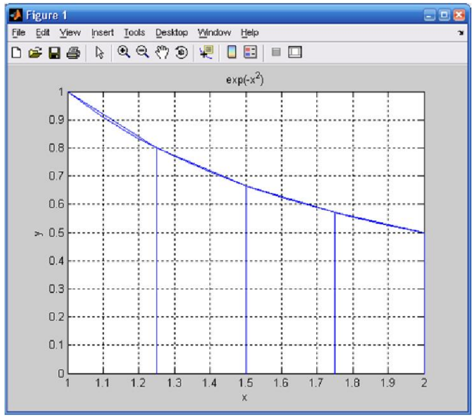
n=1



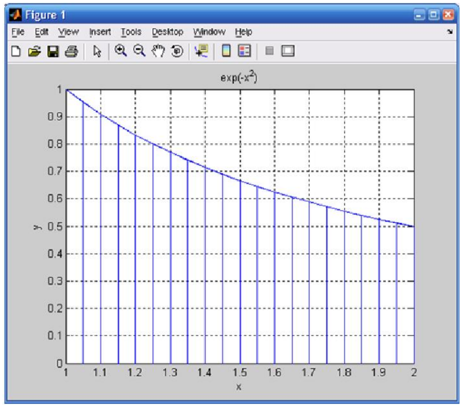
n=2



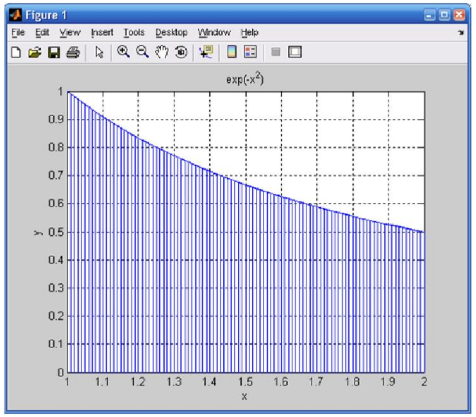
n=3



n=4



n=20



n=100

Similarly for Simpson's Rule

Merits and Demerits

- Trapezoidal rule
  - advantages
    - there can be any number of data points
    - the data points can be arbitrarily spaced
  - disadvantages
    - the error only reduces proportionally to the data spacing

- Simpson's rule
  - advantages
    - the error reduces proportionally to the square of the data spacing
  - disadvantages
    - there must be an odd number of data points
    - the data points must be evenly spaced

In the next lecture we will look in more detail on these and some more methods of numerical integration