# Numerical Differentiation - Lecture 01

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# Outline

- We will develop forward and backward difference approximations to derivatives
  - Taylor series expansions
  - Method of undetermined coefficients
  - Error terms
- Introduce operator notation and generalize first-order accurate one-sided approximations to $n^{th}$ derivatives
- Develop second-order one-sided approximations
- Note that Chapter 23 in text book is on Numerical Differentiation

# Numerical Differentiation

Assume that a function $f(x)$ is analytic in the neighbourhood of some point $x_0$ (i.e., the function $f(x)$ can be expanded in a Taylor series).

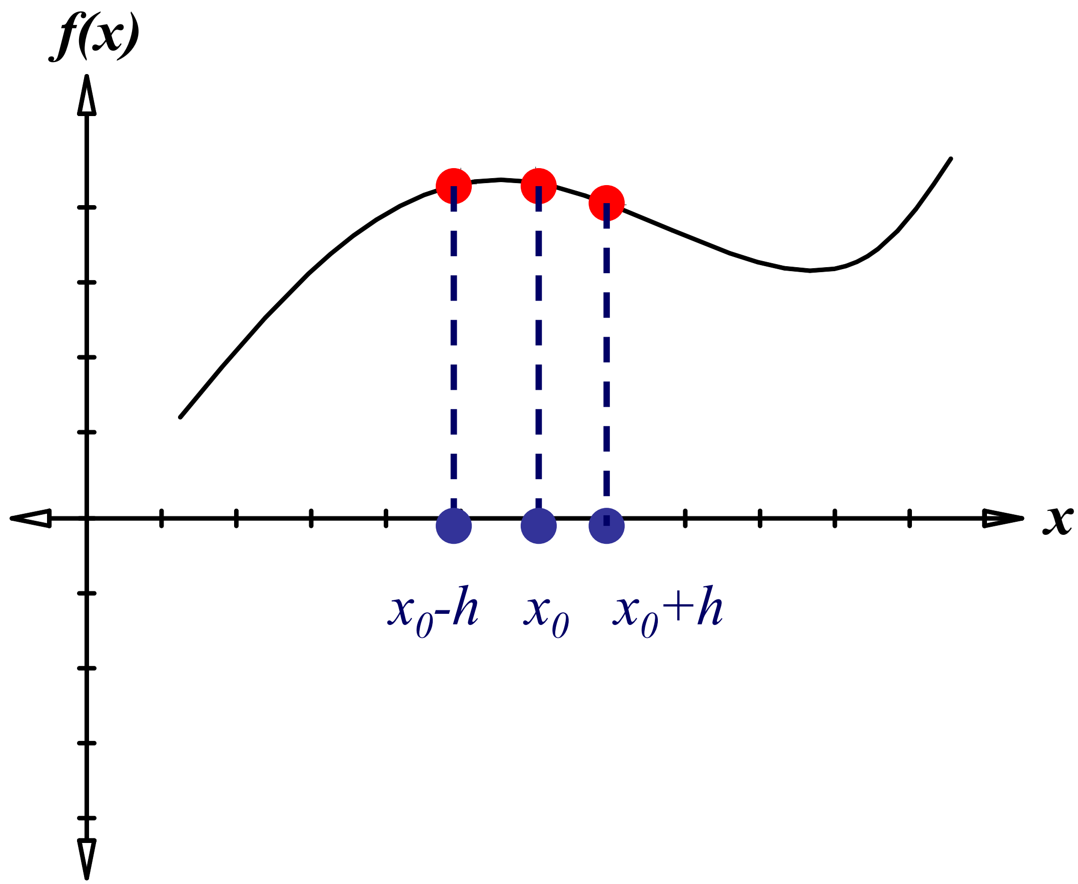
Consider the following data pairs:

$(x_0-h, f(x_0-h))$,

$(x_0, f(x_0))$,

$(x_0+h, f(x_0+h))$.

Expanding the function, $f(x_0+h)$ about $x_0$ in a Taylor's series, we obtain




$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \dots$$

# A Forward Difference Approximation

Solve for $f'(x_0)$:

$$f'(x_0) = \underbrace{\frac{f(x_0+h) - f(x_0)}{h}}_{\textit{Approximation}} \underbrace{- \frac{h}{2!} f''(x_0) - \frac{h^2}{3!} f'''(x_0)}_{\textit{Truncation Error}} + \ldots$$

Thus, a discrete (numerical) approximation for $f'(x_0)$ is:

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

The error $= -\frac{h}{2} f''(\xi)$ where $\xi \in [x_0, x_0 + h]$ $\longrightarrow$ Error is $\vartheta(h)$

In shorthand notation,

$$f_i' = \frac{f_{i+1} - f_i}{h} + \text{Error}$$

$$f_i' \approx \frac{f_{i+1} - f_i}{h} = \frac{\Delta f_i}{h}$$ where $\Delta$ is called the Forward Difference Operator

# A Backward Difference Approximation

Rewriting the data pairs as $(x_{i-1}, f_{i-1})$, $(x_i, f_i)$, $(x_{i+1}, f_{i+1})$ and expanding the function, $f(x_{i-1})$ about the point $x_i$ in a Taylor's series,

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2!} f_i'' - \dots$$

$$f_i' = \frac{f_i - f_{i-1}}{h} + \frac{h}{2!} f_i'' - \frac{h^2}{3!} f''' + \dots$$

where

$$f_i' \approx \frac{f_i - f_{i-1}}{h} \text{ and}$$

$$\text{Error} = \frac{h}{2} f_i'' - \frac{h^2}{6} f''' + \dots \longrightarrow \text{Error is } \vartheta(h)$$

In terms of the backward difference operator

$$f_i' = \frac{f_i - f_{i-1}}{h} = \frac{\nabla f_i}{h}$$

# One-Sided Second Derivative

Let $f_i = f(x_i)$

Expand $f_{i+1}$ about $x_i$ using a Taylor's series,

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!} f_i'' + \frac{h^3}{3!} f_i''' + \ldots \rightarrow (1)$$

and expand $f_{i+2}$ about $f_i$ using a Taylor's series

$$f_{i+2} = f_i + 2hf_i' + \frac{(2h)^2}{2!} f_i'' + \frac{(2h)^3}{3!} f_i''' + \ldots \rightarrow (2)$$

In order to solve for $f_i''$, we need to eliminate $f_i'$.

To do this, multiply (1) by -2 and add to (2) to yield

$$f_{i+2} - 2f_{i+1} = -f_i + 0 + h^2 f_i'' + h^3 f_i''' + \vartheta(h^4)$$

Solving for $f_i''$ yields

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} - hf_i''' + \ldots$$

# Operator Notation

The approximation for the second derivative of $f_i$ is:

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2}$$

The error is $\vartheta(h)$

This term can be regrouped as:

$$f_i'' = \frac{f_{i+2} - f_{i+1} - f_{i+1} + f_i}{h^2}$$

$$= \frac{\Delta f_{i+1} - \Delta f_i}{h^2} \qquad where\ \Delta f_i = f_{i+1} - f_i$$

$$= \frac{\Delta(f_{i+1} - f_i)}{h^2}$$

$$= \frac{\Delta(\Delta f_i)}{h^2} \quad \Rightarrow \quad f_i'' = \frac{\Delta^2 f_i}{h^2}$$

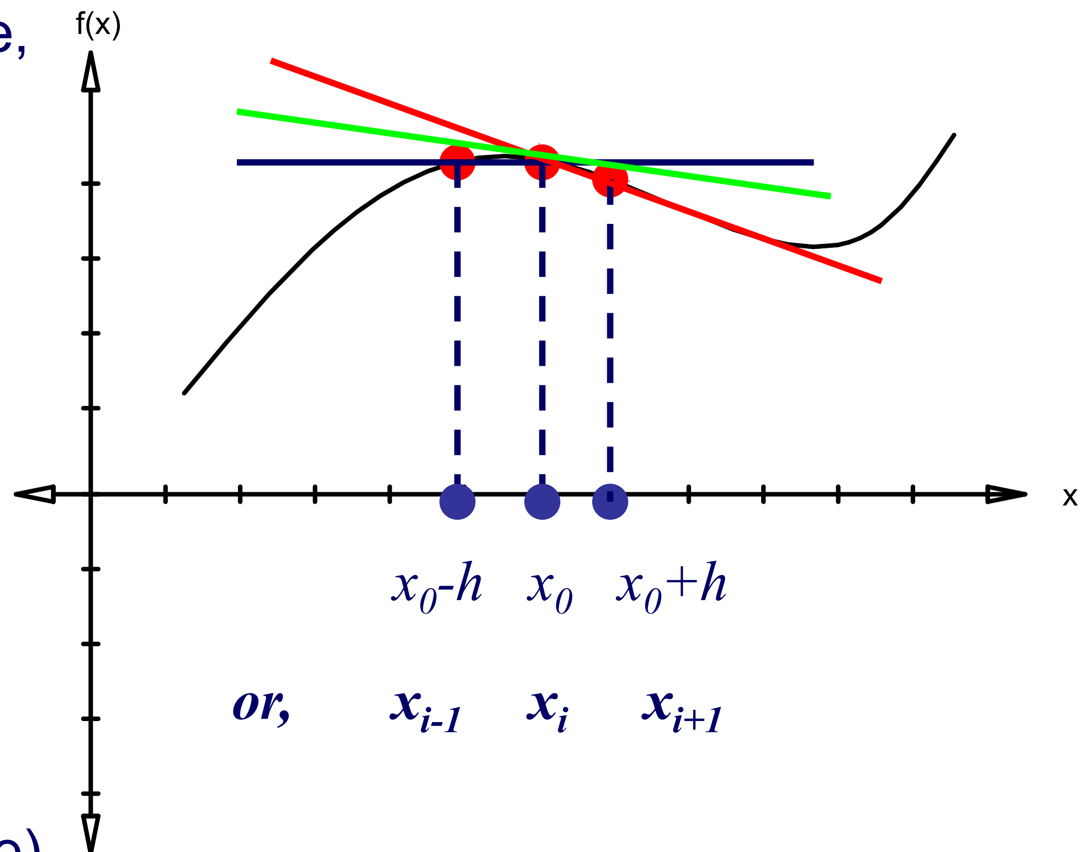
# Generalization to the $n^{th}$ derivative

Generalizing to the $n^{th}$ derivative,

$$f_i^{(n)} = \frac{\Delta^n f_i}{h^n} + \vartheta(h)$$

Using the Backward Difference operator, one obtains,

$$f_i^{(n)} = \frac{\nabla^n f_i}{h^n} + \vartheta(h)$$




The principle of the 1st order forward (red) and backward (blue) difference is depicted in the adjacent figure. We notice that the centered scheme (in green) approximates the slope better.

# Higher Order Numerical Methods

To find the ***2<sup>nd</sup>*** order approximation of $f'_i$

$$f_i' = \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f_i'' - \frac{h^2}{6} f_i''' - \dots$$

Substituting $f_i'' = \dfrac{f_{i+2} - 2f_{i+1} + f_i}{h^2} - hf''' - \cdots$

$$f_i' = \frac{f_{i+1} - f_i}{h} - \frac{h}{2}\left[\frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} - hf''' - \cdots\right] - \frac{h^2}{6} f''' - \dots$$

$$f_i' = \left(\frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}\right) + \frac{h^2}{3} f_i''' + \cdots$$

$$f_i' = \left(\frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}\right) + \vartheta(h^2)$$

Note that in this approach, one simply substitutes a difference approximation into the leading term of the truncation error of a lower order approximation. Many formulas can result from this approach.

# Method of Undetermined Coefficients (1)

Find an expression for $f_i'$ using data at ***i, i+1,*** and ***i+2*** .

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!} f_i'' + \frac{h^3}{3!} f_i''' + \ldots \rightarrow (1)$$

$$f_{i+2} = f_i + 2hf_i' + \frac{(2h)^2}{2!} f_i'' + \frac{(2h)^3}{3!} f_i''' + \ldots \rightarrow (2)$$

$$(1) + \alpha(2) \Rightarrow$$

$$f_{i+1} + \alpha f_{i+2} = (1+\alpha) f_i + (1+2\alpha) h f_i' + \left(\frac{1}{2} + 2\alpha\right) h^2 f_i'' + \left(\frac{1}{6} + \frac{4}{3}\alpha\right) h^3 f_i'''$$

Choose $\alpha$ such to eliminate the leading term of the truncation error, i.e.,

find $\alpha$ from $\quad \frac{1}{2} + 2\alpha = 0$

$$\Rightarrow \alpha = -\frac{1}{4}$$

# Method of Undetermined Coefficients (2)

$$\text{Using } \alpha = -\frac{1}{4}$$

$$\Rightarrow f_i' = 2\left(\frac{f_{i+1} - \left(\tfrac{1}{4}\right)f_{i+2} - \left(\tfrac{3}{4}\right)f_i}{h}\right)$$

$$= \left(\frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}\right) + \vartheta(h^2)$$

Note this is what we got when we substituted a difference approximation into the leading truncation error term of the first order method.

**Yet another (and often quite useful) approach:**

Higher order differences can also obtained by passing the Lagrange polynomial through the points of interest, in this case $f_i, f_{i+1}, f_{i+2}$. This results in $P_2(x)$. One can then differentiate the polynomial to arrive at a difference formula and evaluate it at $x_i$. **What will you get?**

# Summary

- Examined numerical differentiation by using Taylor series expansions
- Discussed one-sided forward and backward difference approximations
- Developed the truncation error terms for the formulas introduced
- Discussed different approaches for obtaining higher order derivative approximations
  - Undetermined coefficients
  - Differentiate the Lagrange polynomial (will see an example in our next lecture)