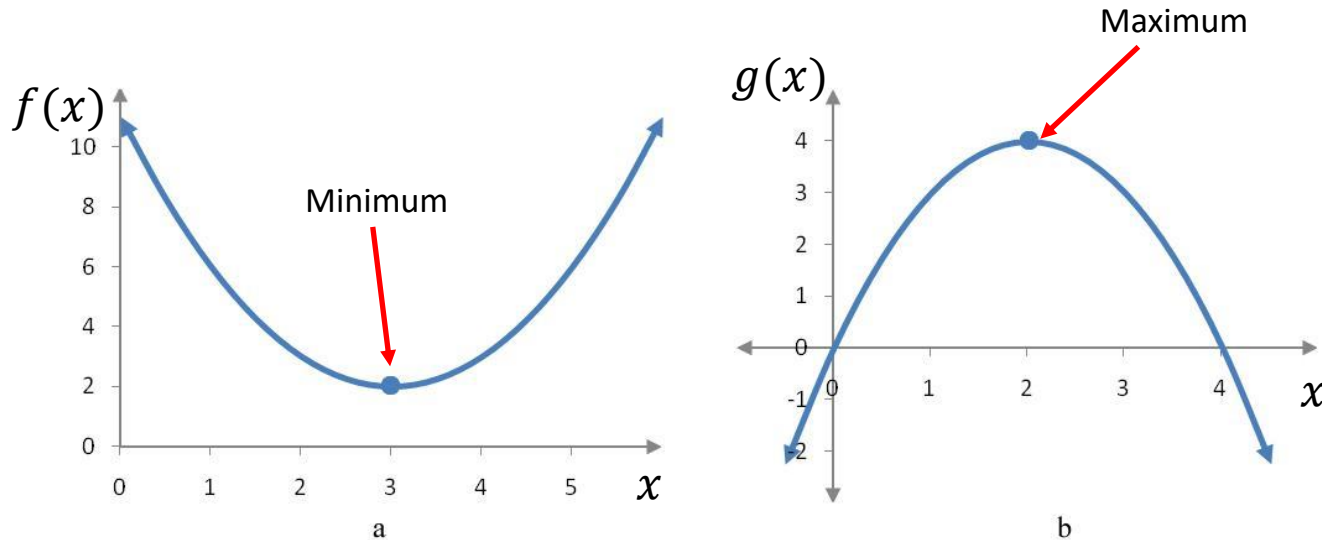


Week 11: Numerical Differentiation

Acknowledgement: Un-copyrighted photos and pictures were taken from the Internet

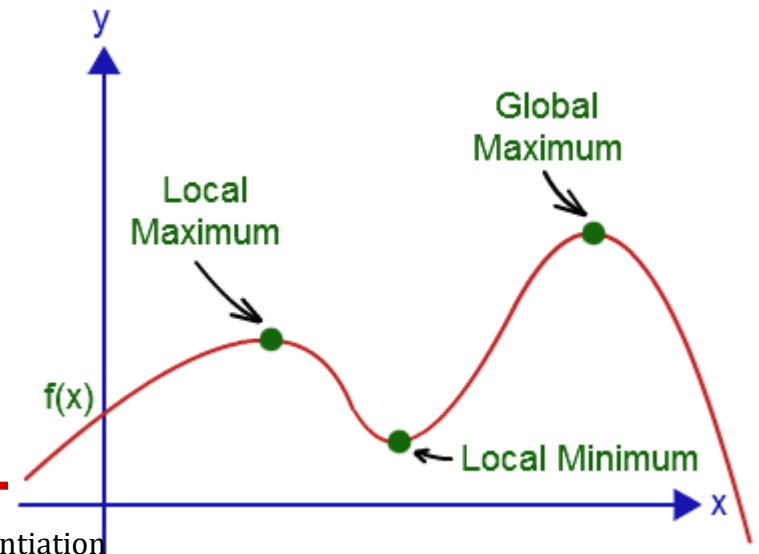
Motivation: Optimization

- **Optimization**: finding the maximum or minimum of a function!
- The **maximum (minimum)** of a function can be found by **differentiation**.
- Many applications in **AI, deep learning**, etc.



Motivation: Optimization Problem

- In many engineering problems, we need to **find the maximum or minimum** of a function.
- The (global) **maximum** is a point that $f(x)$ takes its **largest value**.
- The (global) **minimum** is a point that $f(x)$ takes its **smallest value**.
- The **minimum and maximum** of $f(x)$ are the solutions of $f'(x) = 0$.
- To find them, we need to find the **roots of $f'(x)$** .

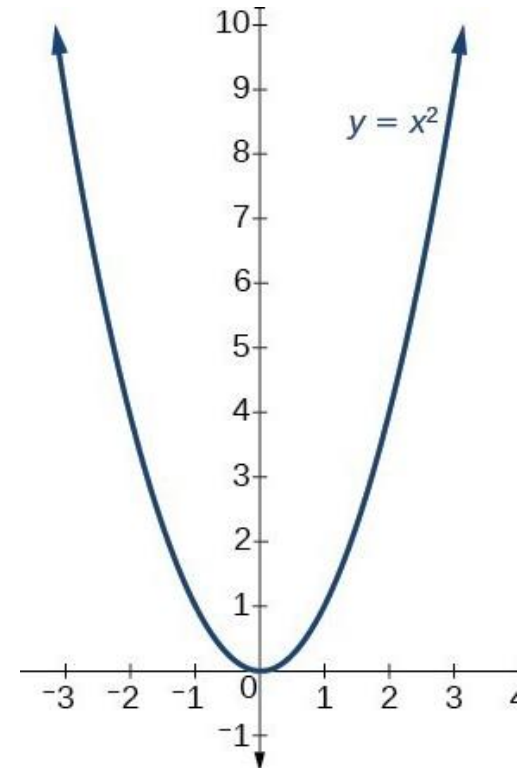


Root Finding: Optimization Problem

- Suppose that you need to find the **minimum** of $f(x) = (x)^2$
- To find it, we find the roots of $f'(x)$.

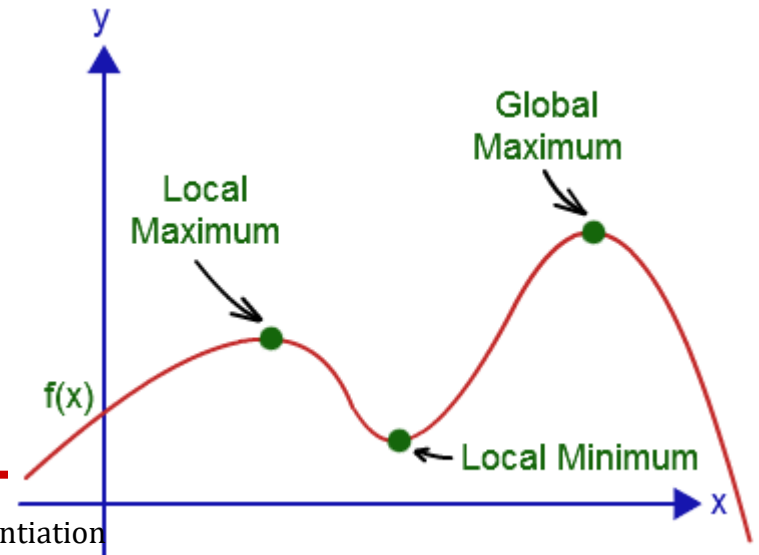
$$f'(x) = 2(x)$$

- So, the minimum is 0.
- In this case, it is easy to find the root of $2x=0$.



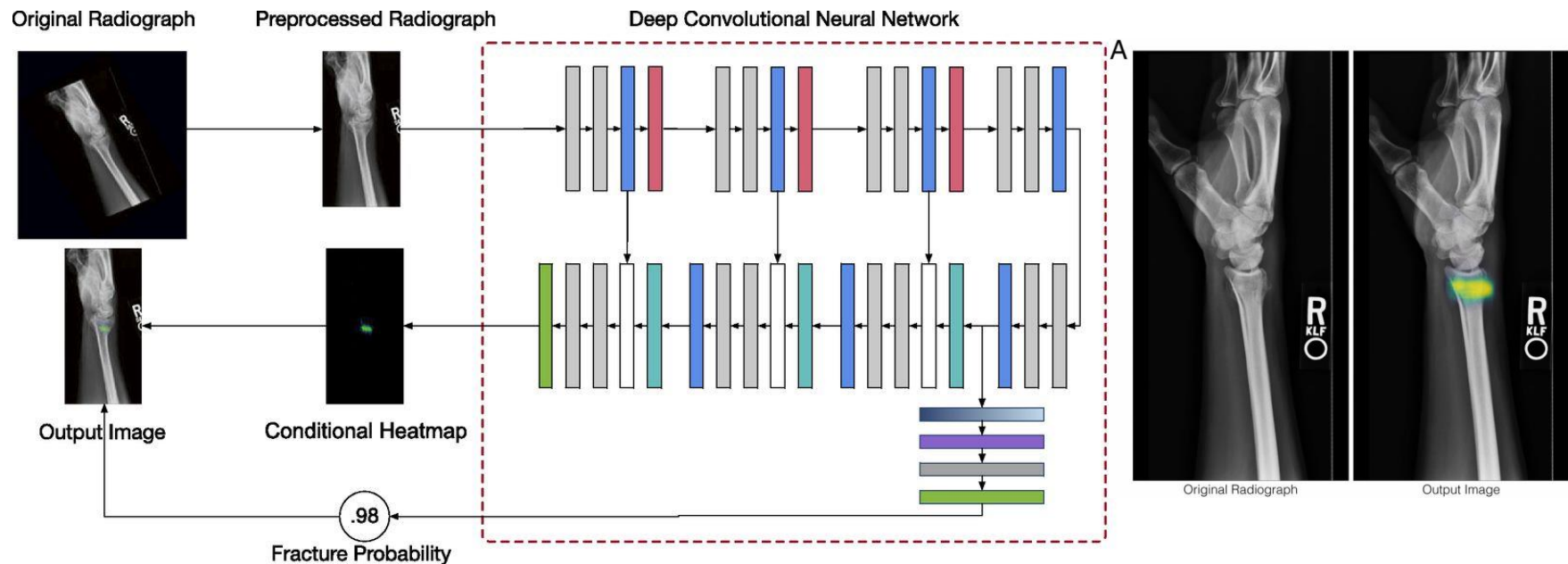
Motivation: Optimization Problem

- The **minimum and maximum** of $f(x)$ are the solutions of $f'(x) = 0$. To find them, we need to find the **roots of $f'(x)$** .
- In many applications, we **cannot find a closed-form** expression for $f'(x)$.
- For example, in **AI and deep learning**, we often cannot explicitly find $f'(x)$.
- In such cases, we can compute the **derivative numerically**.

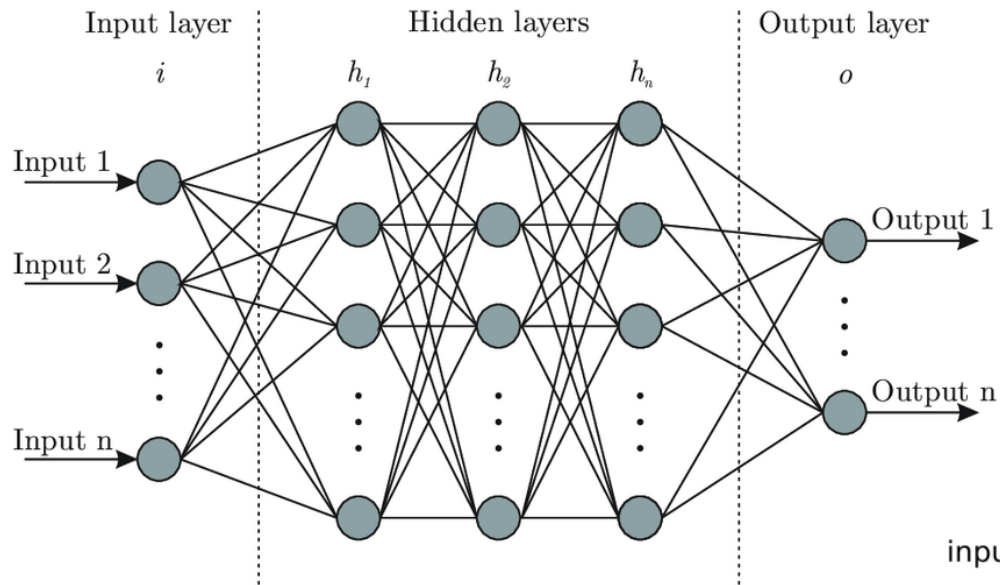


Motivation: Neural Networks

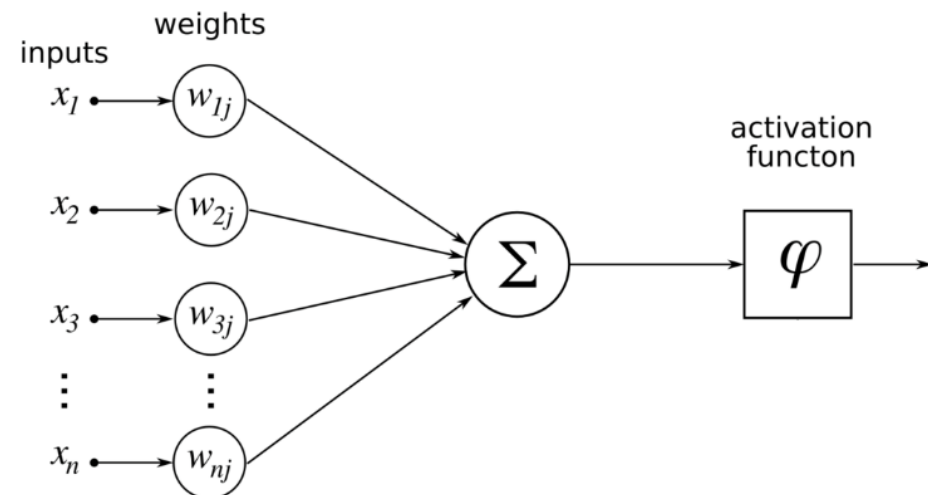
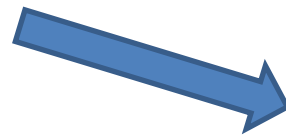
- Neural networks are often designed using **differentiation**.
- Example: **Detecting Bone Fracture and Injuries**



Motivation: Neural Networks

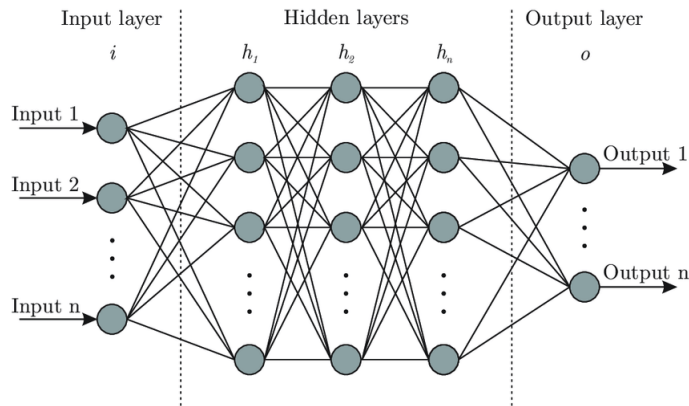


Weights are found by **optimization**.



Motivation: Neural Networks

- Neural networks have many applications in autonomous driving.



Numerical Differentiation

- In lecture 3, we learned 3 different ways for computing the derivative of a function at a given point.
 1. Forward approximation
 2. Backward approximation
 3. Centered approximation
- For certain applications, these methods may not provide an accurate approximation of the derivatives.
- In this lecture, we will learn more accurate ways of computing derivatives.

High-accuracy Computation of the First Derivative

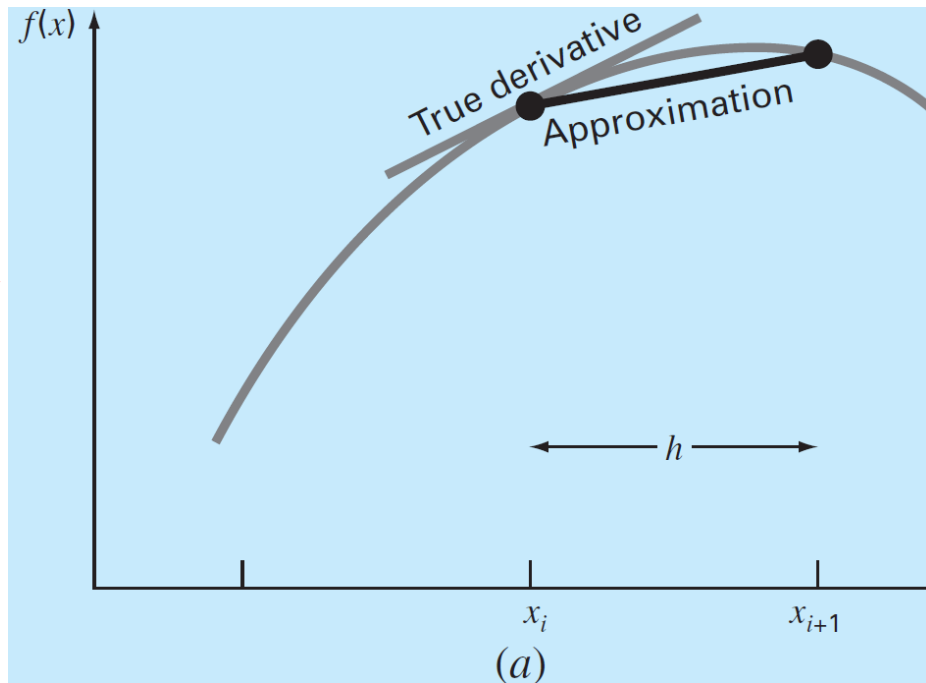
Forward Difference Method

Find the derivative of f at x_i .

1. Select a point x_{i+1} located after x_i
2. Approximate $f'(x_i)$ with

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

- $x_{i+1} - x_i = h$.
- This approximation **may not be accurate** for certain functions.



Numerical Differentiation

- We use **different points** to **compute the derivative** of $f(x)$ at x_i with **high accuracy**.
- h is the step-size.

$$x_{i+5} = x_i + 5h$$

$$x_{i+4} = x_i + 4h$$

$$x_{i+3} = x_i + 3h$$

$$x_{i+2} = x_i + 2h$$

$$x_{i+1} = x_i + h$$

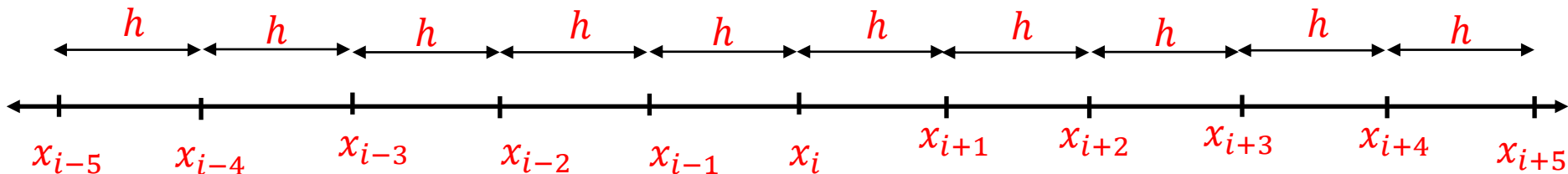
$$x_{i-1} = x_i - h$$

$$x_{i-2} = x_i - 2h$$

$$x_{i-3} = x_i - 3h$$

$$x_{i-4} = x_i - 4h$$

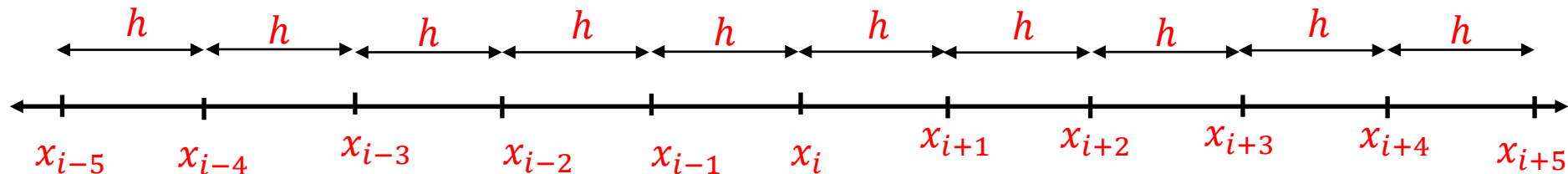
$$x_{i-5} = x_i - 5h$$



High-Accuracy Forward Difference Method

- Suppose that we would like to compute the **first derivative** of $f(x)$ at x_i using the **high-accuracy forward difference** method.
- We use three points x_i, x_{i+1} , and x_{i+2} .

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \quad (\text{High-accuracy})$$



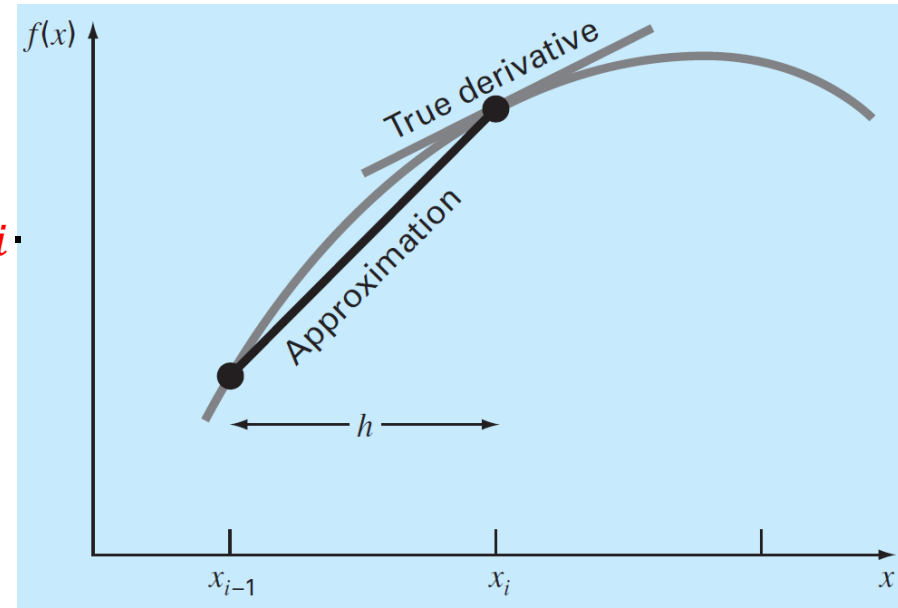
Backward Difference Method

Find the derivative of f at x_i .

1. Select a point x_{i-1} located behind x_i .
2. Approximate $f'(x_i)$ with

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

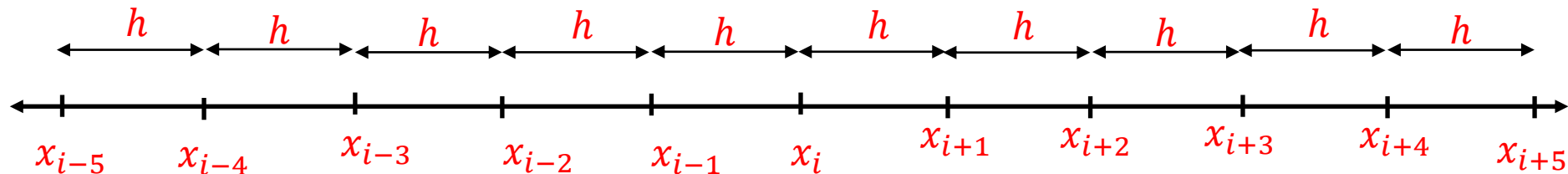
- $x_i - x_{i-1} = h$.
- This approximation **may not be accurate** for certain functions.



High-Accuracy Backward Difference Method

- Suppose that we would like to compute the **first derivative** of $f(x)$ at x_i using the **high-accuracy backward difference** method.
- We use three points x_i, x_{i-1} , and x_{i-2} .

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} \quad (\text{High-accuracy})$$



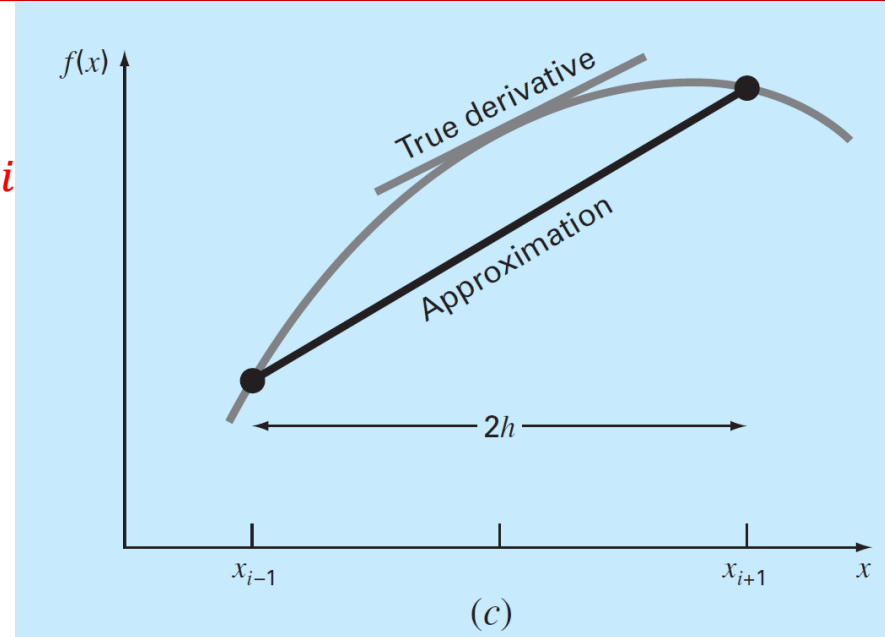
Centered Difference Method

Find the derivative of f at x_i .

1. Select a point x_{i-1} located behind x_i .
2. Select a point x_{i+1} located after x_i .
3. Approximate $f'(x_i)$ with

$$f'(x_i) \cong \frac{f(x_{i+1}) - f(x_{i-1}))}{x_{i+1} - x_{i-1}}$$

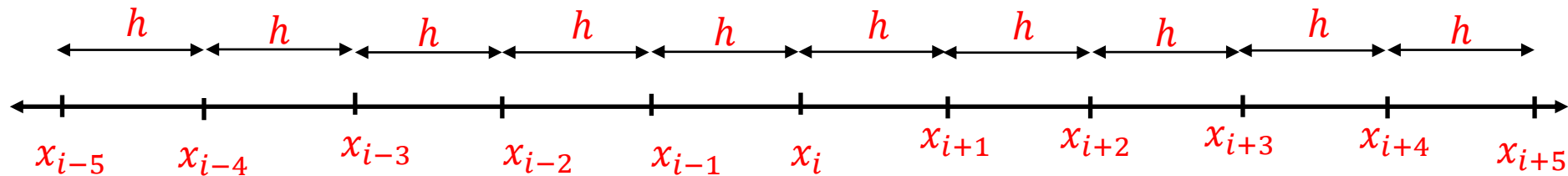
- $x_{i+1} - x_{i-1} = 2h$.
- The centered difference approximation is often **more accurate** than other two approximations.



High-Accuracy Centered Difference Method

- Suppose that we would like to compute the **first derivative** of $f(x)$ at x_i using the **high-accuracy centered difference** method.
- We use four points $x_{i-2}, x_{i-1}, x_{i+1}, x_{i+2}$.

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2}))}{12h} \quad (\text{High-accuracy})$$



Example

Use the **forward, backward and centered** methods to approximate the **first derivative** of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ with the step-size $h = 0.25$. Obtain the **low-accuracy** and **high-accuracy** estimates for each method.

Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

$$x_i = 0.5$$

step-size $h = 0.25$.

$$x_{i-2} = 0$$

$$f(x_{i-2}) = 1.2$$

$$x_{i-1} = 0.25$$

$$f(x_{i-1}) = 1.1035156$$

$$x_i = 0.5$$

$$f(x_i) = 0.925$$

$$x_{i+1} = 0.75$$

$$f(x_{i+1}) = 0.6363281$$

$$x_{i+2} = 1$$

$$f(x_{i+2}) = 0.2$$

Example: Forward Method

Forward method
(low-accuracy)

$$\frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

$$f'(0.5) \cong \frac{0.63632813 - 0.925}{0.25} = -1.155 \quad |\varepsilon_t| = 26.5\%$$

Forward method
(High-accuracy)

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$$

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375 \quad \varepsilon_t = 5.82\%$$

Example: Backward Method

$$\begin{array}{ll} \text{Backward method} & \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \\ \text{(low-accuracy)} & \end{array}$$

$$f'(0.5) \cong \frac{0.925 - 1.10351563}{0.25} = -0.714 \quad |\varepsilon_t| = 21.7\%$$

$$\begin{array}{ll} \text{Backward method} & f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2}))}{2h} \\ \text{(High-accuracy)} & \end{array}$$

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125 \quad \varepsilon_t = 3.77\%$$

Example: Centered Method

Centered method
(low-accuracy)

$$\frac{f(x_{i+1}) - f(x_{i-1}))}{x_{i+1} - x_{i-1}}$$

$$f'(0.5) \cong \frac{0.63632813 - 1.10351563}{0.5} = -0.934 \quad |\varepsilon_t| = 2.4\%$$

Centered method
(High-accuracy)

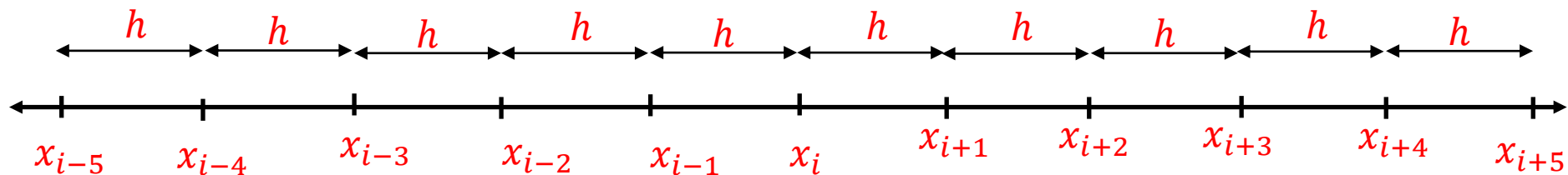
$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2}))}{12h}$$

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125 \quad \varepsilon_t = 0\%$$

Computation of the Second Derivative

Second Derivative

- We can compute the **second derivative** of the function $f(x)$ at point x_i using **backward, forward, and centered methods**.
- Similar to the first derivative, we will obtain **low-accuracy** and **high-accuracy** estimates using the **forward, backward and centered** methods.
- The **high-accuracy** methods use **more points** to estimate the second derivatives.
- They require more computations. They provide more accurate results.



Forward Difference Method

- Suppose that we would like to compute the **second derivative** of $f(x)$ at x_i using the **forward difference** method.
- A **low-accuracy** estimate of $f''(x)$ in the **forward difference** method is obtained using x_i, x_{i+1}, x_{i+2}

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \quad (\text{Low-accuracy})$$

- A **high-accuracy** estimate of $f''(x)$ in the **forward difference** method is obtained using $x_i, x_{i+1}, x_{i+2}, x_{i+3}$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \quad (\text{High-accuracy})$$

Backward Difference Method

- Suppose that we would like to compute the **second derivative** of $f(x)$ at x_i using the **backward difference** method.
- A **low-accuracy** estimate of $f''(x)$ in the **backward difference** method can be obtained using x_i, x_{i-1}, x_{i-2}

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2}))}{h^2} \quad (\text{Low-accuracy})$$

- A **high-accuracy** estimate of $f''(x)$ in the **backward difference** method can be obtained using $x_i, x_{i-1}, x_{i-2}, x_{i-3}$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3}))}{h^2} \quad (\text{High-accuracy})$$

Centered Difference Method

- Suppose that we would like to compute the **second derivative** of $f(x)$ at x_i using the **centered difference** method.
- A **low-accuracy** estimate of $f''(x)$ in the **centered difference** method can be obtained using x_{i-1}, x_i, x_{i+1}

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{h^2} \quad (\text{Low-accuracy})$$

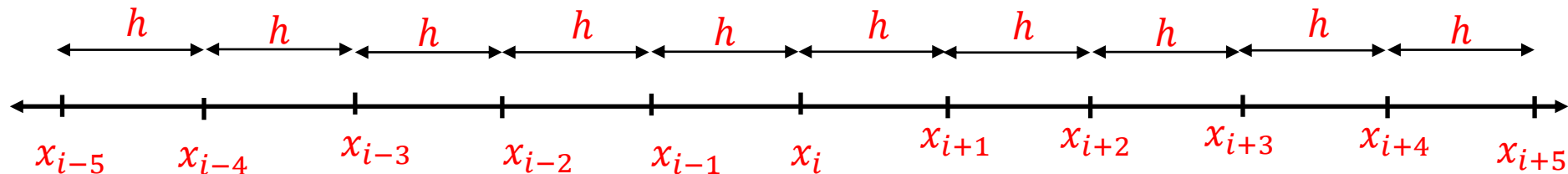
- A **high-accuracy** estimate of $f''(x)$ in the **centered difference** method can be obtained using $x_{i-2}, x_{i-1}, x_i, x_{i+1}, x_{i+2}$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2}))}{12h^2} \quad (\text{High-accuracy})$$

Computation of Higher Derivatives

Higher Derivatives

- We can compute the **third and fourth derivatives** of the function $f(x)$ at point x_i using **backward, forward, and centered** methods.
- We can obtain low-accuracy and high-accuracy estimates using the forward, backward and centered methods.
- The high-accuracy methods use more points to estimate the second derivatives.



Forward Difference Method

- The estimate of the **third derivative** of $f(x)$ at x_i using the **forward difference** method.

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \quad (\text{Low-accuracy})$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \quad (\text{High-accuracy})$$

- The estimate of the **fourth derivative** of $f(x)$ at x_i using the **forward difference** method.

$$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \quad (\text{Low-accuracy})$$

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \quad (\text{High-accuracy})$$

Backward Difference Method

- The estimate of the third derivative of $f(x)$ at x_i using the **backward difference** method.

$$f'''(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3} \quad (\text{Low-accuracy})$$

$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3} \quad (\text{High-accuracy})$$

- The estimate of the fourth derivative of $f(x)$ at x_i using the **backward difference** method.

$$f''''(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4} \quad (\text{Low-accuracy})$$

$$f''''(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4} \quad (\text{High-accuracy})$$

Centered Difference Method

- The estimate of the **third derivative of $f(x)$** at x_i using the **centered difference** method.

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2}))}{2h^3} \quad (\text{Low-accuracy})$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3}))}{8h^3} \quad (\text{High-accuracy})$$

- The estimate of the **fourth derivative of $f(x)$** at x_i using the **centered difference** method.

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2}))}{h^4} \quad (\text{Low-accuracy})$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3}))}{6h^4} \quad (\text{High-accuracy})$$

END

See you next week 😊!