# Chapter4

# Numerical Differentiation

## Approximations of the first derivative

We use the Taylor formula at $x_1 = x_0 + h$ we have:

$$f(x_0 + h) = f(x_0) + hf^{'}(x_0) + \frac{h^2}{2} f^{''}(c)\ , c \in [x_0, x_0 + h]$$

Hence:

$$f^{'}(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f^{''}(c)$$

By substituting $h$ with $-h$ we get:

$$f^{'}(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + \frac{h}{2} f^{''}(c), c \in [x_0 - h, x_0]$$

$$\begin{cases} f^{'}(x_0) = \dfrac{f(x_0 + h) - f(x_0)}{h}, \text{This formula is known as the } \textbf{forward} - \textbf{difference formula} \\ E = -\dfrac{h}{2} f^{''}(c), \quad \textit{This is the error made} \end{cases}$$

$$\begin{cases} f^{'}(x_0) = \dfrac{f(x_0) - f(x_0 - h)}{h}, \text{This formula is known as the } \textbf{backward} - \textbf{difference formula} \\ E = \dfrac{h}{2} f^{''}(c), \quad \textit{This is the error made} \end{cases}$$

## The Central-difference Formulas

A **centered** formula for $f(x_0)$ is obtained by expanding about $x = x_0$ at both $x = x_0 + h$ and $x = x_0 - h$, obtaining

$$f(x_0 + h) = f(x_0) + hf^{'}(x_0) + \frac{h^2}{2} f^{''}(x) + \frac{h^3}{6} f^{'''}(c_1)\ , c_1 \in [x_0, x_0 + h]$$

$$f(x_0 - h) = f(x_0) - hf^{'}(x_0) + \frac{h^2}{2} f^{''}(x) - \frac{h^3}{6} f^{''}{'}(c_2)\ , c_2 \in [x_0 - h, x_0]$$

Then subtracting the second from the first of these two expressions and solving for $f(x_0)$ yields

$$f^{'}(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{h} - \frac{h^3}{12}(f^{'''}(c_1) + f^{'''}(c_2)), c \in [x_0 - h, x_0]$$

then there exists $c \in [x_0 - h, x_0 + h]$ such that

$$f^{'''}(c) = \frac{f'''(c_1) + f^{'''}(c_2)}{2}$$

This permits us to rewrite Equation in its final form

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{h} - \frac{h^3}{6} f'''(c),$$

$$\begin{cases} f'(x_0) = \dfrac{f(x_0+h) - f(x_0-h)}{h}, \text{This formula is known as the } \textbf{centered} - \textbf{difference formula} \\ E = -\dfrac{h^3}{6} f'''(c), \quad \textit{The term E is called the truncation error} \end{cases}$$

## Approximations of the second derivative

We will use Taylor expansion to derive the 2nd-order derivative approximation. Note that

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(c_1), c_1 \in [x_0, x_0+h]$$

$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(c_2), c_2 \in [x_0-h, x_0]$$

Adding these two equations we obtain

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + h^2 f''(x) + \frac{h^4}{24}(f^{(4)}(c_2) + f^{(4)}(c_1))$$

we obtain

$$f''(x) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^4}{24}(f^{(4)}(c_2) + f^{(4)}(c_2))$$

Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$

the Intermediate Value Theorem implies that a number $c$ exists between $c_1$ and $c_2$, and hence in$[x_0 - h, x_0 + h]$, with

$$f^{(4)}(c) = \frac{f^{(4)}(c_1) + f^{(4)}(c_2)}{2}$$

This permits us to rewrite Equation in its final form

$$f''(x) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^4}{12} f^{(4)}(c)$$

$$\begin{cases} f''(x) = \dfrac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}, \textbf{centered} - \textbf{difference formula} \\ E = -\dfrac{h^4}{12} f^{(4)}(c), \quad \textit{the truncation error} \end{cases}$$

**Example**

$f(x) = xe^x$ approximate $f''(0.2)$, $h = 0.1$

**Solution**

$$f''(0.2) = \frac{f(0.2+h) - 2f(0.2) + f(0.2-h)}{h^2} = \frac{f(0.3) - 2f(0.2) + f(0.1)}{0.1^2} = 2.69$$