CMPT-439
Numerical Computation

Fall 2020

Numerical Differentiation

Derivative

- **The derivative of $f(x)$ at x_0 is:**

$$f'(x_0) = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$

- If an analytic expression for a derivative is known, then we can find its values at given data points
- However, if neither for a function, nor for its derivative their analytical expressions are known, then only **numerical methods** can be used to differentiate the function

Numerical Differentiation

The derivative of $f(x)$ at x_0 is:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

$$h = \Delta x = (x_0 + h) - x_0$$

An approximation to this is:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$ **for small values of h.**

Forward Difference Formula

Let $f(x) = \ln x$ and $x_0 = 1.8$

Find an approximate value of $f'(1.8)$

h	$f(1.8)$	$f(1.8+h)$	$\dfrac{f(1.8+h) - f(1.8)}{h}$
0.1	**0.5877867**	**0.6418539**	**0.5406720**
0.01	**0.5877867**	**0.5933268**	**0.5540100**
0.001	**0.5877867**	**0.5883421**	**0.5554000**

The exact value of $f'(1.8) = 0.555$

Numerical Differentiation

- If a function is given only by some data points and the function values at those data points?

Assume that a function fits three points:

$$\left(x_0, f\left(x_0\right)\right), \left(x_1, f\left(x_1\right)\right), \left(x_2, f\left(x_2\right)\right)$$

$$f(x) \approx P(x)$$

$$P\left(x\right) = L_0\left(x\right) f\left(x_0\right) + L_1\left(x\right) f\left(x_1\right) + L_2\left(x\right) f\left(x_2\right)$$

Lagrange Interpolating Polynomial

Lagrange Interpolation

$$P(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$$

$$\begin{aligned} P(x) = {} & \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) \\ & + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ & + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \end{aligned}$$

Differentiation of the Lagrange Polynomial

$$f'(x) \approx P'(x)$$

$$P'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f(x_0)$$

$$+ \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f(x_1)$$

$$+ \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

If the points are equally spaced, i.e.,

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

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

$$+ \frac{2x_0 - x_0 - (x_0 + 2h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 + 2h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 + 2h) - x_0\}\{(x_0 + 2h) - (x_0 + h)\}} f(x_2)$$

$$P'(x_0) = \frac{-3h}{2h^2} f(x_0) + \frac{-2h}{-h^2} f(x_1) + \frac{-h}{2h^2} f(x_2)$$

$$P'(x_0) = \frac{1}{2h}\left(-3f(x_0) + 4f(x_1) - f(x_2)\right)$$

Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\left(-3f(x_0) + 4f(\underbrace{x_0 + h}_{\boxed{x_1}}) - f(\underbrace{x_0 + 2h}_{\boxed{x_2}})\right)$$

Practical Implementation

- Using the Lagrange interpolation in the straightforward way, we can’t estimate the error
- In numerical differentiation, it is very important to estimate the error
- Hence, more sophisticated approach shall be used

Forward Divided Difference

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \dots\dots\dots$$

Taylor series

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

Error

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

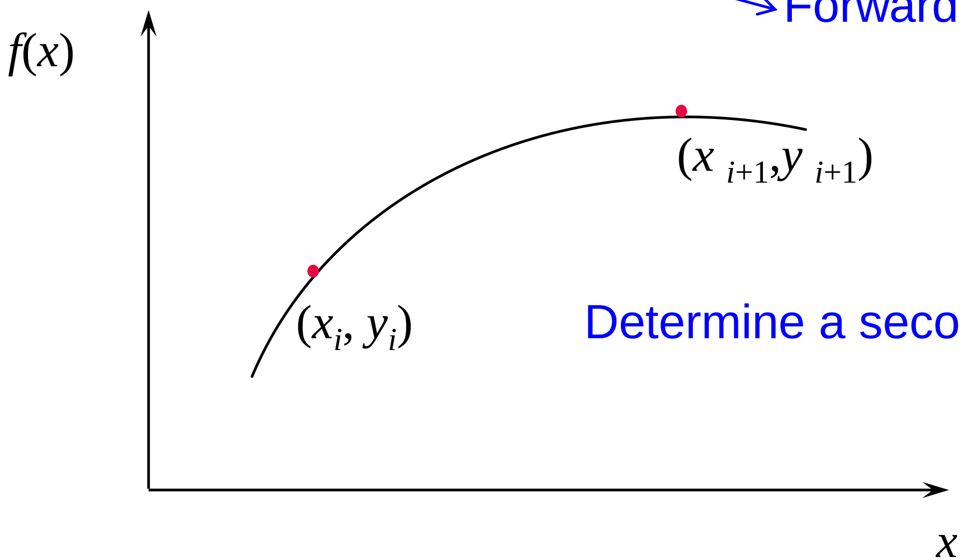
Error

Forward Divided Difference

Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(x_{i+1} - x_i) = \frac{\Delta f_i}{h} + O(h)$$

Forward Divided Difference



Determine a second point

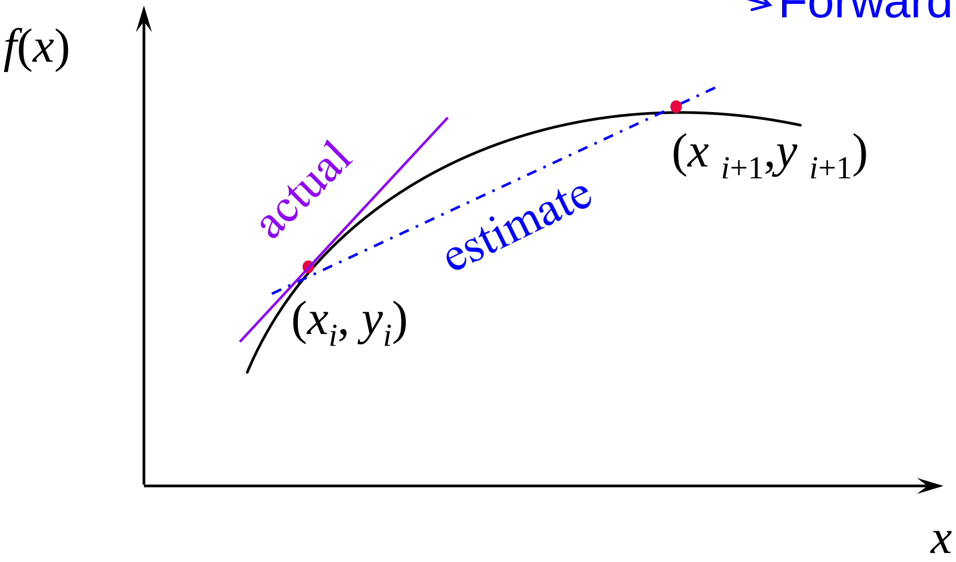
We are looking for a derivative at x_i

Forward Divided Difference

Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(x_{i+1} - x_i) = \frac{\Delta f_i}{h} + O(h)$$

Forward Divided Difference



We are looking for a derivative at x_i

Forward Divided Difference

$$f'(x_i) = \frac{\Delta f_i}{h} + O(h)$$

Error is proportional to the step size

first forward divided difference

O(h^2) error is proportional to the square of the step size

O(h^3) error is proportional to the cube of the step size

Centered Difference Approximation of the First Derivative

Subtract backward difference approximation from forward Taylor series expansion:

$$f\left(x_{i+1}\right) = f\left(x_i\right) + f'\left(x_i\right)h + \frac{f''\left(x_i\right)}{2!}h^2 + \ldots.$$

$$f\left(x_{i-1}\right) = f\left(x_i\right) - f'\left(x_i\right)h - \frac{f''\left(x_i\right)}{2!}h^2 - \ldots.$$

Subtracting $f\left(x_{i-1}\right)$ from $f\left(x_{i+1}\right)$

we obtain:

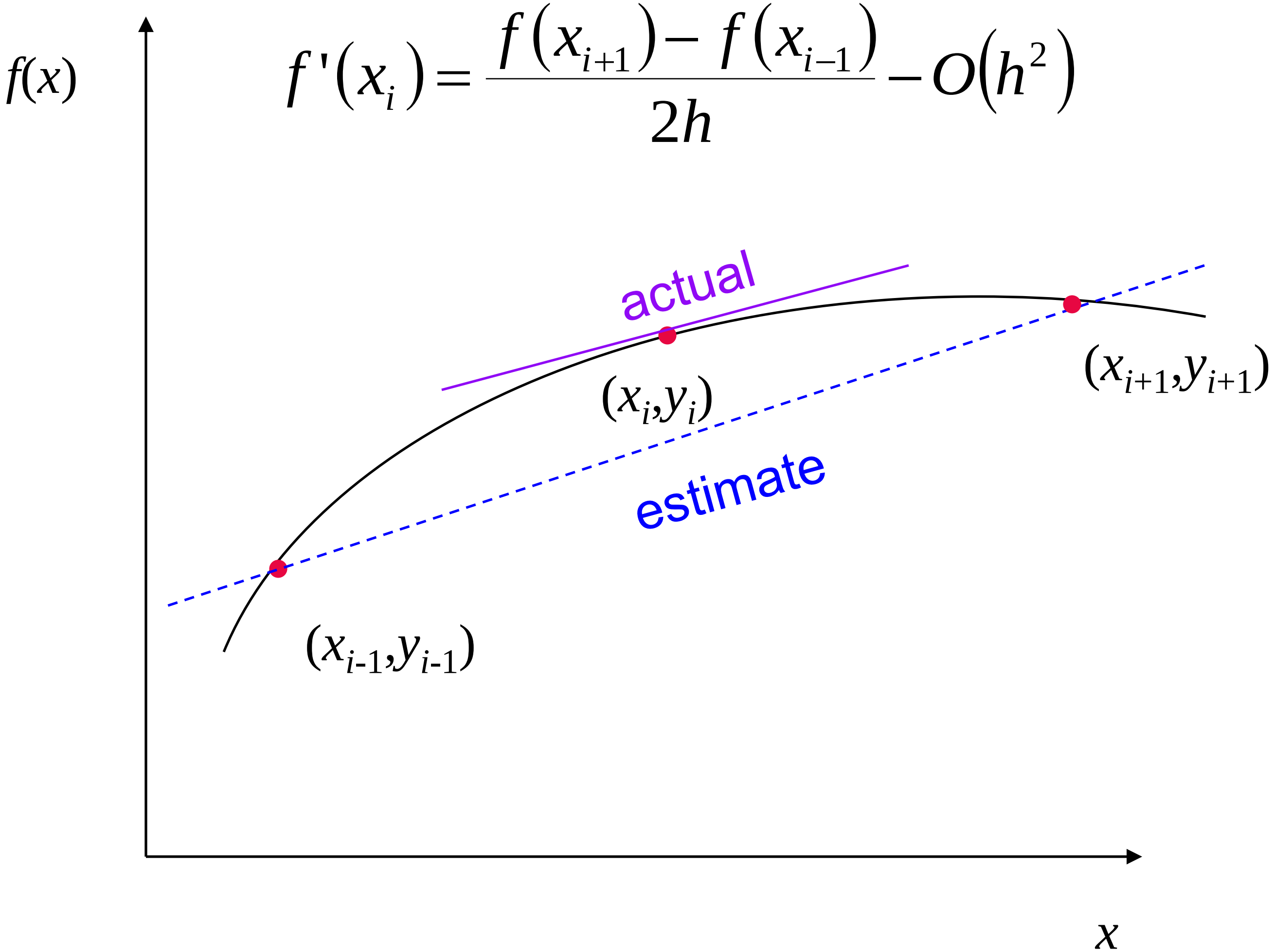
$$f\left(x_{i+1}\right) - f\left(x_{i-1}\right) = 2f'\left(x_i\right)h + O\left(h^2\right)$$

$$f'\left(x_i\right) = \frac{f\left(x_{i+1}\right) - f\left(x_{i-1}\right)}{2h} - O\left(h^2\right)$$

Centered Divided Difference

Centered Difference Approximation of the First Derivative

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



Forward Difference Method

Take Taylor series expansion of *f* (*x*+*h*) about *x*:

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

$$f\left(x_0+h\right)-f\left(x_0\right)=hf'\left(x_0\right)+\frac{h^2}{2}f''\left(x_0\right)+\frac{h^3}{3!}f'''\left(x_0\right)+\cdots$$

$$\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}=f'\left(x_0\right)+\frac{h}{2}f''\left(x_0\right)+\frac{h^2}{3!}f'''\left(x_0\right)+\cdots$$

.... (1)

Forward Difference Method

$$\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}=f'\left(x_0\right)+O\left(h\right)$$

$$f'\left(x_0\right)=\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}-O\left(h\right)$$

$$f'\left(x_0\right)\approx\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}$$ **Forward Difference Formula**

The Error: $$O\left(h\right)=\frac{h}{2}f^{(2)}\left(x\right)+\frac{h^2}{3!}f^{(3)}\left(x\right)+\cdots$$

Three Point Forward Difference

$$f\left(x_0+2h\right)=f\left(x_0\right)+2hf'\left(x_0\right)+\frac{4h^2}{2}f''\left(x_0\right)+\frac{8h^3}{3!}f'''\left(x_0\right)+\cdots$$

$$f\left(x_0+2h\right)-f\left(x_0\right)=2hf'\left(x_0\right)+\frac{4h^2}{2}f''\left(x_0\right)+\frac{8h^3}{3!}f'''\left(x_0\right)+\cdots$$

$$\frac{f\left(x_0+2h\right)-f\left(x_0\right)}{2h}=f'\left(x_0\right)+\frac{2h}{2}f''\left(x_0\right)+\frac{4h^2}{3!}f'''\left(x_0\right)+\cdots$$

.... (2)

Three Point Forward Difference

$$\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}=f'\left(x_0\right)+\frac{h}{2}f''\left(x_0\right)+\frac{h^2}{3!}f'''\left(x_0\right)+\cdots$$

.... (1)

$$\frac{f\left(x_0+2h\right)-f\left(x_0\right)}{2h}=f'\left(x_0\right)+\frac{2h}{2}f''\left(x_0\right)+\frac{4h^2}{3!}f'''\left(x_0\right)+\cdots$$

.... (2)

2 X Eqn. (1) – Eqn. (2)

Three Point Forward Difference

$$2\frac{f\left(x_0+h\right)-f\left(x_0\right)}{h}-\frac{f\left(x_0+2h\right)-f\left(x_0\right)}{2h}$$

$$=f'\left(x_0\right)-\frac{2h^2}{3!}f'''\left(x_0\right)-\frac{6h^3}{4!}f''''\left(x_0\right)-\cdots$$

$$\frac{-f\left(x_0+2h\right)+4f\left(x_0+h\right)-3f\left(x_0\right)}{2h}=$$

$$=f'\left(x_0\right)-\frac{2h^2}{3!}f'''\left(x_0\right)-\frac{6h^3}{4!}f''''\left(x_0\right)-\cdots$$

Error

$$=f'\left(x_0\right)+O\left(h^2\right)$$

Three Point Forward Difference

$$\frac{-f\left(x_0+2h\right)+4f\left(x_0+h\right)-3f\left(x_0\right)}{2h}=f'\left(x_0\right)+O\left(h^2\right)$$

$$f'\left(x_0\right)=\frac{-f\left(x_0+2h\right)+4f\left(x_0+h\right)-3f\left(x_0\right)}{2h}-O\left(h^2\right)$$

$$f'\left(x_0\right)\approx\frac{-f\left(x_0+2h\right)+4f\left(x_0+h\right)-3f\left(x_0\right)}{2h}$$

Three-point (Forward Difference) Formula

The Error: $O\left(h^2\right)=-\frac{2h^2}{3!}f'''\left(x\right)-\frac{6h^3}{4!}f''''\left(x\right)-\cdots$

Three Point Centered Formula

Take Taylor series expansion of *f* (*x*+*h*) about *x*:

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

Take Taylor series expansion of *f* (*x*-*h*) about *x*:

$$f\left(x_0-h\right)=f\left(x_0\right)-hf'\left(x_0\right)+\frac{h^2}{2}f''\left(x_0\right)-\frac{h^3}{3!}f'''\left(x_0\right)+\cdots$$

Subtract one expression from another

$$f\left(x_0+h\right)-f\left(x_0-h\right)=2hf'\left(x_0\right)+\frac{2h^3}{3!}f'''\left(x_0\right)+\frac{2h^6}{6!}f'''''\left(x_0\right)+\cdots$$

Three Point Centered Formula

$$f\left(x_0+h\right)-f\left(x_0-h\right)=2hf'\left(x_0\right)+\frac{2h^3}{3!}f'''\left(x_0\right)+\frac{2h^6}{6!}f''''''\left(x_0\right)+\cdots$$

$$\frac{f\left(x_0+h\right)-f\left(x_0-h\right)}{2h}=f'\left(x_0\right)+\frac{h^2}{3!}f'''\left(x_0\right)+\frac{h^5}{6!}f''''''\left(x_0\right)+\cdots$$

$$f'\left(x_0\right)=\frac{f\left(x_0+h\right)-f\left(x_0-h\right)}{2h}-\frac{h^2}{3!}f'''\left(x_0\right)-\frac{h^5}{6!}f''''''\left(x_0\right)-\cdots$$

Error

Three point Centered Formula

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

The Error: $$O(h^2) = -\frac{h^2}{3!} f'''(x) - \frac{h^5}{6!} f''''''(x) - \cdots$$

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$

Three-point (Centered Difference) Formula

Errors

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}$$ **Forward Difference Formula**

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

Errors

Three-point (Forward Difference) Formula

$$f'(x_0) \approx \frac{-f(x_0+2h)+4f(x_0+h)-3f(x_0)}{2h}$$

Error term $$O(h^2) = -\frac{2h^2}{3!} f'''(x) - \frac{6h^3}{4!} f''''(x) - \cdots$$

Errors

Three-point (Centered Difference) Formula

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$

Error term $O(h^2) = -\frac{h^2}{3!} f'''(x) - \frac{h^5}{6!} f''''''(x) - \cdots$

Summary of Difference Formulas for Numerical Differentiation

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

Forward Difference Formula x_0, x_0+h

Three-point Forward Difference Formula x_0, x_0+h, x_0+2h

$$f'(x_0) \approx \frac{-f(x_0+2h) + 4f(x_0+h) - 3f(x_0)}{2h}$$

Three-point Centered Difference Formula x_0-h, x_0, x_0+h

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$

Example:

$$f(x) = xe^x$$

Find the approximate value of $f'(2)$ **with** $h = 0.1$

x	$f(x)$
1.9	**12.703199**
2.0	**14.778112**
2.1	**17.148957**
2.2	**19.855030**

Using the Forward Difference formula:

$$f'(x_0) \approx \frac{1}{h}\left\{ f(x_0+h) - f(x_0) \right\}$$

$$f'(2) \approx \frac{1}{0.1}\left\{ f(2.1) - f(2) \right\}$$

$$= \frac{1}{0.1}\left\{17.148957 - 14.778112\right\}$$

$$= 23.708450$$

Using the 1st Three-point (Forward Difference) formula:

$$f'(x_0) \approx \frac{1}{2h}\left\{-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}\left[-3f(2)+4f(2.1)-f(2.2)\right]$$

$$= \frac{1}{0.2}\big[-3\times 14.778112+4\times 17.148957$$

$$-19.855030\big]$$

$$= 22.032310$$

Using the 2nd Three-point (Centered Difference) formula:

$$f'(x_0) \approx \frac{1}{2h}\left\{ f(x_0+h) - f(x_0-h) \right\}$$

$$\begin{aligned} f'(2) &\approx \frac{1}{2\times 0.1}\left[f(2.1) - f(1.9) \right] \\ &= \frac{1}{0.2}\left[17.148957 - 12.703199 \right] \\ &= 22.228790 \end{aligned}$$

The exact value of $f'(2)$ is: 22.167168

Comparison of the results with h = 0.1

The exact value of $f'(2)$ is 22.167168

Formula	$f'(2)$	True Absolute Error
Forward Difference	23.708450	1.541282
1st Three-point (Forward Difference)	22.032310	0.134858
2nd Three-point (Centered Difference)	22.228790	0.061622

Higher Order Derivatives

- The same approach can be used to find numerically higher order derivatives
- Let us consider how to find a second-order as an example

Second-order Derivative

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

$$f\left(x_0-h\right)= f\left(x_0\right)-hf'\left(x_0\right)+\frac{h^2}{2}f''\left(x_0\right)-\frac{h^3}{3!}f'''\left(x_0\right)+\cdots$$

Add these two equations.

$$f\left(x_0+h\right)+f\left(x_0-h\right)=2f\left(x_0\right)+\frac{2h^2}{2}f''\left(x_0\right)+\frac{2h^4}{4!}f''''\left(x\right)+\cdots$$

$$\boldsymbol{f\left(x_0+h\right)-2f\left(x_0\right)+f\left(x_0-h\right)=\frac{2h^2}{2}f''\left(x_0\right)+\frac{2h^4}{4!}f''''\left(x_0\right)+L}$$

$$\frac{f\left(x_0+h\right)-2f\left(x_0\right)+f\left(x_0-h\right)}{h^2}=f''\left(x_0\right)+\frac{2h^2}{4!}f''''\left(x_0\right)+\cdots$$

$$f''\left(x_0\right)=\frac{f\left(x_0+h\right)-2f\left(x_0\right)+f\left(x_0-h\right)}{h^2}-\frac{2h^2}{4!}f''''\left(x_0\right)+\cdots$$

$$f''\left(x_0\right)\approx\frac{f\left(x_0+h\right)-2f\left(x_0\right)+f\left(x_0-h\right)}{h^2}$$