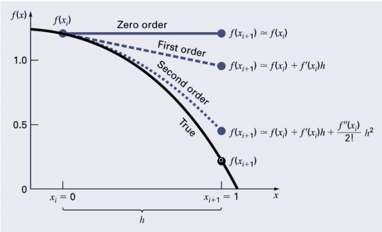
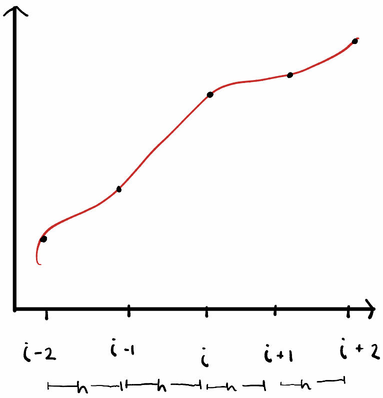
The Taylor Theorem and Series

The *Taylor theorem* states that any smooth function can be approximated as a polynomial.

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n$$





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

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

forward:

$$f_i' = \underbrace{\frac{f_{i+1} - f_i}{h}}_{\text{forward difference}} \underbrace{- \frac{h}{2} f_i'' - \frac{h^2}{3!} f_i''' \dots}_{\text{truncation error}}$$

$O(h) \rightarrow$ first order accurate

Numerical Differentiation using Taylor series Finite difference (FD)

The first order Taylor series can be used to calculate approximations to derivatives:

Given: $$f(x_{i+1}) = f(x_i) + f'(x_i)h + O(h^2)$$

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

This is termed a "forward" difference because it utilizes data at *i* and *i*+1 to estimate the derivative.

Differentiation - FD

There are also backward difference and centered difference approximations, depending on the points used:

Forward:

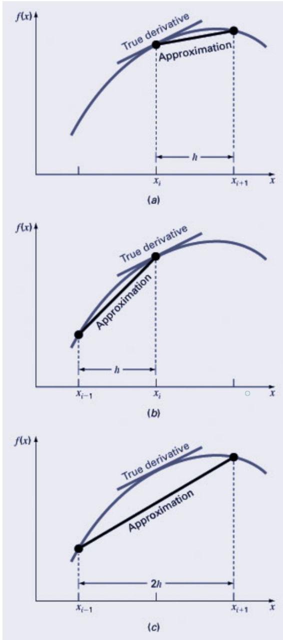
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

Backward:

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

Centered:

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



backward

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

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

$$f_i' = \frac{f_i - f_{i-1}}{h} + \underbrace{\frac{h}{2} f_i'' - \frac{h^2}{3!} f_i'''}_{O(h) \text{ for backward}}$$

centered:

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} + \frac{h^2}{6} f_i^3 + \dots$$

Error Definitions

True error (E_t): the difference between the true value and the approximation.

Absolute error ($|E_t|$): the absolute difference between the true value and the approximation.

True fractional relative error: the true error divided by the true value.

$$\text{True fractional relative error} = \frac{\text{true value} - \text{approximation}}{\text{true value}}$$

Relative error (ε_t): the true fractional relative error expressed as a percentage.

$$\varepsilon_t = \frac{\text{true value} - \text{approximation}}{\text{true value}} 100\%$$

similar to hw

Finite difference error Example

Use forward and backward difference approximations of $O(h)$ and a centered difference approximation of $O(h^2)$ to estimate the first derivative of

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

at $x = 0.5$ using a step size $h = 0.5$.
Repeat the computation using $h = 0.25$.

Note that the derivative can be calculated directly as

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$$

$$f'(0.5) = -0.9125$$

forward:

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

$$f_{(0.5)}' = \frac{f(0.5+1) - f(0.5)}{0.25}$$

$\approx$

For h=0.5

$$x_{i-1} = 0 \qquad f(x_{i-1}) = 1.2$$
$$x_i = 0.5 \qquad f(x_i) = 0.925$$
$$x_{i+1} = 1.0 \qquad f(x_{i+1}) = 0.2$$

Forward: $f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$ $\quad f'(0.5) \cong \frac{0.2 - 0.925}{0.5} = -1.45$ $\quad |\varepsilon_t| = 58.9\%$

Backward $f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$ $\quad f'(0.5) \cong \frac{0.925 - 1.2}{0.5} = -0.55$ $\quad |\varepsilon_t| = 39.7\%$

Centered $f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$ $\quad f'(0.5) \cong \frac{0.2 - 1.2}{1.0} = -1.0$ $\quad |\varepsilon_t| = 9.6\%$

For h=0.25

$$x_{i-1} = 0.25 \qquad f(x_{i-1}) = 1.10351563$$
$$x_i = 0.5 \qquad f(x_i) = 0.925$$
$$x_{i+1} = 0.75 \qquad f(x_{i+1}) = 0.63632813$$

Forward $f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$ $\quad f'(0.5) \cong \frac{0.63632813 - 0.925}{0.25} = -1.155$ $\quad |\varepsilon_t| = 26.5\%$

Backward $f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$ $\quad f'(0.5) \cong \frac{0.925 - 1.10351563}{0.25} = -0.714$ $\quad |\varepsilon_t| = 21.7\%$

Centered $f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$ $\quad f'(0.5) \cong \frac{0.63632813 - 1.10351563}{0.5} = -0.934$ $\quad |\varepsilon_t| = 2.4\%$

can also to 2nd ODE:

$$f_{i+1} + f_{i-1} = 2f_i + h^2 f_i'' + \frac{2h^4}{4!} f_i^4 + \dots$$

$$-h^2 f_i'' = -f_{i+1} - f_{i-1} + 2f_i + \frac{2h^4}{4!} f_i^4 + \dots$$

$$f_i'' = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} - \frac{2h^2}{4!} f_i^4 + \dots$$

Taylor series
MacLaurin series, i.e. Taylor series at $x_i = 0$

With a "trick", i.e. having $x = 0$ & $\Delta x = x$, we can represent any differentiable function as a polynomial series. This series is called the MacLaurin series.

Example: Estimate the values of function exp(x) using MacLaurin series.
Show that by increasing the number of terms in your series, you increase the accuracy of your calculation.

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!}$$

$$e^{0.5} = 1.648721$$

Terms	Result	ε_t, %	ε_a, %
1	1	39.3	
2	1.5	9.02	33.3
3	1.625	1.44	7.69
4	1.645833333	0.175	1.27
5	1.648437500	0.0172	0.158
6	1.648697917	0.00142	0.0158

@ $x = 0$:
$e^0 = 1$

$f(x) = e^x$
$\frac{de^x}{dx} = e^x$

Round-off Errors

Round-off errors arise because digital computers have limitation on storing the digits of a variable.

For example, if the true value of x= 4.3742931023**7203473024**

The computer may store it as, $\tilde{x}$ = 4.3742931023

and the round-off error is e = 0.0000000000**7203473024**

Obviously we have $x = \tilde{x} + e$

Round-off errors and truncation errors

Let's take the example of second-order FD of the first derivative,

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

And since we have round-off errors the values of the function f are saved in computer as $\tilde{f}$ with a truncation of e, and we have,

$$f(x_{i+1}) = \tilde{f}(x_{i+1}) + \tilde{e}_{i+1}$$
$$f(x_{i-1}) = \tilde{f}(x_{i-1}) + \tilde{e}_{i-1}$$

Thus,

$$f'(x_i) = \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} + \frac{\tilde{e}_{i+1} - \tilde{e}_{i-1}}{2h} - \frac{f'''}{6}h^2$$

For a maximum absolute value of ε for $(\tilde{e}_{i+1} - \tilde{e}_{i-1})/2$, and a maximum absolute value of M for $-f'''$ we have,

$$Total\ Error = \left|f'(x_i) - \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h}\right| < \frac{\varepsilon}{h} + \frac{Mh^2}{6}$$

The optimum value of h is found to be, $h = \sqrt[3]{\frac{3\varepsilon}{M}}$