Numerical Differentiation

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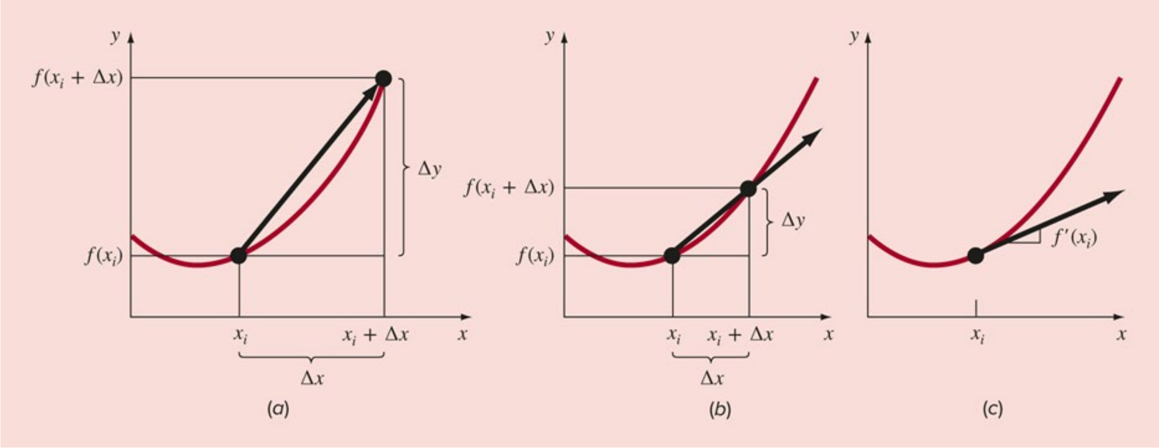
What is Differentiation?

- To differentiate mean to mark off by differences, distinguish, to perceive the difference in or between
- The derivative represents the rate of change.
- The mathematical definition of a derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



and as Δx is allowed to approach zero, the difference becomes a derivative:

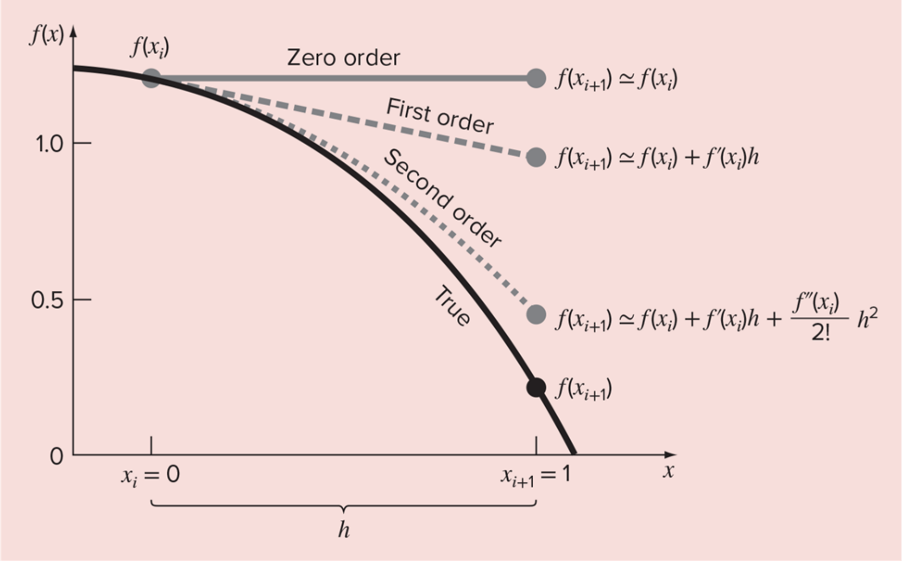
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

The Taylor theorem and series

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

- The *Taylor series* provides a means to express this idea mathematically.

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



Numerical Differentiation

Forward difference approximation of the first derivative

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

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

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

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

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

Numerical Differentiation

Backward difference approximation of the first derivative

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

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

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

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

This is termed a "backward" difference because it utilizes data at $i-1$ and i to estimate the derivative.

Numerical Differentiation

Centered difference approximation of the first derivative

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

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

The first derivative can be approximated by $(1) - (2)$

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

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^{(3)}(x_i)}{6}h^2 + \cdots$$

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

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

Numerical Differentiation

- Forward :

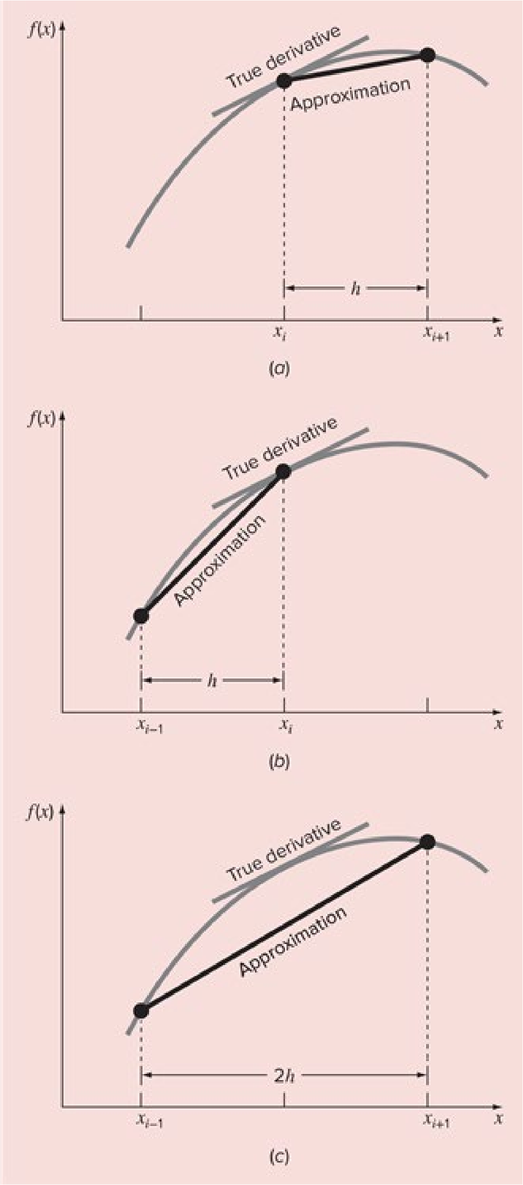
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

- Backward :

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

- Centered :

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



Finite-difference approximations of higher derivatives

Forward difference approximation of the second derivative

A Taylor series expansion for $f(x_{i+1})$ and $f(x_{i+2})$ in terms of $f(x_i)$

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

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

Multiplied (1) by 2 and subtracted from (2)

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

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

Finite-difference approximations of higher derivatives

Backward difference approximation of the second derivative

A Taylor series expansion for $f(x_{i-1})$ and $f(x_{i-2})$ in terms of $f(x_i)$

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

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

Multiplied (1) by 2 and subtracted from (2)

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

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

Finite-difference approximations of higher derivatives

Centered difference approximation of the second derivative

A Taylor series expansion for $f(x_{i-1})$ and $f(x_{i+1})$ in terms of $f(x_i)$

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

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

Adding (1) and (2)

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

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

High-accuracy forward difference formula

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

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

Keep the second-derivative term $$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h + O(h^2)$$

Replace $f''(x_i)$ by forward difference approximation of the second derivative $$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \left(\frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}\right)\frac{h}{2} + O(h^2)$$

More accurate forward difference approximation of the first derivative $$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

Note that the inclusion of the second-derivative term has improved the accuracy to $O(h^2)$

High-accuracy backward difference formula

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

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

Keep the second-derivative term $$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} - \frac{f''(x_i)}{2!}h + O(h^2)$$

Replace $f''(x_i)$ by backward difference approximation of the second derivative $$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \left(\frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}\right)\frac{h}{2} + O(h^2)$$

More accurate backward difference approximation of the first derivative $$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2)$$

Note that the inclusion of the second-derivative term has improved the accuracy to $O(h^2)$

High-accuracy centered difference formula

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

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

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

$$f(x_{i-2}) = f(x_i) - f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 - \frac{f^{(3)}(x_i)}{3!}(2h)^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}(2h)^n + R_n \quad \longrightarrow (4)$$

(1) – (2) $\quad f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{2}{3!}h^3 f^{(3)}(x_i) + \frac{2}{5!}h^5 f^{(5)}(x_i) + \cdots \quad \longrightarrow (5)$

(3) – (4) $\quad f(x_{i+2}) - f(x_{i-2}) = 2(2h)f'(x_i) + \frac{2}{3!}(2h)^3 f^{(3)}(x_i) + \frac{2}{5!}(2h)^5 f^{(5)}(x_i) + \cdots \longrightarrow (6)$

(6) – 8x(5) $\quad f(x_{i+2}) - f(x_{i-2}) - 8f(x_{i+1}) - 8f(x_{i-1}) = -12hf'(x_i) + Ch^5 f^{(5)}(x_i) + \cdots$

More accurate centered difference approximation of the first derivative with the improved accuracy to $O(h^4)$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + Ch^4 f^{(5)}(x_i) + \cdots$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4)$$

Example : Finite-difference approximations of derivatives

Estimate the first derivatives of $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

At $x = 0.5$ using a step size $h = 0.5$ and 0.25 using forward and backward $O(h)$, and centered $O(h^2)$ difference approximations

Note that the derivative can be calculated directly as $f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$

And can be used to compute the true value as $f'(0.5) = -0.9125$

	$\boldsymbol{h = 0.5}$		$\boldsymbol{h = 0.25}$	
	$x_{i-1} = 0$	$f(x_{i-1}) = 1.2$	$x_{i-1} = 0.25$	$f(x_{i-1}) = 1.10351563$
	$x_i = 0.5$	$f(x_i) = 0.925$	$x_i = 0.5$	$f(x_i) = 0.25$
	$x_{i+1} = 1.0$	$f(x_{i+1}) = 0.2$	$x_{i+1} = 0.75$	$f(x_{i+1}) = 0.6362813$
Method	$\boldsymbol{f'(0.5)}$	$\lvert\boldsymbol{\varepsilon_t}\rvert$	$\boldsymbol{f'(0.5)}$	$\lvert\boldsymbol{\varepsilon_t}\rvert$
Forward				
Backward				
Centered				

Example : Finite-difference approximations of derivatives

Estimate the first derivatives of $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

At $x = 0.5$ using a step size $h = 0.25$ and using high-accuracy formulas for forward and backward $O(h)$, and centered $O(h^2)$ difference approximations

	$\boldsymbol{h = 0.25}$	
	$x_{i-2} = 0$	$f(x_i) = 1.2$
	$x_{i-1} = 0.25$	$f(x_{i+1}) = 1.1035156$
	$x_i = 0.5$	$f(x_{i-1}) = 0.925$
	$x_{i+1} = 0.75$	$f(x_i) = 0.6363281$
	$x_{i+2} = 1$	$f(x_{i+1}) = 0.2$
Method	$\boldsymbol{f'(0.5)}$	$\boldsymbol{\lvert\varepsilon_t\rvert}$
Forward		
Backward		
Centered		

Richardson Extrapolation

- As with integration, the Richardson extrapolation can be used to combine two lower-accuracy estimates of the derivative to produce a higher-accuracy estimate.

- For the cases where there are two $O(h^2)$ estimates and the interval is halved ($h_2 = \frac{h_1}{2}$), an improved $O(h^4)$ estimate may be formed using

$$D = \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)$$

- For the cases where there are two $O(h^4)$ estimates and the interval is halved ($h_2 = \frac{h_1}{2}$), an improved $O(h^6)$ estimate may be formed using

$$D = \frac{16}{15} D(h_2) - \frac{1}{15} D(h_1)$$

- For the cases where there are two $O(h^6)$ estimates and the interval is halved ($h_2 = \frac{h_1}{2}$), an improved $O(h^8)$ estimate may be formed using

$$D = \frac{64}{63} D(h_2) - \frac{1}{63} D(h_1)$$

Example : Finite-difference approximations of derivatives

Estimate the first derivatives of $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

At $x = 0.5$, we have already computed the estimates of the first derivative using a step size $h = 0.5$ and 0.25, now use the Richardson extrapolation to compute an improved estimate with $O(h^4)$.

We will use the $O(h^2)$ estimates from centered differences approximations

	$\boldsymbol{h = 0.5}$		$\boldsymbol{h = 0.25}$	
Method	$\boldsymbol{f'(0.5)}$	$\lvert\boldsymbol{\varepsilon_t}\rvert$	$\boldsymbol{f'(0.5)}$	$\lvert\boldsymbol{\varepsilon_t}\rvert$
Forward	$\frac{0.2 - 0.925}{0.5} = -1.45$	58.9%	$\frac{0.6362813 - 0.925}{0.25} = -1.155$	26.5%
Backward	$\frac{0.925 - 1.2}{0.5} = -0.55$	39.7%	$\frac{0.925 - 1.10351563}{0.25} = -0.714$	21.7%
Centered	$\frac{0.2 - 1.2}{1.0} = -1.0$	9.6%	$\frac{0.6362813 - 1.10351563}{0.5} = -0.934$	2.4%

Richardson extrapolation : Improved estimate with $O(h^4)$ of the first derivative

$D =$

$\varepsilon_t =$