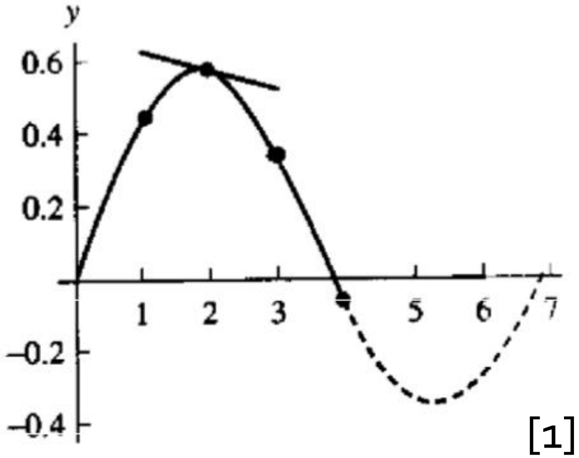
CHAPTER SIX

Numerical Differentiation

Objectives

- Approximate the derivative
- Central-difference formula of order $O(h^2)$
- Optimum step-size

Approximating the Derivative

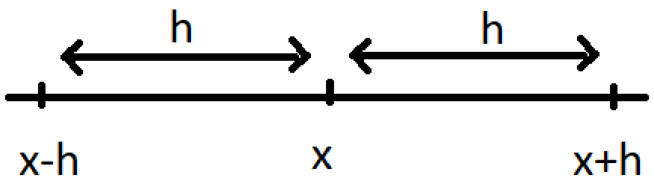


[1]

- Estimate the derivatives (slope) of a function by using the function values at only a set of discrete points
- Represent the function by Taylor polynomials or Lagrange interpolation
- Evaluate the derivatives of the interpolation polynomial at selected points

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(h)}{h}$$, where h is step size

Central-difference formula



- First, start with second-degree Taylor expressions about x for $f(x+h)$ and $f(x-h)$
  - $x_0 = x \quad , \quad x = x + h$

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \boxed{\frac{f'''(c1)}{3!}h^3}$$

Error $O(h^3)$

$$f(x+h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \boxed{\frac{f'''(c2)}{3!}h^3}$$

Error $O(h^3)$

$$\boxed{f'''(c) = \frac{f'''(c1) + f'''(c2)}{2}}$$

$$f(x+h) - f(x-h) = 2f'(x)h + O(h^3) + O(h^3) = 2f'(x)h + O(h^3)$$

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

$Central - differnce\ formula\ of\ order\ O(h^2)$

Central-difference formula - Example

- Let $f(x) = \cos(x)$. Use **central-difference formula of order $\boldsymbol{O}(\boldsymbol{h}^2)$** with step size $h = 0.1$, 0.01 , 0.001 , 0.0001 . To approximate $f'(0.8)$
- Note that the exact value of $f'(0.8) = -\sin(0.8) = -0.717356090899$
- If $h = 0.01$ →
- $f'(0.8) = \dfrac{f(0.81) - f(0.79)}{2 \times 0.01}$

$$= -0.717344150$$

Table 6.2 Numerical Differentiation Using Formu

Step size	Approximation by formula (3)	Error using formula (3)
0.1	−0.716161095	−0.001194996
0.01	−0.717344150	−0.000011941
0.001	−0.717356000	−0.000000091
0.0001	−0.717360000	−0.000003909

[1]

Optimum step-size

- $f(x_0 - h) = y_{-1} + e_{-1}$
- $f(x_0 + h) = y_1 + e_1$

$y_{-1}, y_1 \rightarrow$ approximate values for $f(x_0 - h)$ and $f(x_0 + h)$
$e_{-1}, e_1 \rightarrow$ round-off error

- Central-difference formula of order $O(h^2)$
- $f'(x_0) = \frac{y_1 - y_{-1}}{2h} + E(f,h)$

- $E(f,h)_{\ total\ error} = E(f,h)_{round-off} + E(f,h)_{\ truncated}$

Optimum step-size (cont'd)

- $E(f,h)_{\,total\ error} = E(f,h)_{round-off} + E(f,h)_{\,truncated}$

$$= \frac{e_1 - e_{-1}}{2h} + \frac{h^2 f^{(3)}(c)}{3!}$$

- Assume: $|e_{-1}| \le \epsilon$, $|e_1| \le \epsilon$, $M = \max\{|f^{(3)}(x)|\}$

- Then, error bound: $|E(f,h)| \le \frac{2\epsilon}{2h} + \frac{Mh^2}{6}$

➔To find optimum value of h: $\partial(h) = 0$ ➔ $h = (\frac{3\epsilon}{M})^{\frac{1}{3}}$

Optimum step-size - Example

- Let $f(x) = \cos(x)$ and $\epsilon = 0.5 \times 10^{-9}$. Find optimum step size for Central-difference formula of order $O(h^2)$

- $\left|f^{(3)}(x)\right| \leq |\sin(x)| = 1 \quad \rightarrow \quad M = 1$

- $h = (\frac{3\epsilon}{M})^{\frac{1}{3}} = \left(\frac{3\times0.5\times10^{-9}}{1}\right)^{\frac{1}{3}} = 0.001144714$

- Note that from previous example, optimum step size $h = 0.001$

References

- [1] Mathews J. H. and Fink K. D. (1999). Numerical Methods using MATLAB, NJ: Prentice Hall

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