

Substitution of derivatives with finite differences

Finite differences: Approximations of derivatives $f'(\hat{x})$, $f''(\hat{x})$, ... with function values $f(x_k)$ at some (finite) set of points x_k , $k = 1, \dots, K$.

Taylor theorem: Let the function $f : R \rightarrow R$ be $(n + 1)$ times differentiable at some open interval $I \subset R$ and let the closed interval between points \hat{x} and x lie inside I . Let $h = x - \hat{x}$. Then

$$f(\hat{x} + h) = f(\hat{x}) + f'(\hat{x})h + \frac{f''(\hat{x})}{2!}h^2 + \dots + \frac{f^{(n)}(\hat{x})}{n!}h^n + \mathcal{O}(h^{n+1})$$

Big \mathcal{O} notation $g(h) = \mathcal{O}(h^k)$ describes the limiting behavior of a function $g(h)$ as $h \rightarrow 0$: Function g is said to be $\mathcal{O}(h^k)$, if there exists a constant M such that $|g(h)| < M|h|^k$ at some interval $0 < |h| < h_0$.

Approximation of the first derivative:

Forward difference: Let f be twice differentiable at I , let $h > 0$. Then

$$f'(\hat{x}) = \frac{f(\hat{x} + h) - f(\hat{x})}{h} + \mathcal{O}(h)$$

Backward difference: Let f be twice differentiable at I , let $h > 0$. Then

$$f'(\hat{x}) = \frac{f(\hat{x}) - f(\hat{x} - h)}{h} + \mathcal{O}(h)$$

Proof follows from Taylor theorem immediately.

Central difference: Let f be 3 times differentiable at I , let $h > 0$. Then

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

Proof: $f(\hat{x} + h) = f(\hat{x}) + f'(\hat{x})h + \frac{f''(\hat{x})}{2!}h^2 + \mathcal{O}(h^3)$
 $f(\hat{x} - h) = f(\hat{x}) - f'(\hat{x})h + \frac{f''(\hat{x})}{2!}h^2 + \mathcal{O}(h^3)$

After subtraction: $f(\hat{x} + h) - f(\hat{x} - h) = 2f'(\hat{x})h + \mathcal{O}(h^3)$, then after division by $2h$, the desired result is obtained.

Approximation of the second derivative:

Second Central difference: Let f be 4 times differentiable at I , let $h > 0$. Then

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

Proof: $f(\hat{x} + h) = f(\hat{x}) + f'(\hat{x})h + \frac{f''(\hat{x})}{2!}h^2 + \frac{f^{(3)}(\hat{x})}{3!}h^3 + \mathcal{O}(h^4)$
 $f(\hat{x} - h) = f(\hat{x}) - f'(\hat{x})h + \frac{f''(\hat{x})}{2!}h^2 - \frac{f^{(3)}(\hat{x})}{3!}h^3 + \mathcal{O}(h^4)$

After addition: $f(\hat{x} + h) + f(\hat{x} - h) = 2f(\hat{x}) + f''(\hat{x})h^2 + \mathcal{O}(h^4)$, then after division by h^2 , the desired result is obtained.