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L04

CS5016
Computational Methods
and Applications

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Numerical Differentiation
and Integration

Differentiation

Consider $f(x) = \sin(e^{x^2})$

The derivative of $f(x)$, on application of chain rule will be

$$\frac{d f(x)}{dx} = f'(x) = \frac{d}{d(e^{x^2})} \sin(e^{x^2}) \cdot \frac{d(e^{x^2})}{d(x^2)} \cdot \frac{d(x^2)}{dx}$$

$$f'(x) = \cos(e^{x^2}) \cdot e^{x^2} \cdot 2x$$

Computers can perform numerical methods to differentiate.

Numerical Differentiation

Consider $f: [a,b] \to \mathbb{R}$ that is continuously differentiable in the interval $[a,b]$

We have, by defn

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

We like to approximate this for any point $x \in [a,b]$. For small $h > 0$,

$$\delta_h^+(x) = \frac{f(x+h) - f(x)}{h} \quad \text{... forward finite difference}$$

$$\delta_h^-(x) = \frac{f(x) - f(x-h)}{h} \quad \text{... backward finite difference}$$

Error of approximation

Let f be twice differentiable in $[a,b]$. The from Taylor series expansion, we get

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(\xi), \text{ where } \xi \in [x, x+h].$$

$$\left| \frac{f(x+h) - f(x)}{h} - f'(x) \right| = \frac{h}{2} |f''(\xi)|$$

$$\Rightarrow \underbrace{|\delta_h^+(x) - f'(x)|}_{\text{error of approximation}} = \frac{h}{2} |f''(\xi)|$$

$\therefore$

$f(x) = x^2 \Rightarrow f''(x) = 2$

$\therefore$ error of approximation $= h$

$\therefore$ h has to be small for good approximation

$f(x) = x^3 \Rightarrow f''(x) = 6x$

$\therefore$ error of approximation $= 6xh$ ~ linearly dependent on x & h

$\therefore$ if x is small, h can be somewhat large compared to the case where x is large, where h has to be small enough for good approximation

Centered finite difference

we define

$$\delta_h^c(x) = \frac{f(x+h) - f(x-h)}{2h} \quad \text{for small } h > 0$$

Assuming f is thrice differentiable in $[a,b]$, we get the foll from Taylor series expansion

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(\xi_1) \qquad -①$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(\xi_2) \qquad -②$$

① - ② $\Rightarrow$ where $\xi_1 \in [x, x+h]$, $\xi_2 \in [x-h, x]$

$$f(x+h) - f(x-h) = 2h f'(x) + \frac{h^2}{2}\left(f''(\xi_1) - f''(\xi_2)\right)$$

$$\Rightarrow \frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h}{4}\left(f''(\xi_1) - f''(\xi_2)\right)$$

$$\Rightarrow \underline{\underline{\left|\delta_h^c(x) - f'(x)\right|}} = \frac{h}{4}\left(\left|f''(\xi_1) - f''(\xi_2)\right|\right)$$

where

$\xi_1 \in [x, x+h]$ and

$\xi_2 \in [x-h, x]$

Numerical Integration

We want to evaluate

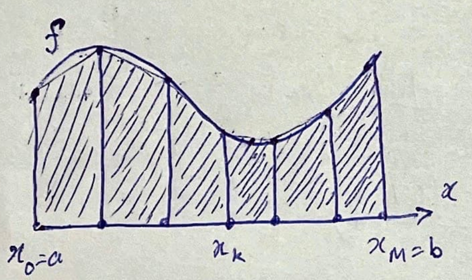
$$I(f) = \int_a^b f(x)\,dx$$

where f is an arbitrary continuous function in $[a,b]$.

Trapezoidal Formula

Divide the interval $[a,b]$ into m intervals of equal length. Let $x_k = a+kM$ for $k \in \{0,1,\dots,M\}$ and $h = \frac{(b-a)}{M}$. Then the approximate integral is given as

$$I_M(f) = \frac{b-a}{2M} \sum_{k=1}^{M} \left[f(x_k) + f(x_{k+1})\right]$$



(M=6)

For twice differentiable (continuously) $f(x)$ on the interval $[a,b]$, we have

$$E_n^T(f) := \int_a^b f(x)\,dx - T_n(f) = -\frac{h^2(b-a)}{12} f''(c_n) \quad \text{for some } c_n \in [a,b]$$

PROOF

Obtaining the error for one (sub) interval:

$$E = \int_\alpha^{\alpha+h} f(x)\,dx - \frac{h}{2}\left[f(\alpha) + f(\alpha+h)\right].$$ Applying Taylor expansion on $f(x)$ & $f(\alpha+h)$,

$$= \int_\alpha^{\alpha+h} \left[f(\alpha) + f'(\alpha)(x-\alpha) + \frac{f''(\xi)}{2}(x-\alpha)^2\right]dx - \frac{h}{2}\left[f(\alpha) + f(\alpha) + hf'(\alpha) + \frac{h^2}{2}f''(\xi)\right]$$

for some $\xi \in [\alpha, \alpha+h]$

$$= \cancel{f(\alpha)h} + \frac{f'(\alpha)}{2}(x-\alpha)^2\Big|_\alpha^{\alpha+h} + \frac{f''(\xi)}{6}(x-\alpha)^3\Big|_\alpha^{\alpha+h} - \cancel{\frac{h}{2}f(\alpha)\times 2} - \frac{h^2}{2}f'(\alpha) - \frac{h^3}{4}f''(\xi)$$

$$= \cancel{\frac{f'(\alpha)}{2}h^2} + \frac{f''(\xi)}{6}h^3 - \cancel{\frac{h^2}{2}f'(\alpha)} - \frac{h^3}{4}f''(\xi) = -\frac{h^3}{12}f''(\xi)$$

$$I(f) = \int_{x_0}^{x_n} f(x)\,dx$$

$$= \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

$$T_n(f) = \frac{h}{2}(f(x_0)+f(x_1)) + \frac{h}{2}[f(x_1)+f(x_2)] + \cdots + \frac{h}{2}(f(x_{n-1})+f(x_n))$$

Then the error

$$E_n^T(f) = \int_a^b f(x)\,dx - T_n(f)$$

can be analysed by adding together errors over each subinterval.

We just showed that

$$\int_\alpha^{\alpha+h} f(x)dx - \frac{h}{2}(f(\alpha)+f(\alpha+h)) = -\frac{h^3}{12} f''(\zeta)$$

Then for each j on $[x_{j-1}, x_j]$

$$\int_{x_{j-1}}^{x_j} f(x)dx - \frac{h}{2}[f(x_{j-1})+f(x_j)] = -\frac{h^3}{12} f''(\gamma_j) \qquad \text{where } x_{j-1} \le \gamma_j \le x_j$$

Combining,

$$E_n^T(f) = -\frac{h^3}{12} f''(\gamma_1) + \cdots + \frac{-h^3}{12} f''(\gamma_n)$$

$$= \frac{-h^3 n}{12} \underbrace{\left(\frac{f''(\gamma_1) + \cdots + f''(\gamma_n)}{n}\right)}_{C_n}$$

This C_n satisfies

$$\min_{a\le x\le b} f''(x) \le C_n \le \max_{a\le x\le b} f''(x)$$

Since $f''(x)$ is continuous, $\exists\, \phi_n \in [a,b]$ for which

$$f''(\phi_n) = C_n$$

We know $hn = b-a$.

Hence,

$$\boxed{E_n^T(f) = \frac{-h^2(b-a)}{12} f''(\phi_n) \qquad \text{where } \phi_n \in [a,b]}$$