Computational Methods and Application

Scribe IV

Numerical Differentiation and Integration

Differentiation

Consider the function

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

Application of chain rule gives us

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

Numerical differentiation

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

First derivative at any point $x \in [a,b]$

By definition

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

For a small value of $h > 0$; good approximations are

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

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

Error of Approximation

Assuming f is twice differentiable in $[a,b]$. Then from Taylor Series expansion

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(\xi)$$

where $\xi \in [x, x+h]$

Thus we have

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

$f(x) = x^2$

$$\delta_h^+(x) = \frac{(x+h)^2 - x^2}{h}$$

$f'(x) = 2x$

$f''(x) = 2$

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

Hence if we want error $< e$ then for $f(x) = x^2$
$h < e$.

when $f(x) = x^3$

$f'' = \cancel{6x}\ 6\xi$

$\therefore$ Error $= 3h\xi$

h has to be small and ξ as close to x.

Centered finite difference

For a small value of $h > 0$

$$\delta_h^c(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Taylor series

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

where $\beta \in [x-h, x]$

so $$|\delta_h^c(x) - f'(x)| = \frac{h^2}{6}\left(f'''(\alpha) + f'''(\beta)\right)$$

where $\alpha \in [x, x+h]$
$\beta \in [x-h, x]$

Error dependent on h^2.

Numerical integration

$$I(f) = \int_a^b f(x)\,dx \quad \text{where } f \text{ is a continuous function in } [a,b]$$

Trapezoidal formula

Divide the interval $[a,b]$ into M equal length intervals

Let $x_k = a + kM$ for $k \in \{0, 1, \ldots M\}$ and $h = (b-a)/M$

then approximate integral is given as

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

For the trapezoidal method with only a single subinterval.

$$\int_{\alpha}^{\alpha+h} f(x)dx - \frac{h}{2}\left[f(\alpha)+f(\alpha+h)\right] = -\frac{h^3}{12} f''(c)$$

for some c in interval $[\alpha, \alpha+h]$

$h = \frac{b-a}{M}$

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

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

$$\approx \frac{h}{2}\left[f(x_0)+f(x_1)\right] + - - - \frac{h}{2}\left[f(x_{n-1})+f(x_n)\right]$$

Errors can be combined

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

$$= \frac{-h^3 M}{12}\left[\frac{f''(\gamma_1) + - - - f''(\gamma_n)}{M}\right]$$

$$= \frac{-h^2 (b-a)}{12} f''(c_n)$$

c_n in $[a, b]$