# Numerical Differentiation.

Numerical differentiation is used in a large number of applications.

Simple approximation:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Error analysis.

From Taylor's theorem

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

$$\therefore \quad f'(x) = \frac{f(x+h) - f(x)}{h} - \underbrace{\frac{h}{2} f''(\xi)}$$

Truncation or discretization error.

error is $O(h)$.

In finite precision, we must also deal with floating point errors.

$$f'(x) \approx \frac{f(x+h)(1+\delta_1) - f(x)(1+\delta_2)}{h}$$

$$= \frac{f(x+h) - f(x)}{h} + \frac{\delta_1 f(x+h) - \delta_2 f(x)}{h}$$

$$|\delta_i| < \epsilon$$

$$\therefore \quad \text{error} \le \frac{\epsilon\,(|f(x)| + |f(x+h)|)}{h} \approx O\left(\frac{1}{h}\right)$$

Truncation error $\propto h$

Rounding error $\propto \frac{1}{h}$.

~~for~~ we get best error when these are roughly equal.

Ignoring constants, we have

$$h \approx \frac{\epsilon}{h} \quad \text{or} \quad h \approx \sqrt{\epsilon}$$

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Approximation 2.

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$

Error analysis.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(\xi), \quad \xi \in [x, x+h]$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(\eta), \quad \eta \in [x-h, x]$$

Subtracting the two.

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12} \left( f'''(\xi) + f'''(\eta) \right)$$

Truncation error is $O(h^2)$

Impact of floating point:

$$\frac{f(x+h)(1+\delta_1) - f(x-h)(1+\delta_2)}{2h}$$

$$= \frac{f(x+h) - f(x-h)}{2h} + \frac{\delta_1 f(x+h) - \delta_2 f(x-h)}{2h}.$$

Error is less than $\dfrac{\epsilon(|f(x+h)| + |f(x-h)|)}{2h}$

$\Rightarrow O(\frac{1}{h})$.

Once again, equating truncation and rounding errors

$h^2 \approx \frac{\epsilon}{h} \Rightarrow h \approx \epsilon^{1/3}$.

at this point, error $\approx h^2 \approx \epsilon^{2/3}$.

This can get accuracy to 2/3 power of floating point accuracy.

Higher derivatives:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{4!} f''''(\xi)$$

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

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{4!} f''''(\eta)$$

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

$$f(x+h) + f(x-h) = 2f(x) + \frac{h^2}{2} f''(x) + \frac{h^4}{12} f''''(\nu), \quad \nu \in [\eta, \xi]$$

$$\Rightarrow f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12} f''''(\nu).$$

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

and error is $O(h^2)$.

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Rounding error is $\frac{\epsilon}{h^2}$.

Equating the two, $h \approx \epsilon^{1/4}$

and overall accuracy is $\sqrt{\epsilon}$

$\therefore$ if $\epsilon \approx 10^{-16}$ $h \approx 10^{-4}$

Say we ~~any~~ are given points

$(x_0, y_0), (x_1, y_1) \dots (x_n, y_n)$.

How do we estimate derivatives.

if $x \in [x_{i-1}, x_i]$, we can use formula above

$$f(x_{i-1}) = f(x) + (x_{i-1} - x) f'(x) + \frac{(x_{i-1} - x)^2}{2!} f''(\xi)$$
$$\xi \in [x_{i-1}, x]$$

$$f(x_i) = f(x) + (x_i - x) f'(x) + \frac{(x_i - x)^2}{2!} f''(\eta)$$
$$\eta \in [x, x_i]$$

Subtracting, we get

$$f'(x) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} - \frac{(x_i - x)^2}{2(x_i - x_{i-1})} f''(\eta) + \frac{(x_{i-1} - x)^2}{2(x_i - x_{i-1})} f''(\xi).$$

$\therefore$ Truncation error is less than

$(x_i - x_{i-1}) \cdot f''(\vartheta)$ $\quad$ $\vartheta$ is where $f''$ has max value in the interval $[x_{i-1}, x_i]$

What happens if $x_i$ s are not evenly spaced or close ?

Interpolate using a polynomial and differentiate it.

Given $(x_0, y_0) \ldots (x_n, y_n)$,

we can fit an n-degree polynomial.

This is problematic unless $x_i$ s are chebyshev points !

Say $p(x)$ is the interpolating polynomial.

$$p'(x) = \frac{-S_1(x) \cdot S_2(x) + S_3(x) \cdot S_4(x)}{(S_1(x))^2}$$

$$S_1(x) = \sum_{i=0}^{n} \frac{w_i}{x - x_i} \qquad S_2(x) = \sum_{i=0}^{n} \frac{w_i}{(x-x_i)^2} y_i$$

$$S_3(x) = \sum_{i=0}^{n} \frac{w_i}{x-x_i} y_i \qquad S_4(x) = \sum_{i=0}^{n} \frac{w_i}{(x-x_i)^2}$$

$$w_i = \frac{1}{\prod_{j \neq i} (x - x_i)} \qquad i = 0, \ldots n.$$

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$$p(x) = \phi(x) \sum_{i=0}^{n} \frac{w_i}{x - x_i} y_i \qquad \phi(x) = \prod_{j=0}^{n} (x - x_j)$$

Richardson Extrapolation.

General technique that applies to many problems

Consider the centered difference formula

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f''''(\xi)$$

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

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f''''(\eta)$$

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

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) + O(h^4)$$

$$f'(x) = \underbrace{\phi_0(h)}_{} - \frac{h^2}{6} f'''(x) + O(h^4) \quad \text{—— } (1)$$

centered difference approximation

$$f'(x) = \phi_0\left(\frac{h}{2}\right) - \frac{(h/2)^2}{6} f'''(x) + O(h^4) \quad \text{—— } (2)$$

(2) $\times$ 4 $-$ (1) ~~gives~~ results in canceling the $h^2$ term!

$$\therefore \quad f'(x) = \frac{4}{3} \phi_0(h/2) - \frac{1}{3} \phi_0(h) + O(h^4)$$

or $$\phi_1(h) = \frac{4}{3} \phi_0(h/2) - \frac{1}{3} \phi_0(h)$$

error is $O(h^4)$.

— Twice as many function evaluation (for ~~at~~ $h$ and $\frac{h}{2}$)

Truncation error goes down much faster : $O(h^4)$.

Rounding error is still $\simeq \frac{\epsilon}{h}$.

$\therefore$ Error is minimized at

$h \simeq \epsilon^{1/5}$

and minimum error is now $\epsilon^{4/5}$