Chapter 9 Numerical Differentiation.

§ 9.1 Numerical Differentiation.

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \Rightarrow \text{for small } h,$$

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

if $h > 0 \Rightarrow$ forward-difference formula

if $h < 0 \Rightarrow$ backward-difference formula.

Let $h > 0$, small. Then

$$f(x+h) \overset{\text{Taylor's}}{=} f(x) + h \cdot f'(x) + \frac{h^2}{2} f''(\xi), \quad \xi \in [x, x+h]$$

$$\Rightarrow f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\substack{\text{approx. of } f \\ \text{(first-order accurate)}}} - \underbrace{\frac{h}{2} f''(\xi)}_{\substack{\text{truncation error} \\ \text{(or discretization error)}, \ O(h)}}$$

Truncation error: results from using approximation formula

Roundoff (or rounding) error:

if h is so small that $x+h$ is rounded to x, then $f(x+h) - f(x) = 0$ in a computer.

If δ_i are roundoff errors for $f(x)$, $f(x+h)$ w/ $|\delta_i| < \varepsilon_m$ (machine precision: single 2^{-23}, double 2^{-52})

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

$$= \frac{f(x+h)-f(x)}{h} + \underbrace{\frac{\delta_1 f(x+h) - \delta_2 f(x)}{h}}_{\text{round. error}}$$

$$\Rightarrow \quad |\text{round. error}| \le \frac{\varepsilon_m \left(|f(x)| + |f(x+h)|\right)}{h}$$

Total error = rounding error + truncation error

$$\Rightarrow \text{Total error } Err = \frac{|f''(\xi)|}{2} h + \frac{\varepsilon_m}{h} \cdot \underset{(|f(x)|+|f(x+h)|)}{\overset{}{C}}$$

$$\frac{d(Err)}{dh} = \frac{|f''(\xi)|}{2} - \frac{\varepsilon_m C}{h^2} = 0$$

$$\Rightarrow \quad h^2 = \frac{2\varepsilon_m C}{|f''(\xi)|} = \underset{\text{machine precision}}{\varepsilon_m} \; \underset{\approx\text{const.}}{\frac{2C}{|f''(\xi)|}}$$

$\Rightarrow$ when $h \approx \sqrt{\varepsilon_m}$ (ignoring C and $|f''(\xi)|/2$) we have the total error minimized.

For example, if $\varepsilon_m = 2^{-52} \approx 2.2 \cdot 10^{-16} \Rightarrow h \approx 10^{-8}$.

Example: $f(x) = \sin x$. Use $\frac{f(\pi/3+h) - f(\pi/3)}{h}$ to approximate $f'(\pi/3) = \cos \pi/3 = 0.5$.

See table 9.1 on p. 214; using $h < \sqrt{\varepsilon_m} \approx 10^{-8}$ makes the error $\left| \frac{\sin(\pi/3+h) - \sin(\pi/3)}{h} - 0.5 \right|$ start increasing, i.e., when $h = 10^{-16}$, the error is 0.5!

Another way:

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

a centered-difference formula

Truncation error using Taylor's theorem:

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

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

$h > 0$

(we assume that f is smooth enough)

Subtract (2) from (1) and solve for $f'(x)$:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \underbrace{- \frac{h^2}{12}\left(f'''(\xi) + f'''(\eta)\right)}_{\text{trunc. error} = O(h^2)}$$

$\Rightarrow$ second-order accurate formula

Roundoff error: $\frac{f(x+h)(1+\delta_1) - f(x-h)(1+\delta_2)}{2h} =$ $\quad \delta_1, \delta_2 \le \varepsilon_m$

$$= \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{\substack{\text{approx.} \\ (\text{error of } O(h^2))}} + \underbrace{\frac{\delta_1 f(x+h) - \delta_2 f(x-h)}{2h}}_{\le \varepsilon_m \left(\frac{|f(x+h)| + |f(x-h)|}{2h}\right)}$$

$$\approx \varepsilon_m / h$$

$\Rightarrow$ total error is minimal, when (ignoring constants)

$$\frac{d}{dh}\left(h^2 + \frac{\varepsilon_m}{h}\right) = 0 \Rightarrow 2h - \frac{\varepsilon_m}{h^2} = 0$$

$$\Rightarrow 2h^3 = \varepsilon_m \Rightarrow$$

$$h^3 \approx \varepsilon_m \Rightarrow \boxed{h \approx \varepsilon_m^{1/3}}$$

So, if $h \approx \sqrt[3]{\varepsilon_m}$ then for $f(x) = \sin x$, $f'(\pi/3) = 0.5$ will be approximated the best when $h \simeq \varepsilon_m^{1/3} \approx 10^{-5}$ in the formula

$$\frac{\sin(\pi/3 + h) - \sin(\pi/3 - h)}{2h} \Rightarrow \text{trunc. error and } O(h^2)$$

round. error are both $O(\varepsilon_m^{2/3})$ $\Rightarrow$ better accuracy than in the forward-diff. formula ($O(\varepsilon_m^{1/2})$)
(ε_m/h)

(See table 9.2, p. 215)

$\Downarrow$

for $h \approx 10^{-5}$, the error was $\approx 8 \cdot 10^{-12}$

What about higher derivatives? Similarly:

Expanding ($h>0$)

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

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

and

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

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

$$\Rightarrow f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{24}\left(f^{(4)}(\xi) + f^{(4)}(\eta)\right)$$

(adding)

$\Rightarrow$ solving for $f''(x)$, we get the approximation formula

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12}f^{(4)}(\nu)$$

where $f^{(4)}(\nu) = \dfrac{f^{(4)}(\xi) + f^{(4)}(\eta)}{2}$, $\nu \in [\eta, \xi]$

(by the IVT, if we assume that $f^{(4)}$ cont.)

So, $\boxed{f''(x) \approx \dfrac{f(x+h) - 2f(x) + f(x-h)}{h^2}}$ w/ trunc. err. $O(h^2)$. The total error (trunc. + rounding) is the best when $h \approx \sqrt[4]{\varepsilon_m}$ $\Rightarrow$ so, h should not be taken less than about 10^{-4}.

h^2 $\quad$ ε_m/h^2

• See <u>Example 9.13</u>, p. 216 for approx. $f''(\pi/3)$ for $f(x) = \sin x$. ⑤

Suppose that we <u>only</u> know f at a <u>fixed</u> set of measurement pts <u>$x_0, x_1, \ldots, x_n$</u> (can't evaluate f anywhere else): $y_i = f(x_i)$, $i = 0, \ldots, n$.

If x_i are not far apart, we can get reasonable approximations of f', f'' by using our data: on $[x_{i-1}, x_i]$,

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

and

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

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

(by subtracting (3) from (4) and dividing by $x_i - x_{i-1}$)

That is, $f'(x) \approx \dfrac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$ (secant slope over $[x_{i-1}, x_i]$)

with trunc. error $\leq (x_i - x_{i-1}) \max\limits_{[x_{i-1}, x_i]} (f''(x))$

If, in addition, $y_{i-1} = f(x_{i-1})(1 + \delta_1)$, $y_i = f(x_i)(1 + \delta_2)$, <u>i.e.</u>, measured w/ errors δ_i (usually larger than roundoff errors), then

$$\left| \underbrace{\frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}}_{\text{exact}} - \underbrace{\frac{y_i - y_{i-1}}{x_i - x_{i-1}}}_{\text{measured}} \right| = \underbrace{\left| \frac{\delta_2 f(x_i) - \delta_1 f(x_{i-1})}{x_i - x_{i-1}} \right|}_{(5)}$$

and $x_i - x_{i-1}$ must be:

1) small enough, s.t. the trunc. error $(x_i - x_{i-1}) \max_{[x_{i-1}, x_i]} f''(x)$ is small, <u>but</u>

2) large enough, s.t. (5) is also small.

In practice, hard to achieve. Gets even worse for higher-order derivatives.

<u>Another option</u>: Interpolate f at given measurement pts $(x_0, y_0), \dots, (x_n, y_n)$ w/ a polynomial $p(x)$ and find $f'(x) \approx p'(x)$!

not recommended for large n

<u>Recall</u> the barycentric formula:

$$p(x) = \left(\sum_{i=0}^{n} \frac{w_i y_i}{x - x_i} \right) \Big/ \left(\sum_{i=0}^{n} \frac{w_i}{x - x_i} \right)$$

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

with $S_1(x) = \sum_{i=0}^{n} \frac{w_i}{x - x_i}$,

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

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

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

<u>Recall</u>: One can use Chebyshev scaled pts.

- See Example 9.1.4, 9.1.5 for $\sin x$, $\frac{1}{1+x^2}$ using package "chebfun" and MATLAB func. "diff".