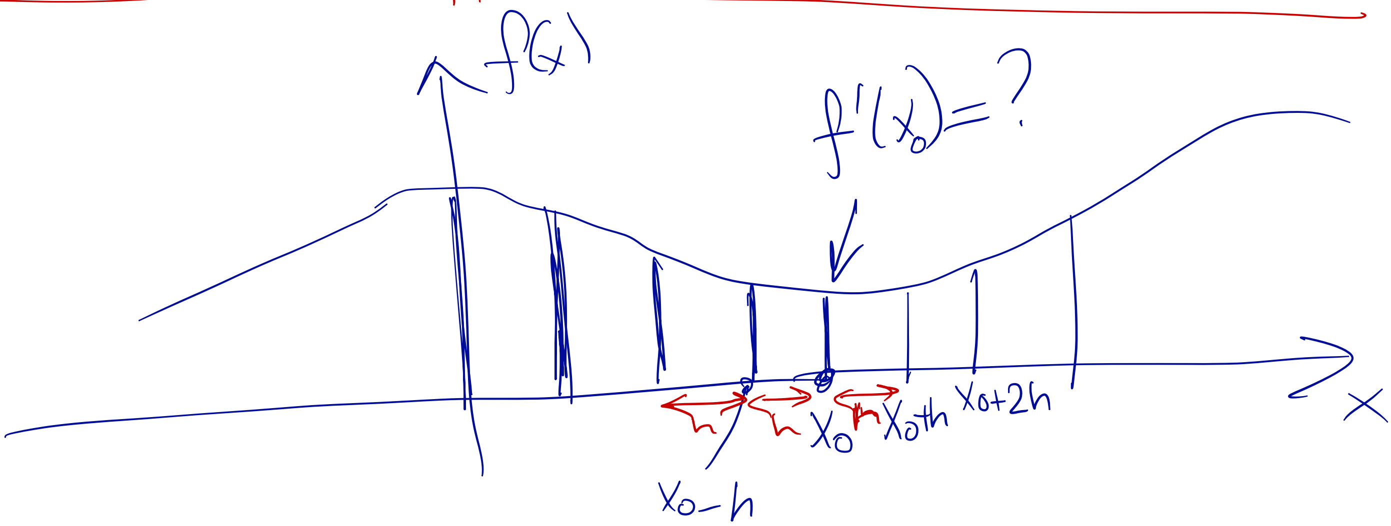
BLG 202E

Numerical Methods

Numerical Differentiation - Part 2

19.04.2016

Numerical Differentiation (Chap 14) - 3/4



① Taylor Series Method:

Forward difference $\boxed{: O(h)}$ ← Truncation error

T.S. expand

$f(x_0+h) = f(x_0) + h\, f'(x_0) + \ldots$

$f(x_0) = \ldots$

=

— 3 pt centered formula. $O(h^2)$

$f(x_0+h) = \ldots$

$f(x_0-h) = \ldots$

② Richardson Extrapolation: Used two methods of lower order at other grid distances (e.g. 2h), to obtain a higher order method.

③. Used polynomial interpolation (today we continue w/ this)

$$f(x) \approx p_n(x)$$

$$f'(x) \approx p_n'(x)$$

Differentiation using Lagrange Interpolation:

$$p(x) = \sum_{j=0}^{n} \underbrace{f(x_j)}_{c_j} L_j(x) \, ;$$

Given interpolation points: $x_0, x_1, \ldots, x_n$

Recall Lagrange polynomials:

$$L_j(x) = \frac{(x-x_0) \ldots (x-x_{j-1})(x-x_{j+1}) \ldots (x-x_n)}{(x_j-x_0) \ldots (x_j-x_{j-1})(x_j-x_{j+1}) \ldots (x_j-x_n)}$$

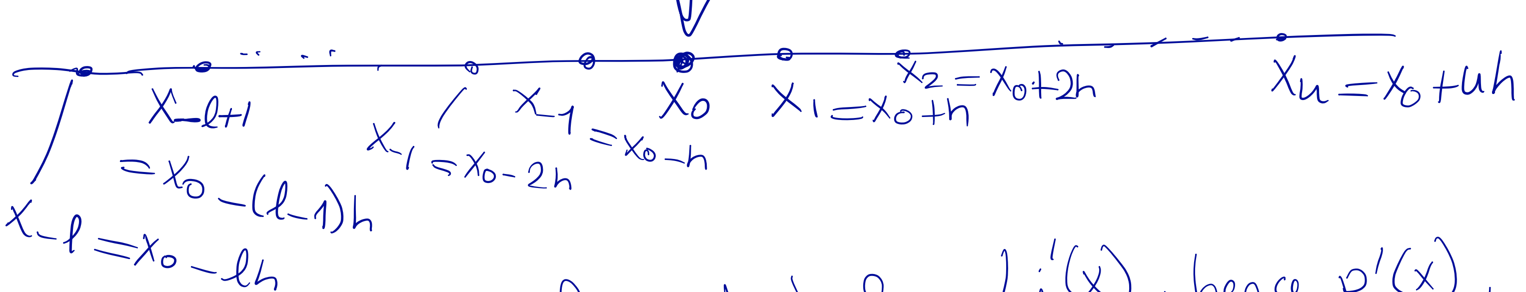
Take the derivative & substitute $x = x_0$

$$\boxed{p'(x_0) = \sum_{j=0}^{n} f(x_j) L_j'(x)}$$

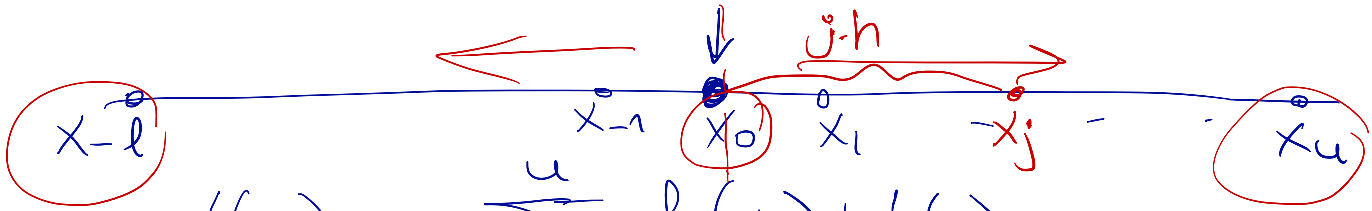
Recall the points $x_0, x_1, \ldots, x_n$ are not required to be equidistant!

Differentiation using equidistant points:

Assume the points are distributed around x_0:



Next, we derive formula's for $L_j'(x)$, hence $p'(x)$, to calculate $f'(x)$.



$$p'(x_0) = \sum_{j=-l}^{u} f(x_j)\, \underbrace{L_j'(x_0)}_{?}$$

$$\boxed{L_j(x)} = \frac{(x-x_{-l})\cdots(x-x_0)\cdots(x-x_u)}{(x_j-x_{-l})\cdots(x_j-x_0)\cdots(x_j-x_0)}$$

Remember $(x-x_j)$ is not included

$j=0$

$$L_0(x) = \frac{(x-x_1)(x-x_2)\cdots(x-x_u)(x-x_{-1})\cdots(x-x_{-l})}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_u)(x_0-x_{-1})\cdots(x_0-x_{-l})}$$

$$L_0'(x_0) = \frac{1}{\underbrace{x_0-x_1}_{-h}} + \frac{1}{\underbrace{x_0-x_2}_{-2h}} + \cdots + \frac{1}{\underbrace{x_0-x_u}_{-u\cdot h}} + \frac{1}{\underbrace{x_0-x_{-1}}_{h}} + \cdots + \frac{1}{\underbrace{x_0-x_{-l}}_{l\cdot h}}$$

$$\underset{j=0}{L_0'(x_0)} = \sum_{\substack{k=-l\\k\neq 0}}^{u} \frac{1}{x_0-x_k} = \frac{1}{h}\sum_{\substack{k=-l\\k\neq 0}}^{u}\left(-\frac{1}{k}\right)$$

$j\neq 0$

$$L_j'(x_0) = \boxed{\frac{1}{\underbrace{x_j-x_0}_{j\cdot h}} \prod_{\substack{k=-l\\k\neq 0\\k\neq j}}^{u} \frac{(x_0-x_k)}{(x_j-x_k)}} = \boxed{\frac{1}{jh}\prod \frac{(-k)}{(j-k)}} \triangleq a_j$$

$= x_0-(x_0+kh) = -kh$

$x_j - x_k = x_0 + jh - (x_0+kh) = (j-k)h$

Exercise: derive this!

Let $\boxed{a_j = h\, L_j'(x_0)}$, $j=-l,\dots,u$; j is a term indep of f and h.

→ These weights can be calculated once & for all.

$$\Longrightarrow \boxed{p'(x_0) = \frac{1}{h}\sum_{j=-l}^{u} a_j f(x_j)}$$

Q: How accurate is this formula (on the previous page)?

We'll use the polynomial interpolation error:

$$f(x) - p_n(x) = f[x_{-\ell}, x_{-\ell+1}, \dots, x_u, x] \prod_{k=-\ell}^{u} (x - x_k)$$

The error in the numerical differentiation formula at $x = x_0$:

$$f'(x) - p_n'(x) = \frac{d}{dx}\left\{ f[x_{-\ell}, \dots, x_u, x] \prod_{i=-\ell}^{u} (x - x_k) \right\}$$

(evaluate at $x = x_0$)

$$= \cancel{\frac{d}{dx} f[\dots] \underbrace{\prod (x - x_k)}_{0 \leftarrow x = x_0}}\Big| \to 0 \quad + f[x_{-\ell}, \dots, x_u, x_0] \cdot \underbrace{\frac{d}{dx}\left\{ (x - x_{-\ell})(x - x_{-\ell+1}) \cdots (x - x_0)(x - x_1) \cdots (x - x_u) \right\}\Big|_{x = x_0}}_{=}$$

$$= \underbrace{f[x_{-\ell}, \dots, x_u, x_0]}_{\Downarrow} \prod_{\substack{k=-\ell \\ k \neq 0}}^{u} (x_0 - x_k)$$

Use the theorem to rewrite the divided diff (p. 312)

$$= \frac{f^{(n+1)}(\xi)}{(n+1)!} \underbrace{(x_0 - x_{-\ell})}_{\ell \cdot h} \underbrace{(x_0 - x_{-\ell+1})}_{(\ell-1)h} \cdots \underbrace{(x_0 - x_{-1})}_{h} \underbrace{(x_0 - x_1)}_{-h} \cdots \underbrace{(x_0 - x_u)}_{-u \cdot h}$$

$$= \left(\frac{f^{(n+1)}(\xi)}{(n+1)!} \, \ell! \, u! \right) h^n (-1)^u \qquad \xi \in [x_{-\ell}, x_u]$$

$\to O(h^n)$ formula.

$$\left| \underbrace{f'(x_0) - \underbrace{\frac{1}{h}\sum_{j=-l}^{u} a_j f(x_j)}_{=p_n'(x_0)}}_{\text{Truncation error}} \right| \leq \underbrace{\frac{l!\,u!}{(n+1)!}\, \|f^{(n+1)}\|_\infty \cdot h^n}$$

Ex: (14.5): Let $l = +1$, $u = 1$; calculate $f'(x_0)$

Given $f(x_{-1}), f(x_0), f(x_1), \ldots \Longrightarrow n = 2$

$x_{-1} = x_0 - h \qquad x_0 \qquad x_0 + h = x_1$

We derived

Recall:

$\boxed{a_j = h\, L_j'(x_0)}$; $L_j'(x_0) = \frac{1}{jh} \prod_{\substack{k=-l \\ k \neq 0 \\ k \neq j}}^{u} \left(\frac{-k}{j-k}\right)$

$$\boxed{P_2'(x_0) = \frac{1}{h} \sum_{j=-l}^{u} a_j f(x_j)}$$

(HW: write a Matlab fn. to calculate a_j)

$$L_0'(x_0) = \frac{1}{h}\left(1 + (-1)\right) \Longleftarrow \left(L_0'(x_0) = \frac{1}{h} \sum_{\substack{k=-l \\ k \neq 0}}^{u} \left(-\frac{1}{k}\right)\right)$$

$L_0'(x_0) = 0 \Longrightarrow a_0 = 0$

$$L_{-1}'(x_0) = \frac{1}{(-1)h}\left(\frac{-1}{-1-1}\right) = -\frac{1}{2h}$$

$$L_1'(x_0) = \frac{1}{h}\left(-\frac{(-1)}{1-(-1)}\right) = \frac{1}{2h}$$

$$\Longrightarrow f'(x_0) = P_2'(x_0) = \frac{1}{h}\left(a_{-1} f(x_0 - h) + a_1 f(x_0 + h) + \cancel{a_0 f(x_0)}\right)$$

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} \Longrightarrow$$

$\Rightarrow$ The error is estimated by $\underline{f'(x_0) - p_2'(x_0)}$

Recall:

$$f'(x_0) - p_n'(x_0) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\, \underline{l!\, u!\, (-1)^u h^n}$$

$$f'(x_0) - p_2'(x_0) = -\frac{1!\, 1!\, h^2}{3!} f'''(\xi)$$

$\Rightarrow O(h^2)$

compare to the result of T.S method (Taylor Series)

Exercise: Take $l = 2$, $u = 2$,

Derive the 1st derivative: (calculate)

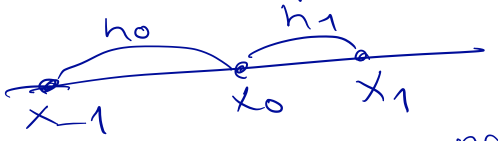
$$f'(x_0) \approx \frac{1}{12h}\left(f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right)$$

Calculate truncation error: $e(h) = \frac{h^4}{30} f^{(v)}(\xi) \Rightarrow O(h^4)$

Compare to T.S. results!

Non-uniformly spaced Points: This is the major advantage of the polynomial differentiation, which is more complicated but useful.

Ex: (14.6): Suppose points $x_{-1} = x_0 - h_0$, $x_1 = x_0 + h_1$



Want to derive a 2nd order formula for $f'(x_0)$.

An ad-hoc approach: $\boxed{f'(x_0) = \frac{f(x_1) - f(x_{-1})}{h_0 + h_1}}$ naive approach

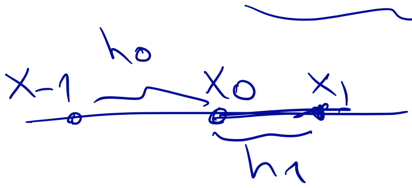
Instead, we'll use polyn. differentiation $\Rightarrow$

$$\Rightarrow P_2'(x_0) = \sum_{j=-1}^{1} f(x_j)\, L_j'(x_0)$$

$L_0'(x_0) = ?$, $L_{-1}'(x_0) = ?$, $L_1'(x_0) = ?$

~~Recall:~~
$$L_0'(x_0) = \sum_{\substack{k=-l \\ k\neq 0}}^{u} \frac{1}{x_0 - x_k} \, , \quad \boxed{\underset{j\neq 0}{L_j'(x_0)} = \frac{1}{x_j - x_0} \prod_{\substack{k=-l \\ k\neq 0 \\ k\neq j}}^{u} \frac{x_0 - x_k}{x_j - x_k}}$$

$$L_0'(x_0) = \frac{1}{\underbrace{(x_0 - x_{-1})}} + \frac{1}{(x_0 - x_1)} = \frac{1}{h_0} + \frac{(-1)}{h_1} = \frac{h_1 - h_0}{h_1 h_0}$$



$$; \; L_{-1}'(x_0) = \frac{1}{(x_{-1} - x_0)} \frac{(x_0 - x_1)}{(x_{-1} - x_1)} = -\frac{1}{h_0} \frac{h_1 \cancel{(-1)}}{(h_0 + h_1)\cancel{(-1)}}$$

$$L_1'(x_0) = \frac{1}{(x_1 - x_0)} \frac{(x_0 - x_{-1})}{(x_1 - x_{-1})} = \frac{1}{h_1} \frac{h_0}{h_0 + h_1}$$

$$\boxed{f'(x_0) = f(x_0) L_0'(x_0) + f(x_{-1}) L_{-1}'(x_0) + f(x_1) L_1'(x_0)}$$

$\hookrightarrow \approx P_2'(x_0)$

$$\boxed{f'(x_0) = \frac{h_1 - h_0}{h_1 h_0} f(x_0) + \frac{1}{h_0 + h_1}\left(\frac{h_0}{h_1} f(x_1) - \frac{h_1}{h_0} f(x_{-1})\right)}$$

eg: Insert $h_1 = h_0$ $\Rightarrow$ this becomes the familiar 3-pt centered formula

$\Rightarrow$ Compare the naive approach to the principled approach in Table 4.2:

$\sim O(h)$ $\Longleftarrow$ $O(h^2)$

Formulas for Higher Order Derivatives:

$$f^{(k)}(x_0) \approx p^{(k)}(x_0) = \sum_{j=-l}^{u} f(x_j)\, L_j^{(k)}(x_0)$$

End of 14.3

14.4 Round-off errors & Data errors in Numerical Differentiation.

Ex 14.7 $f'(x_0) \cong \dfrac{f(x_0+h) - f(x_0-h)}{2h} = D_h$

$\bar{D}_h$: calculated value for D_h.

* Let $\bar{f}(x) = fl(f(x))$: floating pt approx for $f(x)$ at each x.

$$\bar{f}(x) = f(x) + \underbrace{e_r(x)}_{\text{round-off error term}},$$

We'll assume that $\boxed{|e_r(x)| \le \varepsilon}$ → depends on the rounding unit η.

(Recall: $\dfrac{|x - \bar{x}|}{|x|} \le \eta$, $\bar{x} = fl(x)$) for the IEEE fl pt. std.

$\eta = 2^{-52}$

Consider the centered diff. formula: $\bar{D}_h = \dfrac{\bar{f}(x_0+h) - \bar{f}(x_0-h)}{2h}$

(we neglect the floating pt errors in subtraction & division operations) for simplicity.

*Want to see how h (the spacing parameter) affects the round-off error & truncation error & the interplay between the two errors, ⟹

$$\Rightarrow |\bar{D}_h - D_h| = \left| \frac{\bar{f}(x_0+h) - \bar{f}(x_0-h)}{2h} - \frac{f(x_0+h) - f(x_0-h)}{2h} \right|$$

$$= \left| \frac{er(x_0+h) - er(x_0-h)}{2h} \right|$$

$$\leq \underbrace{\left| \frac{er(x_0+h)}{2h} \right|}_{\leq \frac{\varepsilon}{2h}} + \underbrace{\left| \frac{er(x_0-h)}{2h} \right|}_{\leq \frac{\varepsilon}{2h}}$$

$$\leq \frac{\varepsilon}{h}$$

(Note: The round-off error $er(x)$ is not smooth, i.e. signs of $er(x_0+h)$, $er(x_0-h)$ may differ).

* The actual error in our approx:

$$|f'(x_0) - \bar{D}_h| = |\underbrace{(f'(x_0) - D_h)}_{\text{truncation error}} + \underbrace{(D_h - \bar{D}_h)}_{\text{round-off error}}|$$

$$\leq \underbrace{|f'(x_0) - D_h|} + |D_h - \bar{D}_h|$$

Recall truncation error $= -\frac{h^2}{6} f'''(\xi)$, assume $|f'''(\xi)| \leq M$, $\xi \in [x_0-h, x_0+h]$

truncation error bound; round-off error bound

$$\leq \frac{h^2 M}{6} + \frac{\varepsilon}{h} \Rightarrow$$

see Fig. 14.2: ideal round-off error $\propto \frac{1}{h}$

ideal truncation error $\propto h^2$

Derive an optimal h: define

$$E(h) \triangleq \frac{h^2 M}{6} + \frac{\varepsilon}{h} \Rightarrow E'(h) = 0$$

$$\frac{dE}{dh} = \frac{h}{3} M - \frac{\varepsilon}{h^2} = 0 \rightarrow \boxed{h_* = \left(\frac{3\varepsilon}{M}\right)^{1/3}}$$ optimal h value

(verify this is a minimizer $\frac{d^2 E}{dh^2}(h_*) > 0$)

⇒ Actual choice of h: depends on the rounding unit, also on the order of truncation error, also on the derivative bounds.

$$\left(h_* = \left(\frac{3\varepsilon}{M}\right)^{1/3}\right) \quad \frac{1}{q+1}$$

$$|f'(x_0) - \bar{D}_h| \le \frac{h^2}{6}M + \frac{\varepsilon}{h}$$

$f'(x_0)$: actual (true) value of derivative

$\bar{D}_h$: calculated value in the finite precision arithmetic

$\frac{h^2}{6}M$: truncation error ⇒ $O(h^2)$

$\frac{\varepsilon}{h}$: in the round-off error h is in denominator

— h should not be too close to η — rounding unit: too small! (error will blow up!)

(we don't know ε and M values)

⇒ Rule of thumb: keep h well above $\eta^{(1/q+1)}$ for a method of accuracy q.

(Note $q=2$ for the above example)

Also Note:

— We want the truncation error to dominate the round-off error, which has an oscillating characteristic.

Summary: We've seen how the choice of h affects the truncation errors & round-off errors (their relative magnitudes).

Note that: As h is reduced, truncation error shrinks by h^2 while round-off error grows by $\frac{1}{h}$.

∴ If h is very small, the round-off error term dominates, we don't want this to happen.

We've seen this in Fig. 14.2.

The measured error ≃ truncation error + round-off error

$h \searrow$ $\quad\searrow\quad\nearrow$