4.1 Numerical Differentiation

Derivative is defined as $f'(x_0) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}$

To approx this, construct a Lagrange poly. between $[a,b]$, where x_0 and $x_1 = x_0 + h$ are both in $[a,b]$

So

$$f(x) = \frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

$$= \frac{(x-x_0-h)\, f(x_0)}{-h} + \frac{(x-x_0)\, f(x_0+h)}{h} + \frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))$$

Taking the deriv of both sides yields

$$f'(x) = \frac{f(x_0)}{-h} + \frac{f(x_0+h)}{h} + D_x\left[\frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))\right]$$

$$= \frac{f(x_0+h)-f(x_0)}{h} + \underbrace{\left(\frac{2(x-x_0)-h}{2}\right) f''(\xi(x)) + \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x)))}_{\text{Remainder}}$$

Note: this says that $f'(x) \approx \frac{f(x_0+h)-f(x_0)}{h}$ for all $x \in [a,b]$.

This isn't always the best approx, especially if x is far from x_0. It's hard to approx truncation error as a result. However, if we let $x = x_0$, we can eliminate the $D_x f''$ term.

Thus,

Note $\left[\frac{2(x_0-x_0)-h}{2} f''(\xi)\right]$

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

When $h>0$, we call this est the forward difference formula
" $h<0$, " " " " " backward " "

<u>Ex:</u> Let $f(x) = \ln x$ and est $f'(1.8) = \frac{1}{1.8} = .55\bar{5}$

$\to f'(x) = \frac{1}{x}$, $f''(x) = \frac{-1}{x^2}$

$$f'(1.8) \approx \frac{f(1.8+h) - f(1.8)}{h}$$, where error term is bounded by

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} \leq \frac{|h|}{2(1.8)^2}, \quad \xi \in (1.8, 1.8+h)$$

Try for a few h values:

h	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\lvert h\rvert}{2(1.8)^2}$
.1	.5406722	.0154321
.01	.5540180	.0015432
.001	.5554013	.0001543

real ans: $f'(1.8) = \frac{1}{1.8} = .\bar{5}$

What if we use more points instead of two? Let's use $n+1$ pts and take the derivative again.

$$f(x) = \sum_{j=0}^{n} f(x_j) L_j(x) + \frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!} f^{(n+1)}(\xi(x)), \text{ where } \xi \in I$$

L_k = Lagrange poly.

Differentiating this yields

$$f'(x) = \sum_{j=0}^{n} f(x_j) L_j'(x) + D_x\left[\frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) + \frac{\prod_{i=0}^{n}(x-x_i)}{(n+1)!} D_x f^{(n+1)}(\xi(x))$$

Note the middle term can be simplified using log. diff.

$$g(x) = \prod_{i=0}^{n}(x-x_i) \Rightarrow \ln g(x) = \sum_{i=0}^{n} \ln(x-x_i) \Rightarrow \frac{g'(x)}{g(x)} = \sum_{i=0}^{n} \frac{1}{x-x_i}$$

$$\text{So } g'(x) = \sum_{i=0}^{n} \frac{g(x)}{x-x_i} = \sum_{i=0}^{n} \frac{\prod_{j=0}^{n}(x-x_j)}{x-x_i} = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x-x_j)$$

bottom cancels when $j=i$, so

It follows that

$$f'(x) = \sum_{j=0}^{n} f(x_j) L_j'(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j\neq i}}^{n} (x-x_j) + \frac{\prod_{i=0}^{n} (x-x_i)}{(n+1)!} D_x f^{(n+1)}(\xi)$$

Note we have the same issue as before where [the last term] is hard to est as we don't know structure of ξ.

However, if we let $x = x_k$, then $\prod_{i=0}^{n} (x-x_i) = 0$ (since $x_k = x_i$ for one of them)

Also, when $x = x_k$, $\sum_{i=0}^{n} \prod_{\substack{j=0 \\ j\neq i}}^{n} (x_k - x_j) = \prod_{\substack{j=0 \\ j\neq k}}^{n} (x_k - x_j)$ (All terms drop out except $i=k$)

So let $x = x_k$, then

$$\underbrace{f'(x_k) = \sum_{j=0}^{n} f(x_j) L_j'(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{\substack{j=0 \\ j\neq k}}^{n} (x_k - x_j)}_{\text{called } (n+1)\text{-point formula}}$$

More evaluation pts give more accuracy, but at the expense of more function evaluations and growth of rounding error. Most common numbers are 3 and 5.

So, suppose $n=3$. Then

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{x^2 - x_1 x - x_2 x + x_1 x_2}{(x_0-x_1)(x_0-x_2)} \Rightarrow L_0'(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

similarly, $L_1'(x) = \dfrac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}$ and $L_2'(x) = \dfrac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}$

Thus

$$f'(x_k) = f(x_0)\left[\frac{2x_k - x_1 - x_2}{(\underbrace{x_0-x_1}_{-h})(\underbrace{x_0-x_2}_{-2h})}\right] + f(x_1)\left[\frac{2x_k - x_0 - x_2}{(\underbrace{x_1-x_0}_{h})(\underbrace{x_1-x_2}_{-h})}\right] + f(x_2)\left[\frac{2x_k - x_0 - x_1}{(\underbrace{x_2-x_0}_{2h})(\underbrace{x_2-x_1}_{h})}\right] \qquad (*)$$

$$+ \frac{1}{6} f^{(3)}(\xi_k) \prod_{\substack{j=0 \\ j\neq k}}^{2} (x_k - x_j)$$

The formulas become more useful when the points are equally spaced. So let $x_1 = x_0 + h$, $x_2 = x_1 + h = x_0 + 2h$

suppose

$$f'(x_0) = f(x_0)\left[\frac{\cancel{2x_0} - \cancel{x_0} - h - \cancel{x_0} - 2h}{(-h)(-2h)}\right] + f(x_1)\left[\frac{\cancel{2x_0 - x_0 - x_0} - 2h}{(h)(-h)}\right] + f(x_2)\left[\frac{2x_0 - x_0 - x_0 - h}{(2h)(h)}\right] + \text{error}$$

$$= f(x_0)\left[\frac{-3h}{2h^2}\right] + \underset{\substack{\uparrow \\ x_0+h}}{f(x_1)}\left[\frac{-2h}{-h^2}\right] + f(x_2)\left[\frac{-h}{2h^2}\right] + \frac{1}{6} f^{(3)}(\xi_k)\underbrace{(x_0 - x_1)}_{(-h)}\underbrace{(x_0 - x_2)}_{(-2h)}$$

$$= \frac{1}{h}\left[-\frac{3}{2} f(x_0) + 2f(x_1) - \frac{1}{2} f(x_2)\right] + \frac{1}{3} h^2 f^{(3)}(\xi_0)$$

the power is bigger

(1) $$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] + \frac{1}{3} h^2 f^{(3)}(\xi)$$

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

Compare to the 2 pt formula

Instead of choosing $k=0$, what if $k=1$, Then (*) becomes

$$f'(x_1) = f(x_0)\left[\frac{2x_1 - x_1 - x_2}{(-h)(-2h)}\right] + f(x_1)\left[\frac{2x_1 - x_0 - x_2}{-h^2}\right] + f(x_2)\left[\frac{2x_1 - x_0 - x_1}{2h^2}\right] + \text{error}$$

$$= f(x_0)\left[\frac{x_1 - x_1 - h}{2h^2}\right] + f(x_1)\left[\frac{2(\cancel{x_0+h}) - \cancel{x_0} - \cancel{x_0 - 2h}}{-h^2}\right] + f(x_2)\left[\frac{x_0 + h - x_0}{2h^2}\right] + \text{error}$$

$$= f(x_0)\left[\frac{-1}{2h}\right] + f(x_1)\left[0\right] + f(x_2)\left[\frac{1}{2h}\right] + \frac{1}{6} f^{(3)}(\xi_1)\underbrace{(x_1 - x_0)}_{h}\underbrace{(x_2 - x_1)}_{-h}$$

(2) $$f'(x_1) = \frac{1}{2h}\left[-f(x_0) + f(x_2)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Similarly,

(3) $$f'(x_2) = \frac{1}{h}\left[\frac{1}{2} f(x_0) - 2 f(x_1) + \frac{3}{2} f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$$

The three formulas summarized, where $x_1 = x_0 + h$

$x_2 = x_0 + 2h$

(1) $f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$

(2) $f'(x_0+h) = \frac{1}{2h}\left[-f(x_0) + f(x_0+2h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1)$

(3) $f'(x_0+2h) = \frac{1}{2h}\left[\frac{1}{2}f(x_0) - 4f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$

We'd like to center all formulas around x_0, so
subtract $-h$ from all arguments in (2)
subtract $-2h$ from all arguments in (3), which gives

(1) $f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{1}{3} h^2 f^{(3)}(\xi_0)$

(2) $f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{1}{6} h^2 f^{(3)}(\xi_1)$

(3) $$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) + 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$$

<u>Note</u>: If h is replaced by $-h$ in (3), then (3) = (1), so we really only have two formulas:

$$\boxed{\begin{aligned} &(1) \quad f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0) \\ &(2) \quad f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \end{aligned}}$$

Three pt-estimations for $f'(x_0)$

Similarly, there are 5 pt formula:

(4) $f'(x_0) = \frac{1}{12h}\left[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)\right] + \frac{h^4}{30} f^{(5)}(\xi)$

(5) $f'(x_0) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)\right] + \frac{h^4}{5} f^{(5)}(\xi)$

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(5) is used to estimate the derivatives on the endpoints for the clamped version

when x_0 is near the center, use (4)

when x_0 is near the endpoints, use (5)

Example

x	f(x)
1.2	−0.2890399
1.5	0.3648997
1.8	0.2849914
2.1	0.4853357
2.4	0.6529012

Estimate

$f'(1.3)$ using (1), (2), (4), (5)

$f'(1.9)$ using (1), (2), (4), (5)

$f'(2.35)$ using (1), (2), (4), (5)

What is the error? Use the error bound if

last term of each formula

$\max f^{(3)}(x) = 3.245$ and

$\max f^{(5)}(x) = 41.3897$

Taylor Series Method

we can derive formulas using Taylor series expansions

The derivations are algebraically tedious, so only one will be shown:

Expand using h form of Taylor's Series:

$$(*)\quad f(x_0+h) = f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2}h^2 + \frac{f^{(3)}(x_0)h^3}{6} + \frac{f^{(4)}(\xi_1)h^4}{24}$$

Substitute $-h$ for h in $(*)$ gives

$$(**)\quad f(x_0-h) = f(x_0) - f'(x_0)h + \frac{f''(x_0)h^2}{2} - \frac{f^{(3)}(x_0)h^3}{6} + \frac{f^{(4)}(\xi_2)}{24}h^4$$

Adding $(*)$ to $(**)$ gives

$$f(x_0+h)+f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \left(\frac{f^{(4)}(\xi_1)+f^{(4)}(\xi_2)}{24}\right)h^4$$

Solving for $f''(x_0)$ gives

$$\frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \underbrace{\frac{(f^{(4)}(\xi_1) + f^{(4)}(\xi_2))}{24}}\, h^4 = f''(x_0)$$

The intermediate value thm says that can be written as $\dfrac{f^{(4)}(\xi_3)}{12}$.

So

$$(6) \quad \boxed{f''(x_0) = \frac{1}{h^2}\left[f(x_0-h) - 2f(x_0) + f(x_0+h)\right] - \frac{1}{12} h^2 f^{(4)}(\xi_3)}$$

We should analyze roundoff error & truncation error.

If we assume roundoff error is bounded by $\varepsilon > 0$ and $f^{(3)}(x) \le M$, then for

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right],$$ it follows

Truncation error

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6} M$$

roundoff error

Note: If we want to lower truncation error, we make h smaller. But when h gets smaller, the roundoff error increases!

Let's minimize $e(h) = \dfrac{\varepsilon}{h} + \dfrac{h^2}{6} M$

In practice, M is <u>not</u> known (max of $f^{(3)}$) so we can't always use this.

$$e'(h) = \frac{-\varepsilon}{h^2} + \frac{2h}{6}M \overset{\text{set}}{=} 0$$

$$-3\varepsilon + h^3 M = 0$$

$$h^3 M = 3\varepsilon \Rightarrow h = \sqrt[3]{\frac{3\varepsilon}{M}}$$

<u>Conclusion?</u>

- can't be too small or lose accuracy
- can't be too large or lose accuracy
- Numerical Differentiation is <u>unstable</u>
- We still need to do it!
- Tread lightly!