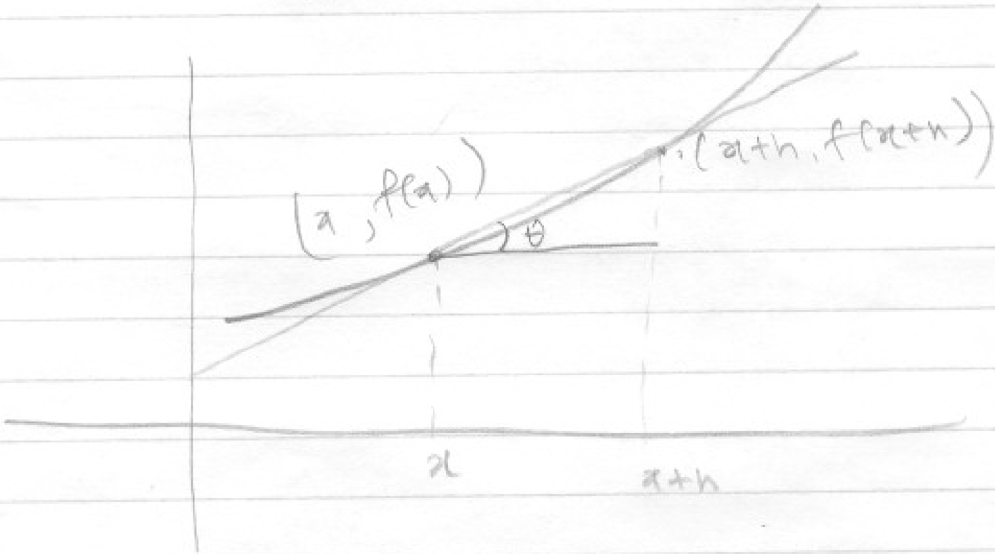
Estimating Derivatives
&
Richardson Extrapolation

$f \in C^2[a,b]$: f is a function where $f'(x)$ is continuous in $[a,b]$

Interested in computing the derivative of a function at a given point x. From the definition of the derivative,

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \quad \text{for some } h < 1.$$

$$\approx \frac{f(x+h) - f(x)}{h} \quad \text{for small } h \qquad (1)$$



slope of the secant line : $\dfrac{f(x+h) - f(x)}{h}$

Which gets closer & closer to being a the slope of the tangent lines

We need to estimate the error. To find out, consider the Taylor's theorem:

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(\xi) \quad \text{for some}$$

ξ in the interval $[x, x+h]$, $f''(\xi) \neq 0$

Rearranging the equation gives

$$f'(x) = \frac{1}{h}\left[f(x+h) - f(x)\right] - \frac{h}{2!} f''(\xi). \qquad (2)$$

Hence the approximation $f'(x) \approx \frac{f(x+h)-f(x)}{h}$ (1)

has error term $-\frac{h}{2} f''(\xi)$ where $\xi \in [x, x+h]$

If $|f''(t)| \leq M \; \forall \, t \in [x, x+h]^2$, error $\leq \left|\frac{Mh}{2}\right|$.

Thus, as $h \to 0$, the difference between $f'(x)$ & $\frac{1}{h}(f(x+h)-f(x))$ approach zero at the same rate as h does i.e. $O(h)$

What happens when $f''(x) = 0 \;\; \forall \, x \in [x, x+h]$?

Then

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

$f''(x) = 0$ & $\xi \in [x, x+h]$

$$\therefore \; f'(x) = \frac{1}{h}\left[f(x+h) - f(x)\right] - \frac{h^2}{6} f'''(\xi).$$

Error term $\left|\frac{M' h^2}{6}\right|$ i.e. $O(h^2)$

We would like convergence rate $O(h^2)$ at least!

i.e. Want an approximation of $f'(x)$ where the error term is $O(h^2)$.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(\xi_1)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(\xi_2)$$

where $\xi_1 \in [x, x+h]$

$\xi_2 \in [x-h, x]$.

$$\therefore \quad f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3!}\left(f'''(\xi_1) + f'''(\xi_2)\right)$$

$$\text{i.e. } f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{12}\left(f'''(\xi_1) + f'''(\xi_2)\right)$$

$$= \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}\left(\frac{f'''(\xi_1) + f'''(\xi_2)}{2}\right)$$

Error term can be simplified by the following reasoning: The expression $\frac{f'''(\xi_1) + f'''(\xi_2)}{2}$ is the average of two values of f''' on the interval $[x-h, x+h]$. If $f'''(x)$ is continuous, the average value is assumed at some point ξ.

$$\therefore\ f'(x) = \frac{1}{2h}\left[f(x+h) - f(x-h)\right] - \frac{1}{6}h^2 f'''(\xi)$$

This is based on the assumption that $f'''(x)$ is continuous on $[x-h, x+h]$. i.e. $f(x) \in C^3[x\pm h]$
has 3 continuous derivatives

The error term is $O(h^2)$.

Objective: higher order error term.

Using Taylor series:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \frac{1}{3!}h^3 f^{(3)}(x) + \frac{1}{4!}h^4 f^{(4)}(x) + \cdots$$

$$f(x-h) = f(x) - hf'(x) + \frac{1}{2}h^2 f''(x) - \frac{1}{3!}h^3 f^{(3)}(x) + \frac{1}{4!}h^4 f^{(4)}(x) - \cdots$$

$$\therefore\ f(x+h) - f(x-h) = 2hf'(x) + \frac{2}{3!}h^3 f^{(3)}(x) + \frac{2}{5!}h^5 f^{(5)}(x) + \frac{2h^7}{7!}f^{(7)}(x)$$

$f^{(i)}(x)$ are bounded in $[x_0-h, x_0+h]$.

$$\therefore\ f'(x) = \frac{f(x+h) - f(x-h)}{2h} + a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots$$

Here the constants $a_2, a_4, \cdots$ depend on f & x. When such information is available about a numerical process, it is possible to use a powerful technique known as the Richardson's extrapolation.

Let $\phi(h) = \dfrac{f(x+h) - f(x-h)}{2h}$ — (1)

$\therefore \quad f'(x) = \phi(h) + a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots$

i.e. $\phi(h) = f'(x) - a_2 h^2 - a_4 h^4 - a_6 h^6 - \cdots$

& $\phi(h/2) = f'(x) - a_2 (h/2)^2 - a_4 (h/2)^4 - a_6 (h/2)^6 - \cdots$

Now $\phi(h) - 4\phi(h/2) = -3f'(x) - \frac{3}{4} a_4 h^4 - \frac{15}{16} h^6 - \cdots$

$\therefore \quad \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h) = f'(x) + b_4 h^4 + b_6 h^6$

Therefore,

$$\frac{4}{3}\phi(h/2) - \frac{\phi(h)}{3} \quad \text{approximates}$$

$f'(x)$ & the error term is $O(h^4)$

We can continue the process:

Let $\Psi(h) = \frac{4}{3}\phi(h/2) - \frac{\phi(h)}{3}$ — ② where $\phi(h)$ is given by ①

$$\therefore \Psi(h) = f'(a) + b_4 h^4 + b_6 h^6 + \cdots$$

Now $\Psi(h/2) = f'(x) + b_4 \cdot (h/2)^4 + b_6 (h/2)^6 + \cdots$

$$\therefore \Psi(h) - 16\Psi(h/2) = -15 f'(x) - \frac{7}{8} b_6 h^6 - \cdots$$

$$\therefore \frac{16}{15}\Psi(h/2) - \frac{1}{15}\Psi(h) = f'(x) + \frac{7}{8\times15} b_6 h^6 + \cdots$$

We can approximate $f'(x)$ by $\frac{16}{15}\Psi(h/2) - \frac{1}{15}\Psi(h)$

where $\Psi(h)$ is given by ②. The error term is $O(h^6)$. $\boxed{\text{We can repeat this process}}$

Another angle (using Lagrange interpolation polynomial)

We know

Polynomial through $(n+1)$ points. $(x_0, f(x_0))$, $\ldots$, $(x_n, f(x_n))$

is. $P_{0,n}(x) = \sum_{k=0}^{n} L_{n,k}(x) f(x_k)$

where $L_{n,k}(x) = \dfrac{(x-x_0)(x-x_1)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)(x_k-x_1)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)}$

$$= \frac{\prod_{\substack{j=0\\ j\neq k}}^{n} (x-x_j)}{\prod_{\substack{j=0\\ j\neq k}}^{n} (x_k-x_j)} = \prod_{\substack{j=0\\ k\neq j}}^{n} \frac{(x-x_j)}{(x_k-x_j)}$$

~~& $f(x) = P_n(x) +$~~

& $f(x) = P_{0,n}(x) + \dfrac{(x-x_0)(x-x_1)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$

where $\xi \in [x_0, x_n]$.

Now $f(x) = P_{0,1}(x) + \dfrac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$

Where $P_{0,1}(x) = \dfrac{x-x_1}{x_0-x_1} f(x_0) + \dfrac{x-x_0}{x_1-x_0} f(x_1)$

To approximate $f'(x_0)$

Let ~~$x_0 = x$~~ & $x_1 = x_0+h$ & $f \in C^2[x_0, x_0+h]$, $h \neq 0$ & is small.

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

$$\text{Now } f'(x) = \frac{f(x_0)}{-h} + \frac{f(x_0+h)}{h} + \frac{d}{dx}\left[\frac{(x-x_0)(x-(x_0+h))}{2!} f''(\xi(x))\right]$$

$$\Downarrow$$

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

$$= \frac{f(x_0+h)-f(x_0)}{h} + \frac{2(x-x_0)-h}{2!} f''(\xi(x)) + \frac{(x-x_0)^2-(x-x_0)h}{2!} \underbrace{\frac{d}{dx}\left(f''(\xi(x))\right)}_{A}$$

The difficulty is A can not be calculated since we have no information about $D_x f''(\xi(x))$. Can't estimate the truncation error.

But $f'(x_0) = \dfrac{f(x_0+h) - f(x_0)}{h} - \dfrac{h}{2} f''(\xi(x)) \quad — \text{(A)}$

$\therefore$ $\dfrac{f(x_0+h) - f(x_0)}{h}$ is an approximation of $f'(x)$ with truncation error of $\left|\dfrac{h}{2} M\right|$ where M is an upper bound of $f''(x)$ in $[x_0, x_0+h]$.

(h is assumed to be small

(A) is the same as the one using the Taylor series.

<u>Three-point formula</u>

$$f(x) = f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} +$$

$$f(x_2)\cdot\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!} f'''(\xi(x))$$

$$\therefore f'(x) = \frac{f(x_0)}{(x_0-x_1)(x_0-x_2)}(x-x_2+x-x_1) + \frac{f(x_1)}{(x_1-x_0)(x_1-x_2)}\cdot(2x-x_0-x_2)$$

$$+ f(x_2)\cdot\frac{(2x-x_0-x_1)}{(x_2-x_0)(x_2-x_1)} + \frac{1}{6}\Big[(x-x_1)(x-x_2) + (x-x_0)(x-x_2) + (x-x_0)(x-x_1)\Big] f'''(\xi(x))$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_2)}{6} D_x f'''(\xi(x))$$

$$\therefore\; f'(x_j) = \frac{f(x_0)\cdot(2x_j - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)(2x_j - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$+ \frac{f(x_2)(2x_j - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} + \frac{1}{6} f^{(3)}(\xi(x_j)) \cdot \prod_{\substack{k=0 \\ j \neq k}}^{2} (x_j - x_k)$$

Let $x_0 = x_1 - h$ & $x_2 = x_1 + h$

$$\therefore f'(x_1) = \frac{f(x_1-h)(2x_1 - x_1 - x_1 - h)}{(x_1 - h - x_1)(x_1 - h - x_1 - h)}$$

$$+ \frac{f(x_1)(2x_1 - x_1 + h - x_1 - h)}{(x_1 - x_1 + h)(x_1 - x_1 - h)}$$

$$+ \frac{f(x_1+h)(2x_1 - x_1 + h - x_1)}{(x_1 + h - x_1 + h)(x_1 + h - x_1)}$$

$$+ \frac{1}{6} f^3(\xi(x_1)) \cdot (x_1 - x_1 + h)(x_1 - x_1 - h)$$

$$= -\frac{f(x_1-h)}{2h} + \frac{f(x_1) \cdot 0}{\times\times\times} + \frac{f(x_1+h)}{2h} + \frac{1}{6} f^3(\xi(x_1)) \times h^2$$

$$\cancel{-\frac{1}{6} f^3(\xi(x_1))}.$$

$$= \frac{f(x_1+h) - f(x_1-h)}{2h} - \frac{1}{6} h^2 f^3(\xi(x))$$

(Same as Taylor Series)

Summary

$f \in C^2[a,b]$; Interested in computing $f'(x)$ for a given x_0.

Let $h>0$ be a small value < 1.

$f'(x_0)$ can be approximated by examining ~~some~~ the values of $f(x)$ at some points in the neighborhood of x_0, $[x_0-h, x_0+h]$. These values are used ~~to~~ in estimating $f'(x_0)$ with the help of

a) Taylor polynomial, or

b) Lagrange polynomial.

Approximation	Error term
1. $f'(x_0) \approx \dfrac{f(x_0+h)-f(x_0)}{h}$ (forward difference formula)	$O(h)$
2. $f'(x_0) \approx \dfrac{f(x_0-h)-f(x_0)}{-h}$ (Backward difference formula)	$O(h)$
3. $f'(x_0) \approx \dfrac{f(x_0+h)-f(x_0-h)}{2h}$	$O(h^2)$
4. $f'(x_0) \approx \frac{4}{3}\phi(h/2) - \frac{1}{3}\phi(h)$ where $\phi(h) = \dfrac{f(x_0+h)-f(x_0)}{2h}$	$O(h^4)$
5. $f'(x_0) \approx \frac{16}{15}\psi(h/2) - \frac{1}{15}\psi(h)$ where $\psi(h) = \frac{4}{3}\phi(h/2) - \frac{\phi(h)}{3}$	$O(h^6)$

- These results can be obtained using Taylor equation & Richardson extrapolation.
- Lagrange polynomial also can be used.