**Example** For $f(x)=\tan^{-1}x$, estimate $f'(\sqrt{2})$ using a sequence of $h \to 0$. $\left( f'(x) = \frac{1}{1+x^2} \text{ so } f'(\sqrt{2}) = \frac{1}{3} \right)$

Using $h = 2^{-k}$, set $r = \dfrac{f(\sqrt{2}+h) - f(\sqrt{2})}{h}$

| $k$ | $h$ | $r$ |
|---|---|---|
| 4 | $0.62 \cdot 10^{-1}$ | 0.32374 |
| 12 | $0.24 \cdot 10^{-3}$ | 0.33325 $\approx 1/3$ |
| 20 | $0.95 \cdot 10^{-6}$ | 0.31250 |
| 24 | $0.60 \cdot 10^{-7}$ | 1.00000 |
| 26 | $0.15 \cdot 10^{-7}$ | 0.00000 |

(Why do we see $r=0$?)

Error $= \mathcal{O}(h)$!

Error $= \mathcal{O}(h^2)$ would work better:

Note
$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \overbrace{\frac{h^3}{3!} f'''(y_1)}^{\text{Error}}$$
$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \underbrace{\frac{h^3}{3!} f'''(y_2)}$$

$$\Rightarrow f(x+h) - f(x-h) = 2h f'(x) + \frac{h^3}{3!}\left(f'''(y_1) + f'''(y_2)\right)$$

$$\Rightarrow f'(x) = \underbrace{\frac{1}{2h}\left(f(x+h) - f(x-h)\right)}_{\text{Estimate}} - \underbrace{\frac{h^2}{12}\left(f'''(y_1) + f'''(y_2)\right)}_{\text{Error}}$$

Error $= \mathcal{O}(h^2)$ but applicable only if $f'''$ exists.

In fact, if $f \in C^3[x-h, x+h]$ then

$$\exists\ x-h < y < x+h \text{ s.t. } \frac{f'''(y_1) + f'''(y_2)}{2} = f'''(y)$$ (Why?)

Then
$$f'(x) = \underbrace{\frac{1}{2h}\left(f(x+h) - f(x-h)\right)}_{\text{"formula"}} - \underbrace{\frac{h^2}{6} f'''(y)}_{\text{Error}}$$

(Similarly, we can obtain
$$f''(x) = \frac{1}{h^2}\left(f(x+h) - 2f(x) + f(x-h)\right) - \frac{h^2}{12} f^{(4)}(y) \text{ )}$$

**Example** For $f(x)=\tan^{-1}x$, estimate $f'(\sqrt{2})$ using a sequence of $h \to 0$. (Recall $f'(\sqrt{2}) = \frac{1}{3}$)

Using $h = 2^{-k}$, set $r = \dfrac{f(\sqrt{2}+h) - f(\sqrt{2}-h)}{2h}$

| $k$ | $h$ | $r$ |
|---|---|---|
| 2 | 0.25 | 0.33719 |
| 10 | $0.98 \cdot 10^{-3}$ | 0.33334 $\approx 1/3$ |
| 18 | $0.38 \cdot 10^{-5}$ | 0.32813 |
| 26 | $0.15 \cdot 10^{-7}$ | 0.00000 |

Note that even if we compute $x \pm h$ very accurately, the error in $f(x \pm h)$ (or $f(x+h) - f(x-h)$) gets multiplied by $\frac{1}{2h}$. This magnifies the error since $h$ is very small. Thus, we should be very careful with numerical differentiation of empirical data. In fact, we should avoid it if possible.

Differentiation via Polynomial Interpolation

Recall: Lagrange form of interpolation polynomial

$$p(x) = \sum_{i=0}^{n} f(x_i)\, \ell_i(x) \qquad \text{where } \ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

Recall: Thm 2 of Section 6.1:

$y_x$ depends on $x$! $\quad \frac{dy_x}{dx}$ not necessarily 0.

$$f(x) = p(x) + \underbrace{\frac{1}{(n+1)!} f^{(n+1)}(y_x)\, w(x)}_{\text{Error}} \qquad \text{where } w(x) = \prod_{i=0}^{n} x - x_i$$

$$\Rightarrow f'(x) = \sum_{i=0}^{n} f(x_i)\, \ell_i'(x) + \frac{1}{(n+1)!} \frac{d}{dx}\left(f^{(n+1)}(y_x)\right) w(x) + \frac{1}{(n+1)!} f^{(n+1)}(y_x)\, w'(x).$$

Since $w(x) = \prod_{i=0}^{n} (x - x_i)$, ① $w(x_k) = 0$

② $w'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j)$

$$\left(f_1(x) f_2(x) f_3(x) \cdots f_n(x)\right)' = f_1'(x) f_2(x) \cdots f_n(x) + f_1 f_2' f_3 \cdots f_n + \cdots + f_1 f_2 \cdots f_n'$$

② $\Rightarrow$ ③ $w'(x_k) = \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j)$

$$\text{① \& ③} \Rightarrow f'(x_k) = \underbrace{\sum_{i=0}^{n} f(x_i)\, \ell_i'(x_k)} + \underbrace{\frac{f^{(n+1)}(y_{x_k})}{(n+1)!} \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j)}$$

**Example**: $(n=2,\ k=1)$ $\quad x_0, x_1, x_2$

$$\ell_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \qquad \ell_0'(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

$$\ell_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \quad \Rightarrow \quad \ell_1'(x) = \frac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}$$

$$\ell_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \qquad \ell_2'(x) = \frac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}$$

$$\ell_0'(x_1) = \frac{x_1 - x_2}{(x_0-x_1)(x_0-x_2)}$$

$$\Rightarrow \ell_1'(x_1) = \frac{2x_1 - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}$$

$$\ell_2'(x_1) = \frac{x_1 - x_0}{(x_2-x_0)(x_2-x_1)}$$

Thus,
$$f'(x_1) = f(x_0)\frac{x_1 - x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{2x_1 - x_0 - x_2}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{x_1 - x_0}{(x_2-x_0)(x_2-x_1)} + \text{Error}$$

$(x_1 - x_0) + (x_1 - x_2)$

where $\text{Error} = \frac{1}{6} f'''(y_x)(x_1-x_0)(x_1-x_2)$ $\qquad \omega'(x_1) = (x_1-x_0)(x_1-x_2)$

Example Say $x_0, x_1, x_2$ are equally spaced, that is $x_0 = x_1 - h$, $x_2 = x_1 + h$ for some $h > 0$. Then

$$f'(x_1) = f(x_1-h)\frac{(-h)}{(-h)(-2h)} + f(x_1)\frac{\cancel{h-h}^{\,0}}{-h\cdot h} + f(x_1+h)\frac{h}{2h(h)} + \frac{1}{6} f'''(y_x)\, h\, h$$

or
$$= \frac{f(x_1+h) - f(x_1-h)}{2h} + \frac{1}{6} f'''(y_x) h^2 \quad \text{as before!}$$

## Richardson Extrapolation

Taylor series: $f(x+h) = \sum_{k=0}^{\infty} \frac{1}{k!} h^k f^{(k)}(x) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{3!}h^3 \ldots$

$f(x-h) = \sum_{k=0}^{\infty} \frac{1}{k!}(-h)^k f^{(k)}(x) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{3!}h^3 \ldots$

$\Rightarrow f(x+h) - f(x-h) = 2f'(x)h + \frac{f'''(x)}{3}h^3 + O(h^5)$

$$\Rightarrow \underbrace{f'(x)}_{\text{Quantity of interest}} = \underbrace{\frac{f(x+h) - f(x+h)}{2h}}_{\text{Estimate with param. } h} \underbrace{- \frac{f'''(x)}{3}h^2 + O(h^4)}_{\text{Error term in powers of } h \,=\, O(h^2)}$$

$\rightarrow L = \varphi(h) + \underbrace{a_2 h^2}_{} + \underbrace{a_4 h^4 + a_6 h^6 + \cdots}_{} \quad \forall h$

$\Rightarrow L = \varphi\left(\frac{h}{2}\right) + \underbrace{a_2 \frac{h^2}{4}}_{} + a_4 \frac{h^4}{16} + a_6 \frac{h^6}{4^3} + \cdots$

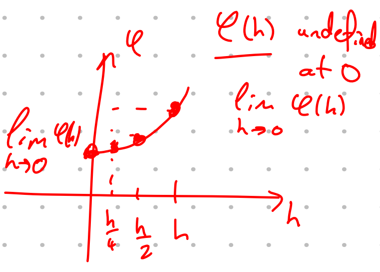
$\Rightarrow \underset{3L}{4L - L} = 4\varphi\left(\frac{h}{2}\right) - \varphi(h) + 4a_2\frac{h^2}{4} - a_2 h^2 + \frac{4a_4 h^4}{16} - a_4 h^4 + \frac{4a_6 h^6}{2^6} - a_6 h^6 \ldots$

$$\Rightarrow L = \underbrace{\frac{4}{3}\varphi\left(\frac{h}{2}\right) - \frac{1}{3}\varphi(h)}_{\text{formula for } L} \underbrace{- \frac{1}{4}a_4 h^4 - \frac{5}{16}a_6 h^6 - \cdots}_{\text{Error } = O(h^4)}$$

$L = \psi(h) + b_4 h^4 + b_6 h^6 + b_8 h^8 + \cdots$ where $\psi(h) = \frac{4}{3}\varphi\left(\frac{h}{2}\right) - \frac{1}{3}\varphi(h)$

$\Rightarrow L = \psi\left(\frac{h}{2}\right) + b_4\frac{h^4}{4^2} + b_6\frac{h^6}{4^3} + \cdots$

$\Rightarrow 4^2 L - L = 4^2\psi\left(\frac{h}{2}\right) - \psi(h) + O(h^6)$




$$\Rightarrow L = \underbrace{\frac{4^2\psi\left(\frac{h}{2}\right)}{4^2-1} - \frac{\psi(h)}{4^2-1}}_{\text{formula for } L} + \underbrace{O(h^6)}_{\text{Error term}}$$

$L = \theta(h) + O(h^6)$ where $\theta(h) = \frac{16\psi\left(\frac{h}{2}\right)}{15} - \frac{\psi(h)}{15}$

The same process can be repeated over and over again to produce error terms with higher powers of $h$.

This is called the Richardson extrapolation.

The algorithm:

$M$: number of steps, $\varphi$: the initial "formula"

1. Select a value for $h$ (e.g. $h=1$)

   for $0 \le n \le M$, compute $D(n,0) = \varphi(h/2^n)$.

2. for $k = 1$ to $M$ $\qquad$ (the second param represents which "formula" we are using $\varphi, \psi, \theta, \ldots$)

   for $n = k$ to $M$

   $$D(n,k) = \frac{4^k}{4^k-1} D(n,k-1) - \frac{1}{4^k-1} D(n-1,k-1)$$

   end for

end for

$D(1,1) = \frac{4}{3}\varphi\left(\frac{h}{2}\right) - \frac{1}{3}\varphi(h) = \psi(h)$

e.g. $D(0,0) = \varphi(h)$

$D(1,0) = \varphi\left(\frac{h}{2}\right) \rightarrow D(1,1) = \psi(h)$

$D(2,0) = \varphi\left(\frac{h}{4}\right) \rightarrow D(2,1) = \psi\left(\frac{h}{2}\right) \rightarrow D(2,2) = \theta(h)$

**Thm** (on Richardson extrapolation)

$D(n,k-1) = L + O(h^{2k})$ as $h \to 0$

more precisely,

$$D(n,k-1) = L + \sum_{j=k}^{\infty} A_{jk}\left(\frac{h}{2^n}\right)^{2j}$$

Example Approximate $\left.\frac{d}{dx}\tan^{-1}x\right|_{x=\sqrt{2}}$

| n | D(n,0) | D(n,1) | D(n,2) | D(n,3) |
|---|---|---|---|---|
| 0 | 0.39269 91 | | | |
| 1 | 0.34877 10 | 0.33412 83 | | |
| 2 | 0.33719 38 | 0.33333 48 | 0.33328 19 | |
| 3 | 0.33429 81 | 0.33333 29 | 0.33333 28 | 0.33333 36 |

Warning: Richardson extrapolation is still vulnerable to subtractive cancellation.

## 7.2 Numerical Integration Based on Interpolation

FTC: If $h$ is an antiderivative of $f$, $\int_a^b f(x)dx = h(b) - h(a)$

However, many elementary functions do not have simple antiderivatives.

e.g. $\int e^{x^2}dx = \sum_{k=0}^{\infty} \frac{x^{2k+1}}{(2k+1)k!} + C$ $\quad \left(e^{x^2} = \sum \frac{x^{2k}}{k!}\right)$

Computing the Taylor series is also not always possible
e.g. if we only know $(x, f(x))$ at finitely many points.

One robust strategy is replace $f$ with $g$ s.t. $g \approx f$ and $g$ is easy to integrate. Of course, we will use polynomial interpolation.

Given $[a,b]$, we select nodes $x_0, x_1, \dots, x_n$. Then

$$f(x) \approx p(x) = \sum_{i=0}^{n} f(x_i)\,\ell_i(x)$$

$$\Rightarrow \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} f(x_i) \int_a^b \ell_i(x)\,dx$$

Set $A_i = \int_a^b \ell_i(x)\,dx$. Then $\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$

Note that $A_i$ is independent of $f$! so the formula

$$(*) \quad \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i)$$

can be used on any function $f$!

If $x_0, x_1, \dots, x_n$ are equally spaced, $(*)$ is called a Newton-Cotes formula.

Trapezoid Rule

If $n=1$, $x_0 = a$, $x_1 = b$, then

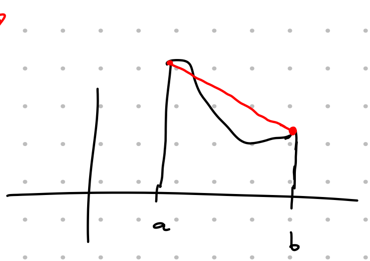
$$\ell_0(x) = \frac{b-x}{b-a} \qquad \ell_1(x) = \frac{x-a}{b-a}$$

$$\Rightarrow A_0 = \int_a^b \ell_0(x)\,dx = -\frac{1}{2}\frac{(b-x)^2}{(b-a)}\Big|_a^b = \frac{1}{2}(b-a)$$

$$A_1 = \int_a^b \ell_1(x)\,dx = \frac{1}{2}\frac{(x-a)^2}{(b-a)}\Big|_a^b = \frac{1}{2}(b-a)$$

Thus, the quadrature formula is → a formula that gives the area.

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f(a) + f(b)\right]$$




$$\left(\text{Error} = -\frac{1}{12}(b-a)^3 f''(y) \qquad y \in (a,b)\right)$$