Can we do better than $O(h)$?

Try step of $h/2$

$$f(x+h/2) = f(x) + \frac{h}{2} f'(x) + \frac{h^2}{2^2 \cdot 2} f''(x) + \frac{h^3}{2^3 \cdot 6} f'''(x) + \ldots$$

$$f(x-h/2) = f(x) - \frac{h}{2} f'(x) + \frac{h^2}{8} f''(x) + \ldots$$

Subtract and solve for $f'(x)$

$$f'(x) = \frac{f(x+h/2) - f(x-h/2)}{h} \underbrace{- \frac{h^2}{24} f'''(x) + \ldots}_{+ O(h^2)}$$

"Central difference approx"

$O(h^2) \ll O(h)$ since $h \ll 1$

$\mathcal{E}_{ro}$ same as before but $\mathcal{E}_{app} = \frac{h^2}{24} |f'''(x)|$

$$\mathcal{E}_{TOT} = q h^2 + p/h$$

[ See code example using

$$f(x) = e^{\sin(2x)}$$

$$f'(x) = 2 \cos(2x) e^{\sin(2x)}$$ ]

Can we do better than $\Theta(h)$ for forward diff approx?

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \dots$$

$$\left[ f(x+h/2) = f(x) + \frac{h}{2} f'(x) + \frac{h^2}{8} f''(x) + \dots \right] -4 \quad \text{add}$$

$$f(x+h) - 4 f(x+h/2) = -3f(x) - h f'(x) + O(h^3)$$

$$f'(x) = \frac{4 f(x+h/2) - f(x+h) - 3f(x)}{h} + \Theta(h^2)$$

We improved forward diff to $\Theta(h^2)$ but now we require 3 evaluations of function

Trade off in precision vs computing time

## Calculate 2nd derivative

Look at central diff again

$$f(x+h/2) = f(x) + \frac{h}{2} f'(x) + \frac{h^2}{8} f''(x) + \frac{h^3}{48} f'''(x) + \frac{h^4}{384} f^{(4)}(x)$$

$$+ \left[ f(x-h/2) = f(x) - \frac{h}{2} f'(x) + \frac{h^2}{8} f''(x) - \frac{h^3}{48} f^{(3)}(x) + \frac{h^4}{384} f^{(4)}(x) \right]$$

$$f(x+h/2) + f(x-h/2) = 2f(x) + \frac{h^2}{4} f''(x) + \frac{h^4}{192} f^{(4)}(x) + \dots$$

$$f''(x) = 4\, \frac{f(x+h/2) + f(x-h/2) - 2f(x)}{h^2} + \Theta(h^2)$$

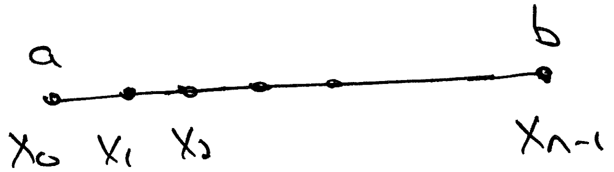
## Practical Considerations

Often we are given $n$ data points of the form $(x_i, f(x_i))$ $i = 0, 1, \dots n-1$

We don't choose the grid or spacing

usually equally spaced so $x_i = a + ih$

$$h = \frac{b-a}{n-1}$$




For example, let $x_i$ be 101 points from 0 to 5 $\Rightarrow$ $h = 5/100 = 0.05$

$(0, 0.05, 0.10, 0.15, \dots 4.95, 5.00)$

We want $f'(3.7)$

forward diff $\quad f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h} + O(h)$

great, use $f(3.75)$ and $f(3.70)$ to get $f'(3.70)$ and $h = 0.05$

central diff $\quad f'(x_i) = \dfrac{f(x_{i+1/2}) - f(x_{i-1/2})}{h} + O(h^2)$

We need $f(3.75 \pm \frac{0.05}{2})$, don't have them!

We can choose to use $h = 0.10$ in our central diff formula

then we need $f(3.65)$ and $f(3.75)$ to get $f'(3.70)$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \quad h = 0.05$$

[Also works for 2nd deriv central diff

$$f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2} + O(h^2)$$
]

We saw central diff more precise than forward diff when using same step $h$

You can show that central diff should still typically be better using $2h$ as well (can depend specifically on function)

# Richardson Extrapolation

Method to improve accuracy of numerical algorithm

Let's say we want to calculate $G$ (deriv., integral, ...)

$G$ is true or exact answer

We'll call our approximation of $G$, $g(h)$

where $h$ is a small param (step size) $g$ depends on

(like $dx$ for our integral)

$$G = \underbrace{g(h) + \varepsilon_{app}(h)}$$

error term also depends on $h$

Assume $\quad G = g(h) + Ah^p + Bh^{p+q} + Ch^{p+2q} + \ldots$

$A, B, C$ constants

$p$ is order of leading error term

$q$ is increment in order for next terms

Step size $h$ : $\quad G = g(h) + Ah^p + O(h^{p+q})$

step size $h/2$ : $\quad G = g(h/2) + A(h/2)^p + O(h^{p+q})$

$$g(h) + Ah^p = g(h/2) + A(h/2)^p + O(h^{p+q})$$

$$Ah^p = \frac{2^p}{2^p - 1}\left[g(h/2) - g(h)\right] + O(h^{p+q})$$

$$G = g(h) + Ah^p + O(h^{p+q}) \quad (1)$$

$$G = g(h) + \frac{2^p}{2^p - 1}\left[ g(h/2) - g(h) \right] + O(h^{p+q})$$

$$G = \frac{2^p g(h/2) - g(h)}{2^p - 1} + O(h^{p+q}) \quad (2)$$

(1) We started with method to get $G$ with uncertainty ~~$O(h^{p+q})$~~ $O(h^p)$

(2) We ended with $O(h^{p+q})$

Ex Forward Diff

$$g(h) \equiv D_{fd}(h) = \frac{f(x+h) - f(x)}{h} + O(h)$$

$$\Rightarrow p = 1$$

$$G_{fd} = \frac{2^p D_{fd}(h/2) - D_{fd}(h)}{2^p - 1} = 2D_{fd}(h/2) - D_{fd}(h)$$

$$= 2\,\frac{f(x+\frac{h}{2}) - f(x)}{h/2} - \frac{f(x+h) - f(x)}{h} + O(h^2)$$

$$= \frac{4f(x+h/2) - f(x+h) - 3f(x)}{h} + O(h^2)$$

Same result we found on 3-5 for (second) forward diff formula!