

Numerical Differentiation

$$f(x) = x^3 + x^2 + x$$

- What's the order of magnitude of $f(x)$?
- $f(10^{10}) = 10^{30} + 10^{20} + 10^{10} \approx 10^{30}$
- $f(10^{-10}) = 10^{-30} + 10^{-20} + 10^{-10} \approx 10^{-10}$

Richardson Extrapolation

- Suppose

$$L = A(h) + a_1 h^{k_1} + a_2 h^{k_2} + a_3 h^{k_3} + \dots$$

where

- L is a quantity we want to estimate;
- $A(h)$ is an approximation to L ;
- $\lim_{h \rightarrow 0} A(h) = L$;
- a_1, a_2, a_3, \dots may be unknown;
- but k_1, k_2, k_3, \dots are known; and $k_1 < k_2 < k_3 < \dots$

- Example: if f is analytic, then (from Taylor series):

$$f(c+h) = f(c) + f'(c)h + \frac{f''(c)}{2!}h^2 + \frac{f'''(c)}{3!}h^3 + \dots$$

$$f'(c) = \frac{f(c+h) - f(c)}{h} - \frac{f''(c)}{2!}h - \frac{f'''(c)}{3!}h^2 - \dots$$

which has the form

$$L = A(h) + a_1h^{k_1} + a_2h^{k_2} + a_3h^{k_3} + \dots$$

- Since $\lim_{h \rightarrow 0} A(h) = L$,
we may expect to get a better and better approximation with a smaller and smaller h .
- That is not always the case because of limited machine precision and rounding error.
- Now suppose we have computed a sequence of approximations to L ,

$$A(h), A\left(\frac{h}{2}\right), A\left(\frac{h}{2^2}\right), A\left(\frac{h}{2^3}\right), \dots, A\left(\frac{h}{2^n}\right).$$

- Richardson extrapolation is a method to compute an improved approximation from these values.

- Write $A(h)$ as $A_0(h)$.

- Since

$$L = A_0(h) + a_1h^{k_1} + a_2h^{k_2} + a_3h^{k_3} + \dots$$

the error of $A_0(h)$ as an approximation to L is in the order of $O(h^{k_1})$.

- We want to obtain a better approximation $A_1(h)$ with error in the order of $O(h^{k_2})$.
- The idea is to eliminate the $a_1h^{k_1}$ term.

$$(1) \quad L = A_0(h) + a_1 h^{k_1} + a_2 h^{k_2} + a_3 h^{k_3} + \dots$$

$$(2) \quad L = A_0\left(\frac{h}{2}\right) + a_1 \left(\frac{h}{2}\right)^{k_1} + a_2 \left(\frac{h}{2}\right)^{k_2} + a_3 \left(\frac{h}{2}\right)^{k_3} + \dots$$

Multiply the second equation by 2^{k_1} :

$$(3) \quad 2^{k_1} L = 2^{k_1} A_0\left(\frac{h}{2}\right) + a_1 h^{k_1} + 2^{k_1} a_2 \left(\frac{h}{2}\right)^{k_2} + 2^{k_1} a_3 \left(\frac{h}{2}\right)^{k_3} + \dots$$

Subtract, and then divide by $(2^{k_1} - 1)$:

$$L = \left(\frac{2^{k_1} A_0\left(\frac{h}{2}\right) - A_0(h)}{2^{k_1} - 1} \right) + b_2 h^{k_2} + b_3 h^{k_3} + \dots$$

$$= A_1(h) + b_2 h^{k_2} + b_3 h^{k_3} + \dots$$

Now,

$$L = A_1(h) + b_2 h^{k_2} + b_3 h^{k_3} + b_4 h^{k_4} + \dots$$

Repeat the same process,

$$\begin{aligned} L &= \left(\frac{2^{k_2} A_1\left(\frac{h}{2}\right) - A_1(h)}{2^{k_2} - 1} \right) + c_3 h^{k_3} + c_4 h^{k_4} + \dots \\ &= A_2(h) + c_3 h^{k_3} + c_4 h^{k_4} + \dots \\ &\vdots \\ &= A_n(h) + s_{n+1} h^{k_{n+1}} + s_{n+2} h^{k_{n+2}} + \dots \end{aligned}$$

$$A_j\left(\frac{h}{2^i}\right) = \frac{2^{k_j} A_{j-1}\left(\frac{h}{2^{i+1}}\right) - A_{j-1}\left(\frac{h}{2^i}\right)}{2^{k_j} - 1}$$

$$\begin{array}{cccccc}
A_0(h) & & & & & \\
A_0\left(\frac{h}{2}\right) & A_1(h) & & & & \\
A_0\left(\frac{h}{2^2}\right) & A_1\left(\frac{h}{2}\right) & A_2(h) & & & \\
A_0\left(\frac{h}{2^3}\right) & A_1\left(\frac{h}{2^2}\right) & A_2\left(\frac{h}{2}\right) & A_3(h) & & \\
\vdots & \vdots & \vdots & \vdots & \ddots & \\
A_0\left(\frac{h}{2^n}\right) & A_1\left(\frac{h}{2^{n-1}}\right) & A_2\left(\frac{h}{2^{n-2}}\right) & A_3\left(\frac{h}{2^{n-3}}\right) & \cdots & A_n(h)
\end{array}$$

$$L = A(h) + a_1 h^{k_1} + a_2 h^{k_2} + a_3 h^{k_3} + \dots = D(n, n) + O(h^{k_{n+1}})$$

$A(h) = D(0, 0)$					
$A(h / 2) = D(1, 0)$	$D(1, 1)$				
$A(h / 2^2) = D(2, 0)$	$D(2, 1)$	$D(2, 2)$			
$A(h / 2^3) = D(3, 0)$	$D(3, 1)$	$D(3, 2)$	$D(3, 3)$		
\vdots	\vdots	\vdots	\vdots	\ddots	
$A(h / 2^n) = D(n, 0)$	$D(n, 1)$	$D(n, 2)$	$D(n, 3)$	\dots	$D(n, n)$

$$D(i, 0) = A\left(\frac{h}{2^i}\right). \quad D(i, j) = \frac{2^{k_j} D(i, j-1) - D(i-1, j-1)}{2^{k_j} - 1}$$

$A_j\left(\frac{h}{2^i}\right)$ is stored in $D(i + j, j)$

Numerical Differentiation

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- Derivative:

$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

- Numerical approximation:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

- Error:

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

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

Applying Richardson Extrapolation

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x)}{h} - \frac{f''(x)}{2!} h - \frac{f'''(x)}{3!} h^2 - \dots \\ &= A(h) + a_1 h + a_2 h^2 + a_3 h^3 + \dots \end{aligned}$$

- Let $A(h) = \frac{f(x+h) - f(x)}{h}$, and apply Richardson's extrapolation, we can kill the h, h^2, \dots, h^n terms, improving the error from $O(h)$ to $O(h^{n+1})$.
- We can do even better than this.

Derivative Formula Using Central Differences

$$(1) \quad f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \dots$$

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

(1) - (2):

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

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(x)}{3!}h^2 - \frac{f^{(5)}(x)}{5!}h^4 - \dots$$

Applying Richardson Extrapolation

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(x)}{3!}h^2 - \frac{f^{(5)}(x)}{5!}h^4 - \dots \\ &= A(h) + a_1h^2 + a_2h^4 + a_3h^6 + \dots \end{aligned}$$

- Let $A(h) = \frac{f(x+h) - f(x-h)}{2h}$, and apply Richardson's extrapolation, we can kill the h^2, h^4, \dots, h^{2n} terms, improving the error from $O(h^2)$ to $O(h^{2n+2})$.

$$f'(x) = A(h) + a_1 h^2 + a_2 h^4 + a_3 h^6 + \dots = D(n, n) + O(h^{2n+2})$$

$A(h) = D(0,0)$					
$A(h/2) = D(1,0)$	$D(1,1)$				
$A(h/2^2) = D(2,0)$	$D(2,1)$	$D(2,2)$			
$A(h/2^3) = D(3,0)$	$D(3,1)$	$D(3,2)$	$D(3,3)$		
\vdots	\vdots	\vdots	\vdots	\ddots	
$A(h/2^n) = D(n,0)$	$D(n,1)$	$D(n,2)$	$D(n,3)$	\dots	$D(n,n)$

$$D(i,0) = A\left(\frac{h}{2^i}\right). \quad D(i,j) = \frac{4^j D(i, j-1) - D(i-1, j-1)}{4^j - 1}$$

Example

Suppose $f(x) = \cos(x^2)$. $f'(3) = ?$

$$f'(x) \approx A(h) = \frac{f(x+h) - f(x-h)}{2h}, \text{ with } x = 3.$$

Richardson: Let $h = 1/8 = 0.125$ and $n = 3$.

$$D(0,0) = A(h) = \frac{f(3+0.125) - f(3-0.125)}{2 \times 0.125} = -2.1694235858$$

$$D(1,0) = A(h/2) = -2.3942868807$$

$$D(2,0) = A(h/2^2) = -2.4529392187$$

$$D(3,0) = A(h/2^3) = -2.4677575849$$

Richardson extrapolation:

-2.1694235858			
-2.3942868807	-2.4692413123		
-2.4529392187	-2.4724899981	-2.4727065772	
-2.4677575849	-2.4726970403	-2.4727108431	-2.4727109108

- Correct value as computed from $f'(x) = -2x \sin(x^2)$ is

$$f'(3) = -2.47271091145054$$

Second Derivative

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

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

Add the two equations:

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

Rearrange:

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

Again, we can apply Richardson's extrapolation.