Differentiation

Newton's formula for a derivative computation is

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

In numerical computations, we take *h* small. Note that the smallness of h is limited by the numerical precision. We will discuss this issue later.

Following Newton, we can derive a formula:

$$f'(x_{i-1}) \approx \frac{f_i - f_{i-1}}{h_i} \qquad (1)$$

Using three points, we obtain

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h}, \qquad (2)$$

which is more accurate than Eq. (1).

We will show below how to derive formulae to compute derivatives.

Ref: Ferziger

We start with Lagrange polynomial with two points (x_{i-1},x_i):

$$f(x) = \frac{x - x_{1-1}}{x_i - x_{i-1}} f_i + \frac{x - x_i}{x_{i-1} - x_i} f_{i-1}$$

The derivative of the above function is

$$f'(x_{i-1}) \approx D_+ f \approx \frac{f_i - f_{i-1}}{h_i} \quad \text{Forward difference}$$

$$f'(x_i) \approx D\_f \approx \frac{f_i - f_{i-1}}{h_i} \quad \text{Backward difference}$$

where $h_i = x_i - x_{i-1}$. Here forward difference means the derivative computed at x_{i-1} using x_i as the additional point. The backward difference is the derivative computation at x_i using x_{i-1} as the additional point. Note that the derivatives at both the points are equal, which is because the interpolated function is linear.

Now we approximate the function using a polynomial passing through three points:

$$f(x) = \frac{(x-x_i)(x-x_{i+1})}{(h_i+h_{i+1})(h_i)} f_{i-1} + \frac{(x-x_{i-1})(x-x_{1+1})}{h_i(-h_{i+1})} f_i + \frac{(x-x_{i-1})(x-x_i)}{(h_i+h_{i+1})(h_{i+1})} f_{i+1} \qquad (2)$$

The derivative of the above function at x_i is

$$f'(x_i) = -\frac{h_{i+1}}{(h_i + h_{i+1})(h_i)} f_{i-1} + \left(\frac{1}{h_{i+1}} - \frac{1}{h_i}\right) f_i$$

$$+\frac{h_i}{(h_i + h_{i+1})(h_{i+1})} f_{i+1}$$

Note that the derivatives of the function at xi-1 and xi+1 would be different.

Let us illustrate these derivatives for a special case:
$h_i = h_{i+1} = h$

$$f'(x_{i-1}) = D_+ f = \frac{-3f_{i-1} + 4f_i - f_{i+1}}{2h} \quad \text{Forward difference}$$

$$f'(x_{i+1}) = D_- f = \frac{f_{i-1} - 4f_i + 3f_{i+1}}{2h} \quad \text{Backward difference}$$

$$f'(x_i) = \frac{1}{2}(D_+ + D_-)f = \frac{f_{i+1} - f_{i-1}}{2h} \quad \text{Central difference}$$

The second derivative of Eq. (2) yields

$$f''(x_i) = \frac{2}{(h_i + h_{i+1})(h_i)} f_{i-1} - \frac{2}{h_i h_{i+1}} f_i$$

$$+\frac{2}{(h_i + h_{i+1})(h_{i+1})} f_{i+1}$$

For equal interval

$$f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} = D_+ D_- f = D_- D_+ f$$

Derivative	f_{i-2}	f_{i-1}	f_i	f_{i+1}	f_{i+2}	Error
Forward			-1	1		
hf’			-3	4	-1	$O(h^2)$
2hf’			1	-2	1	$O(h^2)$
hf”		-1	1			$O(h)$
Backward						
hf’	1	-4	3			$O(h^2)$
2hf’	1	-2	1			$O(h^2)$
hf”		-1	0	1		$O(h)$
Central						
hf’		-1	0	`1		$O(h^2)$
2hf’	1	-8	0	-8	1	$O(h^4)$
hf”		1	-2	1		$O(h^2)$
$12h^2$ f”	-1	16	-30	16	1	$O(h^4)$

Error

Error in interpolation is $E = f(x) - P(x) = \frac{f^{(n)}(\zeta)}{n!}\prod_i (x - x_i)$

Therefore, error in the derivative computation is

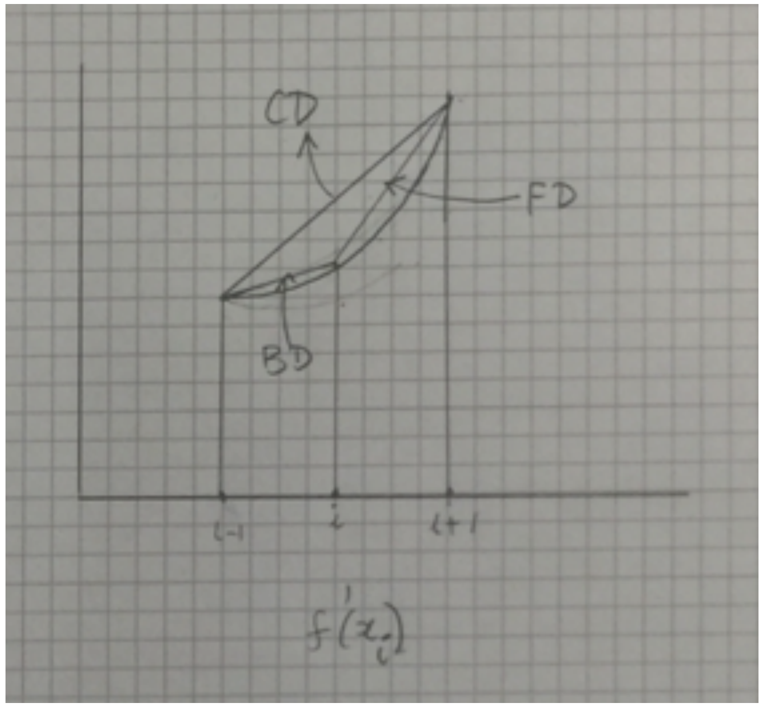
$$E = \frac{f^{(n)}(\zeta)}{n!}\frac{d}{dx}\prod_i (x - x_i)$$

When we compute the above error at x_j, we obtain

$$E_j = \frac{f^{(n)}(\zeta)}{n!}\prod_{i,i\neq j} (x_j - x_i)$$

For equidistant points, $E_j \sim h^{n-1}$

We list the coefficients in the following table (refer to Ferziger)



In Figure 1 se illustrate the numerical derivative computations graphically. Here we compute the derivatives at $x=x_i$. The FD and BD are done using two points.

Derivation using Taylor Series

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2} f''(x) \pm \ldots.$$

$$af(x-h) + bf(x) + cf(x+h)$$

$$= (a+b+c)f(x) + (c-a)hf'(x) + (c+a)\frac{h^2}{2} f''(x)$$

$$+(c-a)\frac{h^3}{6} f'''(x) + HOT$$

Three unknowns a,b,c: Obtain three equations.

$$a + b + c = 0$$

$$c - a = 1/h$$

$$c + a = 0$$

Solution: $b = 0; c = 1/2; a = -1/2.$

Hence

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h}$$

Error: $\frac{h^2}{6} f'''(x)$

Note: $\frac{f(x_i) - f(x_{i-1})}{h_i} = f'(x_i) - \frac{h_i}{2} f''(x_i) + HOT$

So central difference is more accurate.

If we employ higher-order scheme with very small h, the error would be of higher power of h, which could be of the order of machine precision. Hence it is customary that we do not use very high order scheme, which is also expensive computationally. We typically employ 4th order schemes for accurate schemes.

Example exp(x)