Numerical Differentiation

Numeric differentiation is the computation of values of the derivative of a function *f(x)* from given values of *f(x)*. Numeric differentiation should be avoided whenever possible. Whereas integration is a smoothing process and is not very sensitive to small inaccuracies in function values, differentiation tends to make matters rough and generally gives values of that are much less accurate than those of *f(x)*. The difficulty with differentiation is tied in with the definition of the derivative, which is the limit of the difference quotient, and, in that quotient, you usually have the difference of a large quantity divided by a small quantity. This can cause numerical instability. While being aware of this caveat, we must still develop basic differentiation formulas for use in numeric solutions of differential equations.

The derivation of the finite difference approximations for the derivatives of *f(x)* is based on forward and backward Taylor series expansions of *f(x)* about x.

Finite difference formulas

Three forms are commonly considered: forward, backward, and central differences.

A **forward difference** is an expression of the form $f(x+h)-f(x)$

A **backward difference** uses the function values at *x* and *x*−*h*, instead of the values at *x*+*h* and *x*: $f(x)-f(x-h)$

Finally, the **central difference** is given by $f(x+h/2)-f(x-h/2)$

The corresponding approximations to the first derivative are:

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

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

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

It should be noticed that the truncation error of the centered difference is of the order of h^2 in contrast to the forward and backward approximations that are of the order of h.

Despite their practical popularity, finite difference formulas have been harshly criticized by some researchers, because their simplicity must be set against the fact that their accuracy is low - in rough terms, calculations in six-digit precision will produce a slope of only three-digit precision.

An important consideration in practice when the function is calculated using floating point arithmetic is how small a value of h to choose. If chosen too small, the subtraction will yield a large rounding error. In fact all the finite difference formulae are ill-conditioned and due to cancellation will produce a value of zero if h is small enough. If too large, the calculation of the slope of the secant line will be more accurately calculated, but the estimate of the slope of the tangent by using the secant could be worse.

Finite Difference coefficients

https://en.wikipedia.org/wiki/Finite_difference_coefficient
Coefficients of the differences with uniform grid spacing (h)
La suma de los coeficientes siempre es cero.

Second order derivatives $O(h^2)$

Central finite difference

Derivative	-2	-1	0	1	2
1		-1/2		1/2	
2		1	-2	1	
3	-1/2	1	0	-1	1/2
4	1	-4	6	-4	1

For example, the third derivative (with second-order accuracy) is

$$f'''(x_0) = \frac{-\frac{1}{2}x_{-2} + 1x_{-1} - 1x_1 + \frac{1}{2}x_2}{h^3} + O(h^2)$$

Las fórmulas de orden impar son simétricas con respecto al pivote (0) mientras que las de orden par son anti simétricas.

Forward finite difference

Derivative		0	1	2	3	4	5
1		-3/2	2	-1/2			
2		2	-5	4	-1		
3		-5/2	9	-12	7	-3/2	
4		3	-14	26	-24	11	-2

In general, to get the coefficients of the backward approximations, give all odd derivatives listed in the table the opposite sign, whereas for even derivatives the signs stay the same.

Observe that in all finite difference expressions the sum of the coefficients is zero. The effect on the roundoff error can be profound. If h is very small, the values of *f(x)*, *f (x ±h)*, *f(x ±2h)*, and so on, will be approximately equal. When they are multiplied by the coefficients and added, several significant figures can be lost. Yet we cannot make h too large, because then the truncation error would become excessive.

Centered finite-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

Formula	Error
First Derivative	
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) - \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4}$	$O(h^4)$