Automatic/Numerical Differentiation

Frequently we have a program that calculates numerical values of a function.

we would like to obtain [accurate values] for the derivaties of the function. IF we dont want approximation.

Then it is Called "Computational differention" /Algorithmic Differentiation"

Recall:

Standard tylor series Expansion:

Numerically Calculating The derivative:

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

→ first order derivative.

The difference quotient (i) is an approximation of the derivative $f'(x)$ and this approximation gets better as "h" gets Smaller.

→ Geometrically, (i) represents/measures the slope of the Secant line through points $(x, f(x))$, $(x+h, f(x+h))$ on the graph of function;

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \dots\dots \quad \text{(ii)}$$

let $x - x_0 = h$ $\quad |h| <<< 1$ $\quad h > 0$ forward difference

$\Rightarrow x = x_0 + h$ $\quad h < 0$ Backward difference.

This gives :

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

we Say and see that Automatic differentiation and numerically approximating derivatives are two Seperate things.

In numerical derivative (Approximation) we use the tylor series expansion given with (ii) and (ii)-a. while these equations gives us an approximation of $f'(x)$ But we have some loss of error that depends on how we select our "h" for small "h" this should be a good approximation to the slope of the tangent line $f'(x)$.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2 f''(\xi)}{2!} \quad \text{—(iii)} \quad \text{where } \xi \in (x, x+h)$$

Rearrange:

$$\frac{f(x+h) - f(x)}{h} - f'(x) = h\frac{f''(\xi)}{2} \quad \text{—(iii)-a}$$

Question!

How Close an Approximation is the difference Quotient? (i)

From (iii) and (iii)-a

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}h^2 f''(\xi_x) \quad \text{(iii)}$$

$$\frac{f(x+h) - f(x)}{h} - f'(x) = \frac{1}{2} f''(\xi)h \quad \text{(iii)-a}$$

At the point x in (iii)-a we use Cauchy form of Remainder term in which ξ, depends on Both x & h is a point lying B/w x and x+h using (iii)-a we Can Bound the error in finite difference approximation (i) and is Can be bounded by a multiple of the step size

$$\underbrace{\left| \frac{f(x+h) - f(x)}{h} - f'(x) \right|} \le C|h| \quad \text{-(iv)} \qquad C = \max \frac{1}{2} |f''(\xi)|$$

Here The error in (i) Finite difference approximation is bounded By the multiple of step Size: $C|h| \Rightarrow (i) \propto Ch$ "C is a Constant

Here "C" depends on the magnitude of second order derivative of the function over the interval x and x+h: $C = \max \frac{1}{2}|f''(\xi)|$

This Gives us

$O(\ )$ Big O notation

$$f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{Finite difference}} + O(h) \quad \text{-(v)}$$

Equation (v) indicates the approximation (iv) has an error that decreases linearly with "h"

Example: $y = f(x) = \sin x$:

$y' = f'(x) = \cos x$; $\boxed{\text{No we wont use symbolic differentiation.}}$

letus evaluate this derivative with (i) finite difference Quotient at x = 1

$f(x) = \sin x \quad x = 1$ Calculate $f'(x)$ at $x = 1$

$$\underbrace{f'(1) = \cos(1) = 0.5403023\ldots}_{\text{Symbollicaly}} \qquad \underbrace{\cos 1 \simeq \frac{\sin(1+h) - \sin 1}{h}}_{\text{Using (i) finite difference Approximation.}}$$

By the factor of 10

h	0.1	0.01	0.001	0.0001	0.00001	0.000001
Approximation	.497364	.536086	.539881	.540260	.540298	0.540302
Error	-0.042939	-0.004216	-0.000421	-0.000042	-0.000004	-0.000000

By factor of 10

Reducing step size By 10 also reduces the error also By the factor of 10.

To obtain 10 decimal digit accuracy we anticipate step size about $= 10^{-11}$