Numerical Differentiation is Easy

Numerical differentiation is the computation of a slope, the instantaneous rate of change of a function at a point, the quantity

$$f'(c) \equiv \lim_{h\to 0} \frac{f(c+h)-f(c)}{h}.$$

Let's assume (i) that f is differentiable on an interval (a,b) containing c, and (ii) that we can evaluate f at any point in (a,b). All of the commonly used formulas for approximating $f'(c)$ (and f'', etc.) can be derived from the Lagrange interpolation result:

$$f(x) = P_n(x) + R_n(x), \quad \text{where} \quad R(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{j=0}^{n}(x-x_j),$$

$x_j \in (a,b),\ j = 0,1,\ldots,n$, and $\xi = \xi(x) \in (a,b)$.

Differentiating gives

$$f'(x) = P_n'(x) + R_n'(x),$$

which yields the $(n+1)$-point *finite difference* formulae

$$f'(c) \approx P_n'(c).$$

If f is smooth enough, the error in this approximation is $R_n'(c)$, and

$$R_n'(x) \;=\; \frac{f^{(n+1)}(\xi)}{(n+1)!}\left[\sum_{i=0}^{n}\prod_{j\neq i}(x-x_j)\right] \;+\; \left[\frac{f^{(n+2)}(\xi)\ \xi'(x)}{(n+1)!}\right]\prod_{j=0}^{n}(x-x_j).$$

The second term above is rather mysterious (ξ differentiable? Yes!), but we can simplify the analysis by making x one of the nodes:

$$f'(x_i) = P'(x_i) + \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{j\neq i}(x_i-x_j).$$

The 5 differentiation rules below all use the formula above with $c = x_0$ and taking the nodes to be evenly spaced with spacing h. They are just a few of many, and you can easily make up your own (e.g., if you do not have uniformly spaced nodes).

$$\begin{aligned}
f'(x_0) &= \tfrac{1}{h}[f(x_0+h)-f(x_0)] - \tfrac{h}{2}f''(\xi_2)\\
&= \tfrac{1}{2h}[-3f(x_0)+4f(x_0+h)-f(x_0+2h)] + \tfrac{h^2}{3}f^{(3)}(\xi_{3b})\\
&= \tfrac{1}{2h}[f(x_0+h)-f(x_0-h)] - \tfrac{h^2}{6}f^{(3)}(\xi_{3c})\\
&= \tfrac{1}{12h}[-25f(x_0)+48f(x_0{+}h)-36f(x_0{+}2h)+16f(x_0{+}3h)-3f(x_0{+}4h)] + \tfrac{h^4}{5}f^{(5)}(\xi_{5b})\\
&= \tfrac{1}{12h}[f(x_0-2h)-8f(x_0-h)+8f(x_0+h)-f(x_0+2h)] + \tfrac{h^4}{30}f^{(5)}(\xi_{5c})
\end{aligned}$$

The 3^{rd} and 5^{th} of these are called central-difference formulas, the others are forward-difference if $h > 0$, and backward-difference if $h < 0$. Notice that the central difference formulas have |smaller| weights and smaller error coefficients, and that an $(n+1)$-point method has error $O(h^n)$.

This may have been easy, but the title is a lie. Please put on (or adjust) your numerical analysis hat and reconsider assumption (ii), above...