

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

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

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:

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

$x_j \in (a, b)$, $j = 0:n$, 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* formula

$$f'(c) \approx P'_n(c).$$

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 taking x to be one of the nodes:

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

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).

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

The 3rd and 5th 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...