Numerical Differentiation of Functions

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Approximating the Derivative

The simplest way of getting a numerical value for the derivative of a function $y(x)$ or for a set of tabulated values (x_i, y_i) is by using the interpolating polynomials either Newton or Lagrange.

Thus if we use Newton's interpolating polynomial :

$$y(x) \to P(x) = y_0 + s\Delta y_0 + \frac{s(s-1)}{2!}\Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 y_0 + \cdots$$

and the take its derivative we get :

$$\frac{dy}{dx} = \frac{dP}{dx} = \frac{1}{s}\frac{dP(s)}{ds} = \frac{1}{h}\left(\Delta y_0 + \frac{2s-1}{2!}\Delta^2 y_0 + \frac{3s^2-6s+2}{3!}\Delta^3 y_0 + \cdots\right)$$

where $x = x_0 + sh$. Thus for the derivative at x_0 we set $s = 0$ or for the derivative at x_1 we set $s = 1$ and so on, for example

$$y_0' = \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 + \cdots\right) \tag{1}$$

Approximating the Derivative

Depending on the number of terms that we keep we get

$$y_0' = \frac{y_1 - y_0}{h} + O(h) \tag{2}$$

$$y_0' = -\frac{3y_0 - 4y_1 + y_2}{2h} + O(h^2) \tag{3}$$

$$y_0' = -\frac{11y_0 - 18y_1 + 9y_2 - 2y_3}{6h} + O(h^3) \tag{4}$$

In a similar way we can find a formula for the 2nd derivative of $y(x)$ at x_0:

$$\frac{d^2P}{dx^2} = \frac{1}{h^2}\frac{d^2P(s)}{ds^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + (s-1)\Delta^3 y_0 + \cdots\right] \tag{5}$$

thus

$$y_0'' = \frac{y_0 - 2y_1 + y_2}{h^2} + O(h) \tag{6}$$

$$y_0'' = \frac{2y_0 - 5y_1 + 4y_2 - y_3}{h^2} + O(h^2) \tag{7}$$

Prove the above relations

Approximating the Derivative - Error

The error will be estimated by using the formula for the error of the interpolating polynomial, that is

$$E(x) = (x - x_0)(x - x_1)(x - x_2)...(x - x_n)\frac{y^{n+1}(\xi)}{(n+1)!} \tag{8}$$

The error from the numerical estimation of the derivative at a given point, say x_0, will be found by taking the derivative of the above equation

$$E'(x_0) = (x_0 - x_1)(x_0 - x_2)...(x_0 - x_n)\frac{y^{n+1}(\xi)}{(n+1)!} \tag{9}$$

and if we assume equally spaced points i.e. $h = x_{i+1} - x_i$, we get:

$$E'(x_0) = -h(-2h)...(-nh)\frac{y^{n+1}(\xi)}{(n+1)!} = (-1)^n h^n \frac{y^{n+1}(\xi)}{n+1}\,. \tag{10}$$

Thus the error in (2) will be $O(h)$, in (3) will be $O(h^2)$ and in (4) will be $O(h^3)$.

Approximating the Derivative : Error

In a similar way we find the error of the 2nd derivative, which is $O(h^{(n-1)})$ **(Prove it)** .

Thus for the formula (6) will be $O(h)$ and for (7) is $O(h^2)$.

We can use the backward interpolating Newton polynomial also to construct similar relations.

Approximating the Derivative : Example

We will find the 2nd derivative at $x = x_1$ using y_0, y_1, y_2 and y_3.

We will use a 3rd order interpolating Lagrange polynomial and for simplicity we assume that x_0, x_1, x_2,... are equally spaced.

$$\begin{aligned} P(x) = & \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} y_0 + \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)} y_1 \\ & + \frac{(x - x_0)(x - x_1)(x - x_3)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} y_2 + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)} y_3 \end{aligned} \tag{11}$$

then the 2nd derivative will be:

$$\begin{aligned} P''(x) \quad = \quad & \frac{2y_0}{-6h^3}\left[(x - x_1) + (x - x_2) + (x - x_3)\right] + \frac{2y_1}{2h^3}\left[(x - x_0) + (x - x_2) + (x - x_3)\right] \\ + \quad & \frac{2y_2}{-2h^3}\left[(x - x_0) + (x - x_1) + (x - x_3)\right] + \frac{2y_0}{6h^3}\left[(x - x_0) + (x - x_1) + (x - x_2)\right] \end{aligned} \tag{12}$$

and by setting $x = x_1$ we get

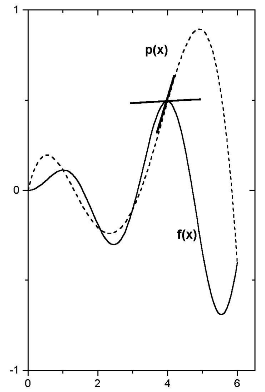
$$P''(x) = \frac{y_0 - 2y_1 + y_2}{h^2} \tag{13}$$

The term y_3, although has been used is absent from the final relation still the error is $O(h^2)$ as it was expected.

Comment about the Error

It should be noticed that although the interpolating polynomial is a very good approximation to a function its derivative does not always approximate accurately the derivative of the function.

This becomes is obvious in the following graph



Central Differences

If a function $f(x)$ can be evaluated at values that lie both to the left and the right of a point x_i then the best formulae are the one coming from **Central Differences**

$$
\begin{aligned}
y(x_0)' &= y_0' = \frac{y_1 - y_{-1}}{2h} + O(h^2) && (14)\\
y(x_0)' &= y_0' = \frac{-y_2 + 8y_1 - 8y_{-1} + y_{-2}}{12h} + O(h^4) && (15)\\
y(x_0)'' &= y_0'' = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + O(h^2) && (16)\\
y(x_0)'' &= y_0'' = \frac{-y_2 + 16y_1 - 30y_0 + 16y_{-1} - y_{-2}}{12h^2} + O(h^4) && (17)\\
y(x_0)''' &= y_0''' = \frac{y_2 - 2y_1 + 2y_{-1} - y_{-2}}{2h^3} + O(h^2) && (18)\\
y(x_0)^{(4)} &= y_0^{(4)} = \frac{y_2 - 4y_1 + 6y_0 - 4y_{-1} + y_{-2}}{h^4} + O(h^2) && (19)
\end{aligned}
$$

These relations can be created with appropriate combinations of Taylor expansions around a given point

Central Differences

Let's assume the Taylor expansions on both sides of x_0 i.e.

$$y(x_0+h) \equiv y_1 = y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{6}y_0''' + \frac{h^4}{24}y_0^{(4)} + \ldots \quad (20)$$

$$y(x_0-h) \equiv y_{-1} = y_0 - hy_0' + \frac{h^2}{2}y_0'' - \frac{h^3}{6}y_0''' + \frac{h^4}{24}y_0^{(4)} - \ldots \quad (21)$$

$$y(x_0+2h) \equiv y_2 = y_0 + 2hy_0' + 2h^2y_0'' + \frac{4}{3}h^3y_0''' + \frac{2}{3}h^4y_0^{(4)} + \ldots \quad (22)$$

$$y(x_0-2h) \equiv y_{-2} = y_0 - 2hy_0' + 2h^2y_0'' - \frac{4}{3}h^3y_0''' + \frac{2}{3}h^4y_0^{(4)} - \ldots \quad (23)$$

Then with appropriate combinations of the above relations one can construct the central difference relations. For example, by subtracting (21) from (20) we get equation (14), while by adding we get the relation (16) which has been proved earlier by using the Lagrange polynomial.

In a similar fashion by multiplying equations (20) and (21) with 8 and by using equations (22) and (23) we get a formula of the form

$$y_{-2} - y_2 + 8\left(y_1 - y_{-1}\right)$$

which leads to equation (15) with error $\sim O(h^4)$.