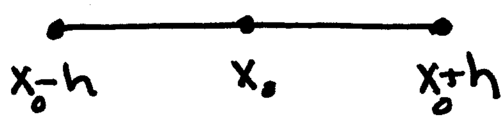
Computing derivatives by Polynomial fitting

Another way to approximate derivatives is to fit a polynomial to nearby points and differentiate <u>that</u>.



If we fit a line to $\begin{array}{cc} x-h & x+h \\ \hline f(x-h) & f(x+h) \end{array}$, we clearly get the central approximation

$$P_1(x) = f(x_0) + f[x_0, x_0+h]\,(x-x_0)$$

and

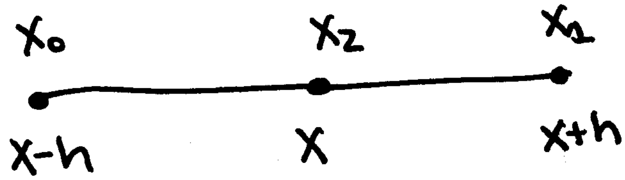
$$f'(x) \approx P_1'(x) = f[x_0, x_0+h]$$

and

$$f'(x_0) \approx P_1'(x_0) = f[x_0, x_0+h]$$

$$= \frac{f(x_0+h) - f(x_0)}{h}$$

Now suppose we interpolate on



If we use x_0, x_1 alone, we get

$$p_1(x) = f(x_0) + f[x_0,x_1](x-x_0)$$

$$p_1'(x) = f[x_0,x_1] = \frac{f(x+h) - f(x-h)}{2h}$$

Now if we interpolate all 3 nodes, we get

$$p_2(x) = f(x_0) + f[x_0,x_1](x-x_0) + f[x_0,x_1,x_2](x-x_0)(x-x_1)$$

$$p_2'(x) = f[x_0,x_1] + f[x_0,x_1,x_2](2x-x_0-x_1).$$

we note that

$$p_2'(x_2) = f[x_0,x_1] = \frac{f(x+h)-f(x+h)}{2h}$$

which is another way of seeing this formula is better than the first one.

So how do we estimate the error in these formulae?

If we let $\omega(x) = \prod_{i=0}^{n}(x-x_i)$, then we recall that our exact formula

$$f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\,\omega(x)$$

involves an $(n+1)$st derivative at some point in (x_0, x_n). We can differentiate to get

$$f'(x) - p_n'(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\,\omega'(x)$$

$$+ \frac{1}{(n+1)!}\,\omega(x)\frac{d}{dx}\left(f^{(n+1)}(\xi)\right).$$

after all, ξ depends on x, so this term is not always zero.

It is pretty clear that this formula can only be of help at a <u>node</u>, where we get

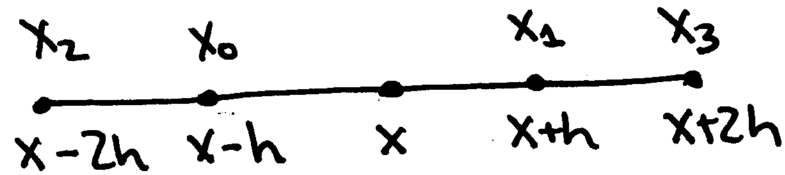
$$f'(x_i) = p_n'(x_i) + \frac{1}{(n+1)!} f^{(n+1)}(\xi)\, \omega'(x_i).$$

For example, for the two node approximation, we get

$$f'(x_0) = p_1'(x_0) + \frac{1}{2} f''(\xi)$$
$$= f[x_0, x_1] + \frac{1}{2} f''(\xi)$$

which is the Taylor theorem error bound from before.

A useful case of this is



We fit

$$P_3(x) = f[x_0] + f[x_0,x_1](x-x_0)$$
$$+ f[x_0,x_1,x_2](x-x_0)(x-x_1)$$
$$+ f[x_0,x_1,x_2,x_3](x-x_0)(x-x_1)(x-x_2).$$

So

$$P_3'(x) = f[x_0,x_1] + f[x_0,x_1,x_2](2x-x_0-x_1)$$
$$+ f[x_0,x_1,x_2,x_3]\big((x-x_0)(x-x_1) + (x-x_0)(x-x_2)$$
$$+ (x-x_1)(x-x_2)\big)$$

If we start actually plugging stuff in, at x we get

$$= f[x_0,x_1] + f[x_0,x_1,x_2](h-h)$$
$$+ f[x_0,x_1,x_2,x_3]\big(h(-h) + h(2h) + (-h)(2h)\big)$$

$$= f[x_0, x_1] \cancel{+} - h^2 f[x_0, x_1, x_2, x_3]$$

If you work this out, you get

$$f'(x) \approx \frac{1}{2h}[f(x+h) - f(x-h)]$$

$$- \frac{1}{12h}\{f(x+2h) - 2[f(x+h) - f(x-h)] - f(x-2h)\}$$

This is a 3rd degree polynomial approx, so the error is $O(h^4)$. How does this compare to the corresponding richardson extrapolation $O(h^4)$ formUla?

<derivative_and_difference.nb>

What about <u>second</u> derivatives?

It's worth noting that we can extract second derivatives as well. Recall

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \ldots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \ldots$$

If we ~~subtract~~ add, we get

$$\frac{f(x+h) + f(x-h) - 2f(x)}{h^2} = f''(x) + \frac{f''''(x)}{12}h^2 + \ldots$$

Of course we have to check this numerically (note that we could use Richardson extrapolation to help here, too).