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A Higher order Approximation for the first derivative :

Central difference approximation for first derivative :

To obtain a second order approximation to the first derivative at $x = x_0$.

we consider three data points x_0, x_1, x_2 they are equally spaced

i.e $x_i = x_0 + ih$, $i = 0, 1, 2, \dots n$

where h be step length

From interpolation theory, we get

$$f(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) +$$

$$\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) + f[x_0, x_1, x_2, x](x-x_0)(x-x_1)(x-x_2) \quad \text{--- (1)}$$

or $f(x) =$ Lagrange interpolation + Error Term.

differentiating eq^n (1) w. r. to x and evaluating at $x = x_0$

$$f'(x) = \frac{(x-x_1)+(x-x_2)}{2h^2} f(x_0) - \frac{(x-x_0)+(x-x_2)}{h^2} f(x_1) +$$

$$\frac{(x-x_0)+(x-x_1)}{2h^2} f(x_2) + \frac{d}{dx} f[x_0, x_1, x_2, x](x-x_0)(x-x_1)(x-x_2)$$

$$+ f[x_0, x_1, x_2, x] \frac{d}{dx}(x-x_0)(x-x_1)(x-x_2)$$

at $x = x_0$

$$f'(x_0) = \frac{(x_0-x_1)+(x_0-x_2)}{2h^2} f(x_0) - \frac{x_0-x_2}{h^2} f(x_1) +$$

$$\frac{(x_0-x_1)}{2h^2} f(x_2) + f[x_0, x_1, x_2, x_0] \frac{d}{dx}(x-x_0)(x-x_1)(x-x_2)\Big|_{x=x_0}$$

$$\Rightarrow \boxed{f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3} f'''(\xi)} \quad — (2)$$

where $x_1 = x_0+h$
$x_2 = x_0+2h$.

or
$$\boxed{f'(x_0) \simeq \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h}}$$

This is known second order Forward ~~central~~ difference approximation for first derivative.

~~Example~~: If h is replaced by $-h$ in eq^n (2) we get Backward second order approximation to first derivative

$$f'(x_0) = \frac{3f(x_0) - 4f(x_0-h) + f(x_0-2h)}{2h} + \frac{h^2}{3} f'''(\xi)$$

or
$$\boxed{f'(x_0) \simeq \frac{3f(x_0) - 4f(x_0-h) + f(x_0-2h)}{2h}}$$

Now suppose that x_2 is placed on the opposite side of x_0, and hence data form x_0-h, x_0, and x_0+h are used to develop an approximation. We obtain

$$\boxed{f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(\xi)}$$

or

$$\boxed{f'(x_0) \simeq \frac{f(x_0+h) - f(x_0-h)}{2h}}$$

This is second order central difference approximation to the first derivative.

Example 6.3: Verify second order approximation for forward, Backward and central difference approximations for first derivative.

Consider the function $f(x) = \ln x$, $x_0 = 2$,

For $h = 0.1$: second order forward difference approximation for first derivative at $x = x_0 = 2$.

$$f'(2) = \frac{-3f(2) + 4f(2.1) - f(2.2)}{0.2}$$

$$= \frac{-3\ln(2) + 4\ln(2.1) - \ln(2.2)}{0.2}$$

$$= 0.499252$$

Error = True value − Approximate value

$$= 0.5 - 0.499252 = 7.4762 \times 10^{-4}.$$

For $h=0.1$: Second order Backward difference of first derivative at $x_0=2$ is

$$f'(2) \simeq \frac{3f(2) - 4f(1.9) + f(1.8)}{0.2}$$

$$\simeq \frac{3\ln(2) - 4\ln(1.9) + \ln(1.8)}{0.2}$$

$$\simeq 0.499063$$

Error Term = True value − Approximate value

$$= 0.5 - 0.499063$$
$$= 9.3669 \times 10^{-4}$$

For $h=0.1$: Second order Central difference approx. of first derivative is

$$f'(2) \simeq \frac{f(2.1) - f(1.9)}{0.2}$$

$$= \frac{\ln(2.1) - \ln(1.9)}{0.2}$$

$$= 0.500417$$

Error $= 4.1729 \times 10^{-4}$

Formula for Second order derivative :

If "f" is interpolated at $x_0 - h$, x_0 and $x_0 + h$.

The second order central difference approximation for the second derivative is

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi)$$

or
$$\boxed{f''(x_0) \approx \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2}}$$

Assignment : Do Q.10, 11, 12, 13, 14. (Ex. problems).

(c) Numerically verify the order of approximation using $f(x) = \ln x$ and $x_0 = 2$.

7. (a) Derive a formula for approximating the first derivative of an arbitrary function at $x = x_0$ using four equally spaced points, with two (2) of those points to the left and one (1) to the right of $x = x_0$.

(b) What is the order of approximation for the formula obtained in part (a)? Completely justify your response.

8. (a) Derive a formula for approximating the first derivative of an arbitrary function at $x = x_0$ by interpolating at $x = x_0 + h$ and $x = x_0 - \alpha h$ for $\alpha > 0$.

(b) Show, analytically, that the formula from part (a) is second order when $\alpha = 1$, but only first order for $\alpha \neq 1$.

9. (a) Derive a formula for approximating the second derivative of an arbitrary function at $x = x_0$ by interpolating at $x = x_0 + h$, $x = x_0$ and $x = x_0 - \alpha h$ for $\alpha > 0$.

(b) Show, analytically, that the formula from part (a) is second order when $\alpha = 1$, but only first order for $\alpha \neq 1$.

W 10. (a) Using $f(x) = \ln x$ and $x_0 = 2$, demonstrate numerically that the central difference approximation for the second derivative given by

$$f''(x_0) \approx \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2},$$

is second order accurate.

(b) Repeat part (a) using $f(x) = e^x$ and $x_0 = 0$.

W 11. Verify that each of the following difference approximations for the first derivative provides the exact value of the derivative, regardless of h, for the functions $f(x) = 1$, $f(x) = x$ and $f(x) = x^2$, but not for the function $f(x) = x^3$.

(a) $f'(x_0) \approx \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}$

(b) $f'(x_0) \approx \frac{3f(x_0)-4f(x_0-h)+f(x_0-2h)}{2h}$

(c) $f'(x_0) \approx \frac{f(x_0+h)-f(x_0-h)}{2h}$

W 12. Verify that the second-order central difference approximation for the second derivative provides the exact value of the second derivative, regardless of the value of h, for the functions $f(x) = 1$, $f(x) = x$, $f(x) = x^2$, and $f(x) = x^3$, but not for the function $f(x) = x^4$.

W 13. (a) Use the formula

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

to approximate the derivative of $f(x) = 1 + x + x^3$ at $x_0 = 1$, taking $h = 1, 0.1, 0.01$, and 0.001. What is the order of approximation?

(b) Repeat part (a) for $x_0 = 0$.

(c) Explain any difference between the results from part (a) and those from part (b).

W 14. (a) Use the formula

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}$$

to approximate the derivative of $f(x) = \sin x$ at $x_0 = \pi$, taking $h = 1, 0.1, 0.01$, and 0.001. What is the order of approximation?

(b) Repeat part (a) for $x_0 = \pi/2$.

(c) Explain any difference between the results from part (a) and those from part (b).

15. Consider the following formula for approximating the first derivative of an arbitrary function:

$$f'(x_0) = \frac{-2f(x_0 - 3h) + 9f(x_0 - 2h) - 18f(x_0 - h) + 11f(x_0)}{6h} + \frac{1}{4}h^3 f^{(4)}(\xi),$$

where $x_0 - 3h < \xi < x_0$.

(a) Suppose that the function values used in the above formula contain roundoff/data errors that are bounded in absolute value by ϵ and that the absolute value of the fourth derivative is bounded by M. Derive a bound for the approximation error associated with the above formula as a function of ϵ, M, and h.

(b) Suppose $\epsilon = 5.96 \times 10^{-8}$ (machine precision in IEEE standard single precision). Determine the value for the step size h that minimizes the bound on the error when approximating the value of the derivative of $f(x) = e^x$ at $x_0 = 1$.

16. Consider the second-order forward difference formula for approximating the first derivative of an arbitrary function:

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} + \frac{1}{3}h^2 f'''(\xi),$$

where $x_0 < \xi < x_0 + 2h$.

(a) Suppose that the function values used in the above formula contain roundoff/data errors that are bounded in absolute value by ϵ and that the absolute value of the third derivative is bounded by M. Derive a bound for the approximation error associated with the above formula as a function of ϵ, M, and h.

(b) Suppose $\epsilon = 1.11 \times 10^{-16}$ (machine precision in IEEE standard double precision). Determine the value for the step size h that minimizes the bound on the error when approximating the value of the derivative of $f(x) = \ln x$ at $x_0 = 2$.

6.3 RICHARDSON EXTRAPOLATION

In the previous section several first- and second-order finite difference approximation formulas for first and second derivatives were obtained. Higher-order formulas can of course be derived by interpolating more data points, but an alternative for obtaining higher-order approximations is to use a procedure known as extrapolation. The basic idea behind extrapolation is that whenever the leading term in the error for an approximation formula is known, we can combine two approximations obtained from that formula using different values of the parameter h to