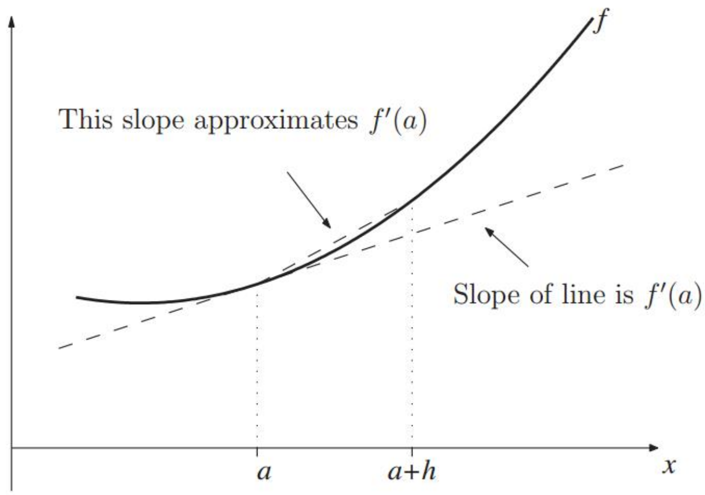
Recitation – 5: Numerical Differentiation

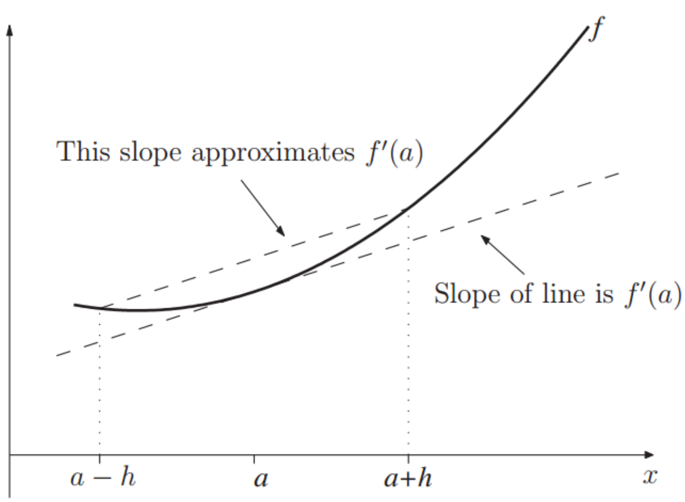
Two-point and Three-point formulas for the First Derivative

Our aim is to approximate the slope of a curve f at a particular point $x = a$ in terms of $f(a)$ and the value of f at a nearby point where $x = a + h$.



This is one-sided, forward difference approximation to the derivative of f.

$$f'(a) = slope\ of\ short\ broken\ line = \frac{difference\ in\ the\ y - values}{difference\ in\ the\ x - values} = \frac{f(a+h) - f(a)}{h}$$



This is called a central difference approximation to $f'(a)$.

$$f'(a) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Deriving Formulas Using Taylor Series

Start from Taylor's Expansion, generally written for a small $h > 0$.

$$f(x_0 \pm h) = f(x_0) \pm hf'(x_0) + \frac{h^2}{2}f''(x_0) \pm \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{(iv)}(x_0) \ldots$$

Truncate this as needed to derive an expression for $f'(x_0)$.

Backward difference is obtained by writing,

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

Hence,

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

One-sided, two point backward and forward formulas are 1st order methods and have truncation error $O(h)$.

Question 1

Let $f(x) = ln(x)$ and $a = 3$. Using both a forward and a central difference, and working to 8 decimal places, approximate $f(a)$ using $h = 0.1$ and $h = 0.01$.

(Note that $\frac{d}{dx}lnx = 1/x$ and $f'(3) = 1/3$.)

Solution

Using the forward difference, for $h = 0.1$

$$f'(a) \approx \frac{\ln(a+h) - \ln(a)}{h} = \frac{1.13140211 - 1.09861229}{0.1} = 0.32789823$$

and for $h = 0.01$ we obtain

$$f'(a) \approx \frac{\ln(a+h) - \ln(a)}{h} = \frac{1.10194008 - 1.09861229}{0.01} = 0.33277901$$

Using central differences the two approximations to $f'(a)$ are

$$f'(a) \approx \frac{\ln(a+h) - \ln(a-h)}{2h} = \frac{1.13140211 - 1.06471074}{0.2} = 0.33345687$$

And,

$$f'(a) \approx \frac{\ln(a+h) - \ln(a-h)}{2h} = \frac{1.10194008 - 1.09527339}{0.02} = 0.33333457$$

Question 2

The distance x of a runner from a fixed point is measured (in metres) at intervals of half a second. The data obtained is

t	0.0	0.5	1.0	1.5	2.0
x	0.00	3.65	6.80	9.90	12.15

Use central differences to approximate the runner's velocity at times $t = 0.5s$ and $t = 1.25s$.

Hint: Velocity is defined as the rate of change of position which is first derivative of position-time function ($V = \frac{dx}{dt}$)

Solution

Our aim here is to approximate $x(t)$. The choice of h is dictated by the available data,

Using data with $t = 0.5s$ at its centre we obtain,

$$x'(0.5) \approx \frac{x(1.0) - x(0.0)}{2 \times 0.5} = 6.80\, m/s, \qquad where\ h = 0.5$$

Data centred at $t = 1.25s$ gives us the approximation,

$$x'(1.25) \approx \frac{x(1.5) - x(1.0)}{2 \times 0.25} = 6.80\, m/s, \qquad where\ h = 0.25$$

Note the value of h used.

Question 3

Estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

At $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$.

Solution

The problem can be solved analytically

$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$ and $f'(0.5) = -0.9125$.

When $h = 0.5$, $x_{i-1} = x_i - h = 0$, and $f(x_{i-1}) = 1.2$; $x_i = 0.5$, $f(x_i) = 0.925$; $x_{i+1} = x_i + h = 1$, and $f(x_{i+1}) = 0.2$.

The forward divided difference:

$$f'(0.5) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{0.2 - 0.925}{0.5} = -1.45$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-1.45)}{-0.9125}\right| \times 100\% = 58.9\%$$

The backward divided difference:

$$f^{'}(0.5) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{0.925 - 1.2}{0.5} = -0.55$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-0.55)}{-0.9125}\right| \times 100\% = 39.7\%$$

The centered divided difference:

$$f^{'}(0.5) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{0.925 - 1.2}{2 \times 0.5} = -1.0$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-1.0)}{-0.9125}\right| \times 100\% = 9.6\%$$

When $h = 0.25$, $x_{i-1} = x_i - h = 0.25$, and $f(x_{i-1}) = 1.1035$; $x_i = 0.5$, $f(x_i) = 0.925$; $x_{i+1} = x_i + h = 0.75$, and $f(x_{i+1}) = 0.6363$.

The forward divided difference:

$$f^{'}(0.5) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{0.6363 - 0.925}{0.25} = -1.155$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-1.155)}{-0.9125}\right| \times 100\% = 26.5\%$$

The backward divided difference:

$$f^{'}(0.5) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{0.925 - 1.1035}{0.25} = -0.714$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-0.714)}{-0.9125}\right| \times 100\% = 21.7\%$$

The centered divided difference:

$$f^{'}(0.5) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{0.6363 - 1.1035}{2 \times 0.25} = -0.934$$

The percentage relative error:

$$|\epsilon_t| = \left|\frac{(-0.9125) - (-0.934)}{-0.9125}\right| \times 100\% = 2.4\%$$

Using centered finite divided difference and small step size achieves lower approximation error.

Three-point formula for the Second Derivative

$$f(x_0+h)=f(x_0)+hf'(x_0)+\frac{h^2}{2}f''(x_0)+\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(iv)}(\xi_1)$$

$$f(x_0-h)=f(x_0)-hf'(x_0)+\frac{h^2}{2}f''(x_0)-\frac{h^3}{6}f'''(x_0)+\frac{h^4}{24}f^{(iv)}(\xi_2)$$

Adding together the two expansions, all the odd powers of h cancel out and we have,

$$f(x_0+h)+\ f(x_0-h)=\ 2f(x_0)+h^2f''(x_0)+\frac{h^4}{24}\left(f^{(iv)}(\xi_1)+f^{(iv)}(\xi_2)\right)$$

So the centered formula for the second derivative,

$$f''(x_0)=\frac{1}{h^2}\left(f(x_0-h)-2f(x_0)+\ f(x_0+h)\right)-\frac{h^2}{12}f^{(iv)}(\xi),\qquad where\ \ x_0-h\ \le\ \xi\ \le\ x_0+h$$

Question 4

The distance x of a runner from a fixed point is measured (in metres) at intervals of half a second. The data obtained is

t	0.0	0.5	1.0	1.5	2.0
x	0.00	3.65	6.80	9.90	12.15

Use central differences to approximate the runner's acceleration at times $t\ =\ 0.5s$ and $t\ =\ 1.25s$.

Hint: Velocity is defined as the rate of change of velocity which is given by the first derivative of position-time function ($a=\frac{dV}{dt}=\frac{d^2\mathrm{x}}{\mathrm{d}t^2}$)

Solution

Our aim here is to approximate $x(t)$.

Using data with $t\ =\ 1.5s$ at its centre we obtain

$$x''(1.5)\approx\frac{x(2.0)-2x(1.5)+x(1.0)}{0.5^2}=-3.40\ m/s^2$$

From which we see that the runner is slowing down.

Richardson Extrapolation

The trick is to compute derivative for 2 different values of h, and combine the results in some appropriate manner. This is to use two derivative estimates to compute a third, more accurate one.

An approximation using h,

$$f'(a) \approx D_0(h) = \frac{f(x+h) - f(x-h)}{2h} = f'(x) + b_1 h^2 + O(h^4)$$

Another approximation using 2h,

$$f'(a) \approx D_0(2h) = \frac{f(x+2h) - f(x-2h)}{4h} = f'(x) + b_1 4h^2 + O(h^4)$$

We can substract these to get

$$D_0(2h) - D_0(h) = 3b_1 h^2 + O(h^4)$$

We divide across by 3 to get

$$\frac{D_0(2h) - D_0(h)}{3} = b_1 h^2 + O(h^4)$$

The righthand side of this equation is simply $D_0(h) - f'(x)$, so we can substitute to get

$$\frac{D_0(2h) - D_0(h)}{3} = D_0(h) - f'(x) + O(h^4)$$

This rearranges (carefully) to obtain

$$f'(x) = D_0(h) + \frac{D_0(h) - D_0(2h)}{3} + O(h^4) \approx \frac{4}{3} D_0(h) - \frac{1}{3} D_0(2h)$$

Question 5

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2, \quad x_i - 0.5, \ \ h_1 = 0.5, \ \ h_2 = 0.25.$$

Solution

With h_1, $x_{i+1} = 1$, $\quad x_{i-1} = 0$, $\quad D(h_1) = \frac{f(x_{i+1} - f(x_i)}{2h_1} = \frac{0.2 - 1.2}{1} = -1.0$, $\epsilon_t = -9.6\%$.

With h_2, $x_{i+1} = 0.75$, $x_{i-1} = 0.25$, $D(h_2) = \frac{f(x_{i+1} - f(x_i)}{2h_2} = -9.34375$, $\quad \epsilon_t = -2.4\%$.

$$D = \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1) = \frac{4}{3} \times (-0.934575) - \frac{1}{3} \times (-1) = -0.9125, \ \ \epsilon_t = 0.$$

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