Numerical Differentiation

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- Numerical differentiation is the problem of finding (as accurately as necessary) a derivative of a function for a given data.
- Major reasons: 1- Approximation of derivatives in different equations; 2- Forming the derivative of a function from empirical data.

Approximation of the derivative of $f(x)$

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

$$(b) \qquad f'(x) \approx \frac{f(x)-f(x-h)}{h}$$

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

$$(d) \qquad f'(x) \approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

$$(e) \qquad f'(x) \approx \frac{-f(x+2h)+4f(x+h)-4f(x-h)+f(x+2h)}{4h}$$

(a-b) are simply related to $f'(x_0) = \lim\limits_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}$, the slope of $f(x)$ at x_0.

Example: Approximate the derivative of $f(x) = e^x$ at $x = 0$

h	formula (a)	error	formula (c)	error
10^{-1}	1.05170918075648	−0.05170918075648	1.00166750019844	−0.00166750019844
10^{-2}	1.00501670841679	−0.00501670841679	1.00001666674999	−0.00001666674999
10^{-3}	1.00050016670838	−0.00050016670838	1.00000016666668	−0.00000016666668
10^{-4}	1.00005000166714	−0.00005000166714	1.00000000166689	−0.00000000166689
10^{-5}	1.00000500000696	−0.00000500000696	1.00000000001210	−0.00000000001210
10^{-6}	1.00000049996218	−0.00000049996218	0.99999999997324	0.00000000002676
10^{-7}	1.00000004943368	−0.00000004943368	0.99999999947364	0.00000000052636
10^{-8}	0.99999999392253	0.00000000607747	0.99999999392253	0.00000000607747
10^{-9}	1.00000008274037	−0.00000008274037	1.00000002722922	−0.00000002722922

At first, the error decreases as h decreases, following closely the expected errors $(a)O(h)$ and $(c)O(h^2)$. However, notice the deterioration of the approximations as h is decreased still further.

First Derivative: Forward/Backward difference formula

We expand $f(x+h)$ using Taylor series

$$f(x+h) = f(x) + hf'(x) + h^2\frac{f''(\xi_1)}{2}$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\xi_1)$$

Similarly

$$f(x-h) = f(x) - hf'(x) + h^2\frac{f''(\xi_2)}{2}$$

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2}f''(\xi_2)$$

First Derivative: Central difference formula (midpoint formula)

$$f(x+h) = f(x) + hf'(x) + h^2\frac{f''(x)}{2} + h^3\frac{f'''(\xi_1)}{6}$$

Similarly

$$f(x-h) = f(x) - hf'(x) + h^2\frac{f''(x)}{2} - h^3\frac{f'''(\xi_2)}{6}$$

Subtracting

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

Second Derivative: Central difference formula (midpoint formula)

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

Similarly

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

Adding

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

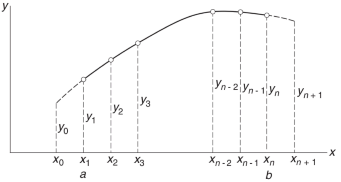
$\xi \in [x-h, x+h]$.

Homework:

1- Write a code for approximating the solution of the differential equation below, i.e. solving Ay=b, where the matrix A and vector b are given below and y is the approximated solution.

$$y'' = -4y + 4x \qquad y(0) = 0 \qquad y'(\pi/2) = 0$$

$$y_i' = \frac{y_{i+1} - y_{i-1}}{2h} \qquad y_i'' = \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$$



$$y_1 = 0$$

$$y_{i-1} - 2y_i + y_{i+1} - h^2\left(-4y_i + 4x_i\right) = 0, \;\; i = 2, 3, \ldots, 10$$

$$2y_{10} - 2y_{11} - h^2(-4y_{11} + 4x_{11}) = 0$$

$$\begin{bmatrix} 1 & 0 & & & \\ 1 & -2+4h^2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2+4h^2 & 1 \\ & & & 2 & -2+4h^2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{10} \\ y_{11} \end{bmatrix} = \begin{bmatrix} 0 \\ 4h^2 x_2 \\ \vdots \\ 4h^2 x_{10} \\ 4h^2 x_{11} \end{bmatrix}$$

A y = b

2- Run the code for n=10,20,40,80, where n is the number of divisions of the solution domain, and plot the solutions, on a single plot, and describe your observation.

Extra credit: Find the extact solution y(x) and compare with your approximated solution.