Fundamentals of Data Science
Practical session #6

This week you will have an opportunity to practice calculus and basic finite difference analysis. You will differentiate and integrate tabulated functions, i.e., functions defined numerically, on a discrete grid, rather than in a symbolic form.

Please, create Python scripts solving Problems 2-3. You can use any environment, such as Spyder, Colab, Jupyter Notebook etc (although, Spyder is preferred).

NB Various math libraries (Numpy, Scipy etc) have ready-to-use functions for differentiation and integration, e.g. numpy.gradient. Please refrain from using them this week, when doing Problems 1-3 below. It would be very useful for you to see how numerical differentiation and integration are done using basic math. Hence, this week please use basic math, array and cycle operations.

Problem 1 (Homework)

This problem involves analytical integration.

Evaluate following definite integrals:

a) $\int_0^{\pi} x \sin(x)\, dx$

b) $\int_0^{1} x^2 \exp(-x)\, dx$

c) $\int_0^{\sqrt{\pi}} x \cos(x^2)\, dx$

d) $\int_{-\pi/4}^{\pi/4} \cos(2x)\ [\sin(2x)]^2\, dx$

e) $\int_{-\sqrt{4}}^{\sqrt{4}} (x^5 + 2x^3 + x)\, dx$

Problems 2-3 need to be solved numerically using basic finite difference techniques.

Problem 2 (Homework+Classwork)

a) Given function $y(x) = x\, e^{-x}$, show that its derivative is $y'(x) = (1-x)\, e^{-x}$;
b) Generate an evenly spaced array X in the interval [0:4] with the step of 0.04;
c) Generate corresponding array Y, where $Y_i = X_i \exp(-X_i)$ (i.e. the function from 1a),
d) Calculate corresponding array DY1, where $DY_i = (1-X_i) \exp(-X_i)$, i.e. derivative of the function from 1a,
e) Calculate derivative DY2 of the tabulated function $Y_i(X_i)$ defined in 1c. Use CD2 scheme (see lecture notes, $Y_i' = (Y_{i+1} - Y_{i-1})/(X_{i+1} - X_{i-1})$). (NB Obviously, your array DY2 would be 2 elements shorter than arrays X and Y)
f) Compare DY1 and DY2, i.e. derivatives of $y(x) = x\, e^{-x}$, calculated analytically and numerically.

Problem 3 (Homework+Classwork)

a) Given function $y(x) = x\,e^{-x}$, show that its definite integral
$\int_0^4 x\,e^{-x}\,dx = [-(1+x)e^{-x}]_0^4 \approx 0.9084$
b) Generate an evenly spaced array X in the interval [0:4] with the step of 0.04;
c) Generate corresponding array Y, where $Y_i = X_i \exp(-X_i)$ (i.e. the function from 1a),
d) Calculate definite integral numerically, using the trapezoidal rule (see lecture notes);
e) Compare the integrals evaluated analytically and numerically