Seminar 6

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Course: KZ4016 Kemisk DataAnalys
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1. Compute an area under the curve that is expressed with the following function:

$$y(x) = \sqrt{1 - x^2}$$

for `x` within `[0, 1]` interval. What do you get if you multiply the result by 4?

2. Find the minimum and maximum of the polynomial $f(x) = x^3 - x^2 - 3x$ in the interval $-2.5 < x < 2.5$. Plot the polynomial to verify the results.

3. When water boils under varying pressures, the heat transfer (per area) changes according to Table 1:

Table 1: Heat transfer for bolining water under various pressures

Pressure p (MPa)	0	1	2	4	6	10	15	20
Heat transfer q (MW/m^2)	1.1	2.4	3.4	3.9	4.0	3.8	3.0	1.2

Perform the polynomial fits with orders from 1 to 4 and plot the results. Estimate the prediction error by taking the sum of squared differences of the reference and predicted values.

4. Calculate the heat Q required to increase the temperature of 1 mole of methane from 533 K to 873 K at 1 bar. The heat capacity equation is given by

$$\frac{C_p}{R} = A + BT + CT^2 + DT^{-2}\,.$$

$A = 1.702$, $B = 9.081 \times 10^{-3}$, $C = -2.164 \times 10^{-6}$ and $D = 0$ are constant parameters. R is the gas constant. The heat is obtained by integrating the heat capacity:

$$Q = n \int_{T_{in}}^{T_f} dT C_p\,.$$

5. Use the data from Table 2 to calculate the vapor pressure of 1-chlorotetradecane at 180 °C.

Table 2: Vapor pressure for 1-chlorotetradecane at varying temperatures

T (°C)	98.5	131.8	148.2	166.2	199.8	215.5
P_0 (mmHg)	1	5	10	20	60	100

Tip: fit a second degree polynomial to construct $P_0(T)$

6. Weak acid dissociation equilibrium is usually written in the following form:

$$\frac{[H^+][A^-]}{[HA]} = K_a$$

where $[H^+]$ is an equilibrium concentration of hydrogen ions, $[A^-]$ is an equilibrium concentration of the conjugate base and $[HA]$ is an equilibrium concentration of the acid HA. The equation above can be expressed in a polynomial form if $[H^+]$ and $[A^-]$ are substituted with x:

$$\frac{x^2}{(C_a - x)} = K_a$$

where C_a is the initial concentration of the acid $[HA]$. Find the equilibrium concentration of the hydrogen ions $[H^+]$ of 0.2 M acetic acid CH_3COOH solution (K_a = 1.8 x 10^{-5}) by finding the roots of the polynomial. Compute the pH of the solution.

Hint: use the `np.roots` function to find the roots of the polynomial.

7. The content of ^{137}Cs has been measured at the Chernobyl nuclear plant after the reactor failure in April 1986. The data can be empirically fitted to an exponential function [*Phys. Rev. E*, 62:4389 (2000)]

$$C_0(t) = Ae^{-t/\tau},$$

where $A = 0.588\,\mathrm{mBq\,m^{-3}}$ and $\tau = 677$ days. When did the amount of cesium fall below 1% from that at $t = 0$ for the first time?

Compare the result to the half-life of ^{137}Cs (30 years).