Problem 1 (50 points)

Vapor-liquid equilibria data are correlated using two adjustable parameters A_{12} and A_{21} per binary mixture. For low pressures, the equilibrium relation can be formulated as:

$$p = x_1 \exp\left(A_{12}\left(\frac{A_{21}x_2}{A_{12}x_1 + A_{21}x_2} \right)^2 \right) p_{water}^{sat} + x_2 \exp\left(A_{21}\left(\frac{A_{12}x_1}{A_{12}x_1 + A_{21}x_2} \right)^2 \right) p_{1,\ 4dioxane}^{sat}.$$

Here the saturation pressures are given by the Antoine equation

$$\log_{10}(p^{sat}) = a_1 - \frac{a_2}{T + a_3},$$

where $T = 20(\circ \mathrm{C})$ and $a_{1,\ 2,\ 3}$ for a water - 1,4 dioxane system is given below.

	a_1	a_2	a_3
Water	8.07131	1730.63	233.426
1,4 dioxane	7.43155	1554.679	240.337

The following table lists the measured data. Recall that in a binary system $x_1 + x_2 = 1$.

x_1	**0.0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**	**1.0**
p	28.1	34.4	36.7	36.9	36.8	36.7	36.5	35.4	32.9	27.7	17.5

Estimate A_{12} and A_{21} using data from the above table:

1. Formulate the least square problem;
2. Since the model is nonlinear, the problem does not have an analytical solution. Therefore, solve it using the gradient descent or Newton's method implemented in HW1;
3. Compare your optimized model with the data. Does your model fit well with the data?

Problem 2 (50 points)

Solve the following problem using Bayesian Optimization:

$$\min_{x_1,\ x_2} \quad \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right)x_1^2 + x_1x_2 + \left(-4 + 4x_2^2\right)x_2^2,$$

for $x_1 \in [-3,\ 3]$ and $x_2 \in [-2,\ 2]$. A tutorial on Bayesian Optimization can be found here (https://thuijskens.github.io/2016/12/29/bayesian-optimisation/)