ME598/494 Homework 3

1. (40 Points, problem from Professor M. Kokkolaras, McGill University) 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:

$$\begin{aligned} p &= x_1 \exp\left(A_{12}\left(\frac{A_{21}x_2}{A_{12}x_1 + A_{21}x_2}\right)^2\right) p_1^{sat} \\ &+ x_2 \exp\left(A_{21}\left(\frac{A_{12}x_1}{A_{12}x_1 + A_{21}x_2}\right)^2\right) p_2^{sat}. \end{aligned} \tag{1}$$

   Here the saturation pressures are given by the Antoine equation

$$\log_{10}(p^{sat}) = a_1 - \frac{a_2}{T + a_3}, \tag{2}$$

   where $T = 20(°\mathrm{C})$ 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 ($x_1 + x_2 = 1$). x_1 is for water.

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 Table 1: (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?

2. Solve the following problem using Bayesian Optimization:

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

   for $x_1 \in [-3, 3]$ and $x_2 \in [-2, 2]$. You can use an off-the-shelf Bayesian Optimization solver.