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 $T = 20(^\circ\text{C})$ 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:

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

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

3. (Bonus 20 Points) Read the ANSYS DOE and Design Optimization Tutorial. Choose **ONE** of the analyses (structural, modal, or thermal) and optimize the related objective (e.g., minimize the maximum Von Mises stress, maximize the first natural frequency, or minimize the maximum temperature) with respect to geometry parameters. Please report the followings:

   - What are your design variables, constraints, and objectives?
   - What design of experiment method do you use?
   - What response surface method do you use?
   - How do you validate your response surface?
   - What optimization method do you use?
   - How do you validate your optimal solution?