ME555 Homework 3

1. (50 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

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

   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. 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 Table 1: (1) Formulate the least square problem; (2) solve using your own gradient descent or Newton's implementation; (3) solve using Matlab functions "lsqnonlin" or "lsqcurvefit".

2. (50 Points, Optional for MAE494) Download the data "homework3data.mat". The data contains a set of topologically optimal brackets. Each row of "X" represents a bracket structure and "y" the corresponding loading force angle. Build a metamodel using "X" as input and "y" as output, by means of a neural network or support vector regression. Instruction: You can use the MATLAB neural net toolbox and the libsvm package. The neural net toolbox automatically reports test performance. In libsvm, enable crossvalidation and report its result.