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

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

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. (30 Points) 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, e.g., using a neural network. Instruction: If your Matlab does not come with the neural net toolbox, you can find it from the CAD lab (on GWC 4th floor). The neural net toolbox automatically reports test performance.

3. (20 Points, Optional for MAE494) Logistic regression is commonly used to approximate systems with binary outputs, e.g., the result of an election, a football game, a purchase on Amazon, etc. The mathematical form of a logistic regression model is as follows:

$$p(y; \mathbf{x}, \theta) = \frac{1}{1 + \exp(-y\theta^T\mathbf{x})}, \tag{3}$$

where y is the output that takes either 1 or -1, $\mathbf{x}$ are the input variables (covariates), θ are the unknown parameters. Given a dataset $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$, the likelihood of θ can be written as

$$L(\theta; D) = \prod_{i=1}^{N} \frac{1}{1 + \exp(-y_i \theta^T \mathbf{x}_i)}. \tag{4}$$

Is the maximum likelihood estimate of θ unique? Hint: To obtain the maximum likelihood estimate of θ, one needs to minimize the negative log-likelihood function.

4. (10 Points) Please go through this tutorial on creating a metamodel using a deep convolutional neural network to predict Young's modulus of sandstone structures. There is an instruction on installing Keras and Tensorflow. Please attach your results.

5. (20 Points, bonus) For the data in Problem 2, can you build a model that takes in "y" and outputs "X" (instead of taking in "X" and output "y"), i.e., can you predict the optimal topology based on the input force angle? Show your attempts. For example, you can plot two data points (two topologies for different angles), and plot a new topology predicted from your model for an angle in between the data points. The ground truth (true optimal topologies) for any input force angles can be computed using this code. **Note:** You can take this problem as your project.