THE UNIVERSITY OF HONGKONG
DEPARTMENT OF PHYSICS

Final Exam

Course: *Machine Learning in Physics (PHYS3151)* – Professor: *Dr. Ziyang Meng*
Date: *May. 13th, 2022* Time: *9:30 am - 11:30 am*

A: Students have to answer all 4 questions. Please submit a pdf file containing all the solutions and submit all your codes used for generating your answers.

B: This is an online open-book exam. Candidates are permitted to refer to the following online/printed/handwritten materials in the examination: textbook, lecture slides, assignment handout, colab examples, and self-made notes.

C: Internet searching and crowdsourcing from group messages, online forums or social media, etc. are strictly forbidden.

1. **Multivariate Linear Regression. (25)**

   (a) What is the hypothesis, the cost function, and the Hessian Matrix of Multivariate Linear Regression?

   (b) Please explain the difference between Gradient Descent, Steepest Descent, and Conjugate Gradient method.

   (c) Quadratic potential is very common in physics systems, for example, the potential energy of a simple harmonic oscillator is quadratic in x (the distance away from the equilibrium position), and therefore physicists are very often asked to perform optimization or finding the minimal of quadratic potentials. Here we have the potential of the form $f(x) = \frac{1}{2}x^T A x - b^T x + c$, where $A = \begin{pmatrix} 30 & 15 & 22 \\ 15 & 26 & 12 \\ 22 & 12 & 25 \end{pmatrix}$, $b = \begin{pmatrix} 8 \\ 2 \\ 6 \end{pmatrix}$, and $c = 12$. Please use the Conjugate Gradient method to find the minimum of the potential. Note that you need to write codes from scratch for this problem.

2. **Logistic Regression and SVM. (30)**
   Classifying states of matter is the task of physics, such as classification of liquid, gas and solid, separating magnet and paramagnet. Logistic regression and SVM are being used by physicists to solve the classification problems with the data generated from experiments or numerical simulations. Solving the following problem will bestow you with the ability of classify physical problems.

   (a) In the course project, we have solved a 2D Ising model with Metropolis algorithm and calculated several physical observables. The magnetization of the system for a certain configuration is defined as

   $$m(C) = \frac{1}{N}\sum_i S_i \tag{1}$$

   If $\langle |m| \rangle > 0.5$ is an ordered phase and else is the disordered phase. Please use the logistic regression to determine the Ising phase transition point T_C for $L = 4, 8, 10$ $m(T)$ data separately and analyze the results. Note that you need to write codes from scratch for this problem. You can download $m(T)$ data at github.

   (b) Please use the two features **SepalLengthCm** and **PetalWidthCm** of Iris.csv to separate the two species **Iris-setosa** and **Iris-versicolor** using SVM and draw the hyperplane and margins. Note that you need to write codes from scratch for this problem. Please find the data here.

3. **PCA and Clustering. (30)**
   The Ising model is named after Ernst Ising, Ph.D. in Physics (1924) from the University of Hamburg under the supervision of Wilhelm Lenz. Ising solved the one-dimensional (1D) Ising model exactly to find no phase transition at finite temperature. He also tried to provide arguments on why there would not

be a phase transition in higher dimensions either. In 1936, Peierls argued that both 2D and 3D Ising models admit phase transitions. And in 1944, Lars Onsager solved the 2D square lattice Ising model and analytically showed that the system undergoes a second order phase transition at the critical temperature $T_c = 2J/\ln(1+\sqrt{2}) \approx 2.269J$ (usually we take $J = 1$). For temperatures less than T_c, the system magnetizes, and the state is called the ferromagnetic or the ordered state. This amounts to a globally ordered state due to the presence of local interactions between the spin. For temperatures greater than T_c, the system is in the disordered or the paramagnetic state. In this case, there are no long-range correlations between the spins.

In the course example, we performed PCA for 2D Ising model, and found the first component yields the magnetization order parameter because PCA finds linear combinations of the features that have the largest variance.

(a) Please randomly choose 100 Ising configurations from conf.csv, then compute the covariance matrix Σ, perform Singular Value Decomposition on Σ, and show all the eigenvalues and eigenvectors of Σ. You can download the data here.

(b) Again, use the data conf.csv, now using PCA to reduce the data to three-dimension and group the reduced data to three clusters using the K-means algorithm and make a 3D plot to represent the clusters. Note that you need to write codes from scratch for this problem. The data is here.

4. **Neural Networks. (15)**
In the question 2(a), we have performed logistic regression to find the continuous phase transition point of 2D Ising model. However, in the modern application of machine learning in Physics, physicists start to employ neural network to detect the different phases. It turns out that the AI is capable of finding the order parameter automatically. In this simple question, we will not be able to solve the Ising model with neural networks, however, one is required to show how to optimize the weights in a neural network with back propagation.

(a) Please draw a schematic plot of perceptron and mark all the essential components.

(b) As for the case in Figure 1, if we have two data: ($x_1^{(1)} = [3,2]$, $y_1^{(1)} = 2$), ($x_2^{(1)} = [5,1]$, $y_2^{(1)} = 1$), and initially we set $\Theta_{k,i}^{(l)} = 1$ for all the neurons. Please use the back propagation algorithm to calculate the partial derivative of the cost function (consider the case without regularization terms) with respect to all $\Theta_{k,i}^{(l)}$ for just one step. Note that the activation function for all the neurons are sigmoid functions. And you need to write codes from scratch for this problem.

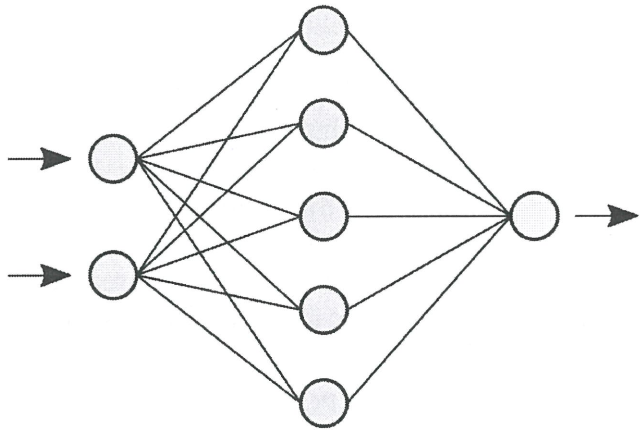

Figure 1: Fully connected feedforward network with one hidden layer and one output layer.

*************** END OF PAPER ***************