THE UNIVERSITY OF HONGKONG DEPARTMENT OF PHYSICS

Assignment 5

Course: *Machine Learning in Physics (PHYS3151)* – Professor: *Dr. Ziyang Meng*Due date: *Apr. 25th, 2023*

This assignment is also a project, you will need to deliver a presentation on how you solve the questions as well as your results.

2D Ising model phases classification

In this assignment, we are going to use Neural Network to classify phases (ordered or disordered) for a given configuration of the 2D Ising model.

In all questions, you need to use data files $Ising_conf.csv$ and $Ising_temp.csv$ from the Github folder $feedforward_neural_network/Ising$. The $Ising_conf.csv$ contains 5000 configurations of a 10×10 system obtained by Monte Carlo simulation, and the 100 columns are spin orientations on every lattice sites. $Ising_temp.csv$ contains the corresponding temperature of each configuration, going from 0.25 to 4 with step 0.25.

For the 2D Ising model, there is a critical temperature $T_c \approx 2.269$, below which system is in ordered state, and disordered above.

1. Data Processing

- (a) Load the data files from Github, use the configurations as features X. Standardize it by subtracting corresponding column-wise means and dividing by column-wise standard deviations.
- (b) Construct the expected output list Y, where Y[i]=1 if its corresponding temperature T[i] is below T_c , and 0 otherwise. i.e. It tells if the system is ordered or disordered.
- 2. **Model Construction** Construct two Neural Networks with the following parameters.
 - (a) 100 input neurons, one hidden layer with 2 neurons, and 1 output neuron.
 - (b) 100 input neurons, two hidden layers with 2 neurons on each layers, and 1 output neuron.

In both cases, the output neuron is a number from 0 to 1. If its value is above 0.5, the model predicts the input configuration to be in ordered state (y=1).

3. **Model Training** Randomly divide the 5000 configurations into training set with 1000 data and testing set with 4000 data. The testing set should only be used to evaluate the models but not in updating the weights. Train the models using back propagation discussed in the lecures. Store lists for the following variables obtained during iteration of each training.

- (a) Cost *J* calculated from training set.
- (b) Accuracy calculated from training set.
- (c) Accuracy calculated from testing set.

Hint: Accuracy is calculated by matching the output value with y[i].

- 4. **Model Evaluation** For each fully trained network, perform forward propagation using all 5000 configuration, log the value of the output neuron.
 - (a) Make a scatter plot of the final output value against temperature.
 - (b) At each temperature, find the mean value of all points with the same temperature. Plot the mean value on the scatter plot.

Sample plots for the two models are as followed.

5. **Discussion** With the above variables and your own experience, compare the performance of the two model.

