THE UNIVERSITY OF HONG KONG
DEPARTMENT OF PHYSICS

Assignment 3

Course: *Machine Learning in Physics (PHYS3151)* – Prof.*Zi Yang Meng*
Tutor: *Mr. Tim Lok Chau*
Due date: *18th March, 2025*

This assignment is a project. You are required to deliver a presentation on how you solve the questions and your results. Efforts beyond the answer of these questions are welcome.

1. Sigmoid function

   In logistic regression, we use the sigmoid function $g(z) = \frac{1}{1+e^{-z}}$. Prove the following properties for the sigmoid function.

   (a) $g(z) + g(-z) = 1$

   (b) $g'(z) = g(z)g(-z) = g(z)[1 - g(z)]$

   (c) $g'(-z) = g'(z)$

   (d) $g''(z) = g(z)g(-z)[g(-z) - g(z)]$

2. One-dimensional Transverse field Ising Model

   The following Hamiltonian describes the one-dimensional transverse field Ising model, a basic quantum spin system,

$$H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x$$

   where σ_i^z and σ_i^x are the Pauli matrices representing spin components at site i, J is the exchange interaction, and h is the transverse magnetic field. At $T = 0$, the system exhibits a quantum phase transition at $h = 1$ for an infinite size system (in units of J).

   You will use the quantum Monte Carlo simulation data at different h with system length $L = 32$. Label the data with absolute magnetization $\langle |m| \rangle > 0.5$ as ordered phase (i.e. set its value to be 1) and else as disorder phase (i.e. set its value to be 0). Perform logistic regression on the data provided and determine the phase transition point h_c from the decision boundary. Compare your results with the figures in (1) and (2).

3. Two-dimensional ferromagnetic square lattice

   In a two-dimensional ferromagnetic square lattice, spin waves arise from collective excitations of spins, which is described by the following energy-momentum relation,

$$E(k_x, k_y) = JS\left(4 - 2\cos(k_x a) - 2\cos(k_y a)\right)$$

where J is the exchange interaction, S is the quantum spin number, a is the lattice constant, and (k_x, k_y) are the x and y component of the momentum. This model is fundamental in understanding magnetism in low-dimensional systems.

We set $J = 1$, $S = \frac{1}{2}$, $a = 1$ and $(k_x, k_y) \in [-\frac{\pi}{a}, \frac{\pi}{a}]^2$ in the following of our calculation. Since the result is symmetric in each quadrant, you are only required to show the result in the first quadrant of (k_x, k_y). Use the function in notebook SVM_Fermi_Surface.ipynb to complete the following question and you may need to try a few times with different random samples of points $\{(k_x, k_y)\}$ to see the effect of randomness.

(a) Plot a function $E(k_x, k_y)$ in the region $(k_x, k_y) \in [-\frac{\pi}{a}, \frac{\pi}{a}]^2$.

(b) Set the energy $E(k_x, k_y) = 2$. Perform logistic regression and support vector machine with feature $X_1 = [k_x, k_y]$, $N = 100$ sample points, 20,000 iteration steps, evaluate the performance of these two methods on drawing the energy contour. Please, the **result of two methods and the energy contour on the** (k_x, k_y) **space.** You can refer to the plots (3), (4).

(c) At energy $E(k_x, k_y) = 0.5$, the straight-line boundary might not be suitable to approximate the energy contour. Also, since x and y directions are equivalent in this model, the Fermi surface should be symmetric along $x = y$. In other words, the coefficients of Θ in k_x and k_y terms should equal, the same goes for k_x^2 and k_y^2. We can manually enforce this condition by introducing symmetric features for the fitting.

Consider the following features $X_2 = [k_x + k_y, k_x^2 + k_y^2, k_x * k_y]$. Perform SVM and logistic regression with $N = 500$ sample points and 20,000 iteration steps, and show the result of two methods and the Fermi surface on the (k_x, k_y) space. You can refer to the plot (5), (6).

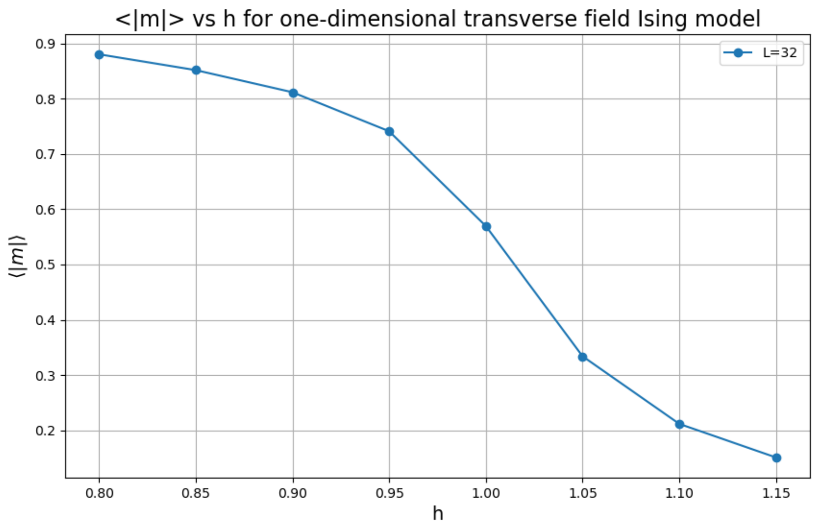


Figure 1: Absolute magnetization versus magnetic field strength h of one-dimensional transverse field Ising model.

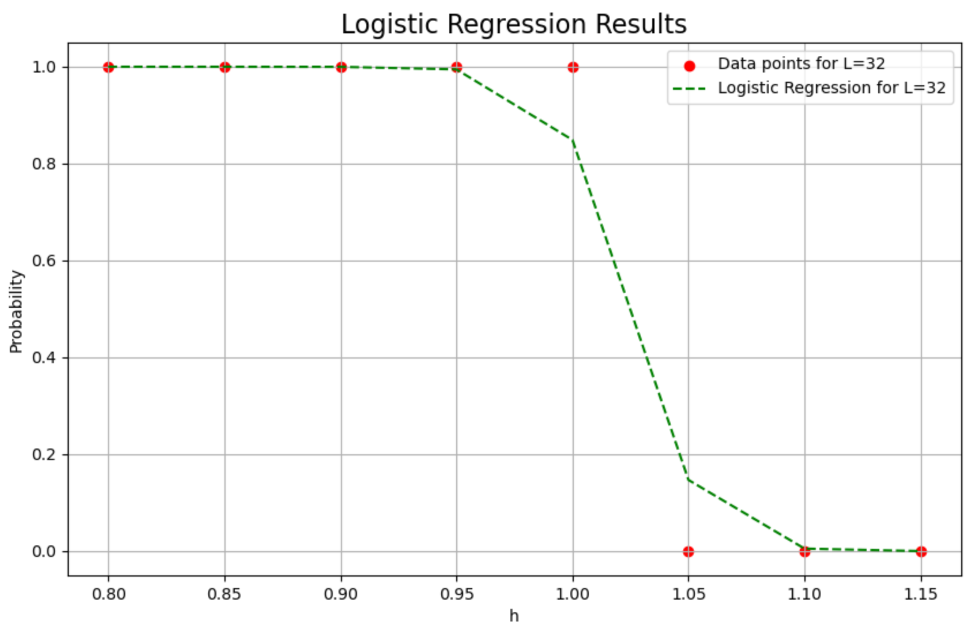
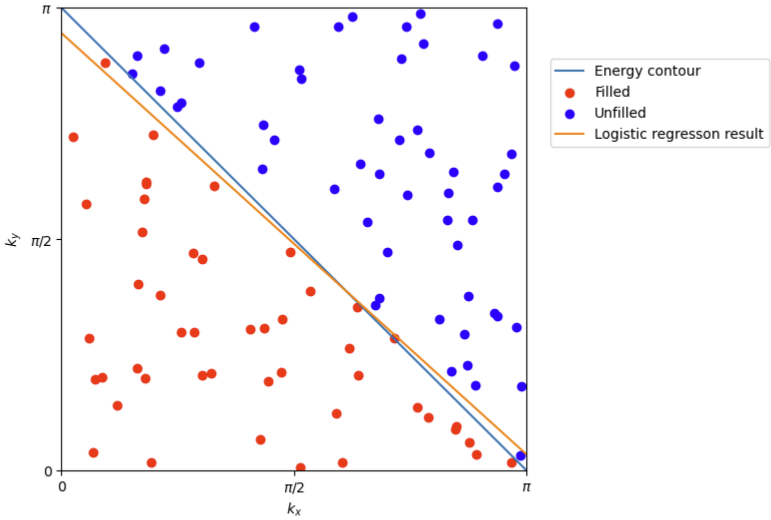
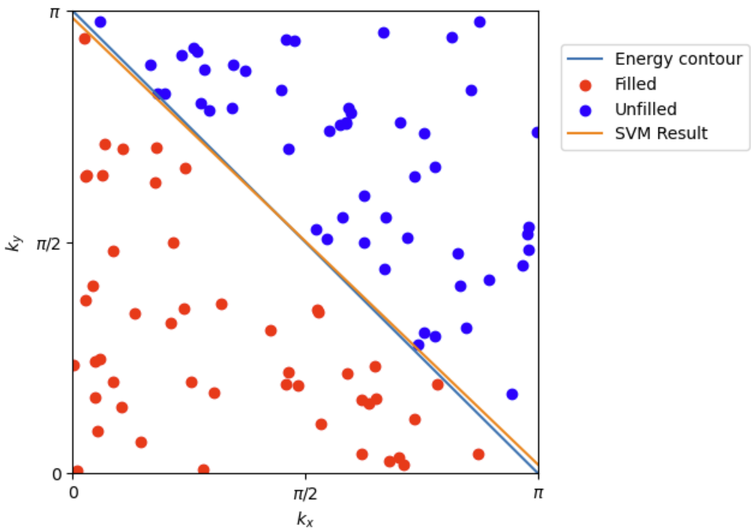


Figure 2: Right: Result of logistic regression after 500,000 iterations.



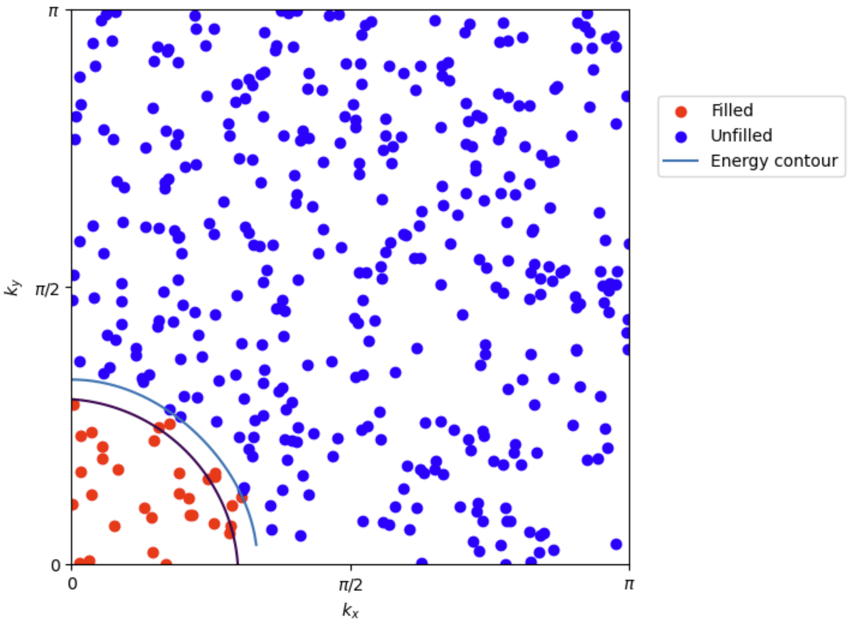
0.5

Figure 3: Question 3b) - Logistic regression result



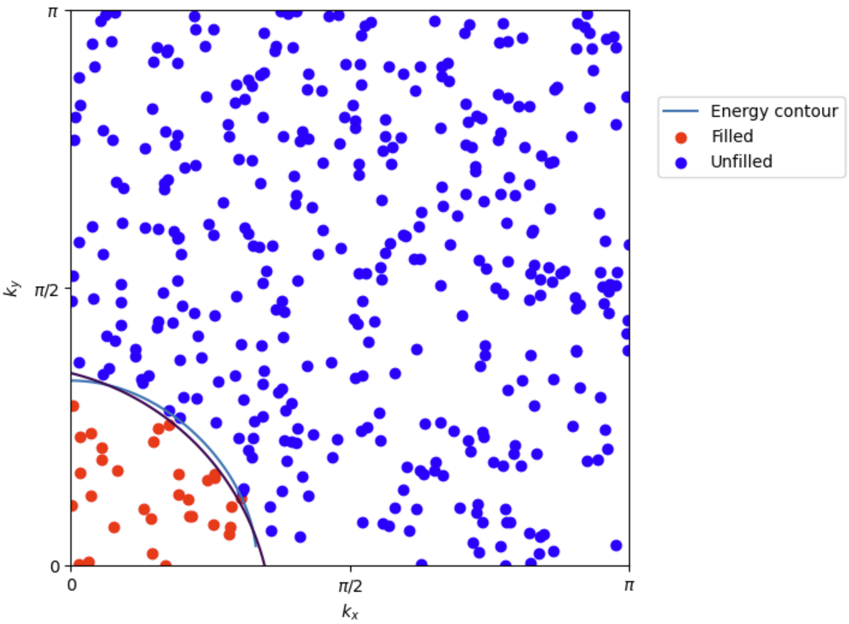
0.5

Figure 4: Question 3b) - SVM result



0.5

Figure 5: Question 3c) - Logistic regression result



0.5

Figure 6: Question 3c) - SVM result