Machine Learning for Phase Transition in 1D Transverse Field Ising model

First Milestone: Data

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In this project, we seek to find the phase transition point in one dimensional Transverse-field Ising model and classify different phases, using Machine Learning methods. For the first milestone, we solve the model numerically in MATLAB using Exact diagonalization (ED) technique, then we calculate quantities that are helpful for our problem and collect them as our data set. In this report, we put some information about the theory of this model, then we'll explain how we produced these data sets and what are some of the statistical properties of them. At the end we will mention some related articles and write about their relevance to our project.

1 Introduction

Spin is a quantum mechanical property of an electron and is related to angular momentum. Since the 20th century, spin has became an important feature for physicists. One of the most important models which includes more and more spins is Ising model. One can calculate some variables such as energy, correlation functions, entanglement entropy, etc. But if we look closely to these models, we can find out a phase transition. Indeed, phase transition is a thermodynamic phenomenon and it occurs in thermodynamic limit of a system. Everyday we observe it in our life, for example melting and evaporating are just some simple examples. In other magnetic systems, the phase transition happens when the magnetic property of the model has changed, i.e, phase transition from paramagnetic order to ferromagnetic one.

Like the other magnetic systems, Ising model does have phase transition. For instance, in 2D classical Ising model, at some critical temperature T_C, we have a phase transition. But what about the quantum mechanical one? In the next section, we will study the exact solution of the quantum Ising model, but before that, we should mention that there will be a critical point which is independent from the temperature because of the transverse field. In sections 2 and 3 we'll find this critical point theoretically and explain our method for numerical solution.

2 Analytical Exact Solution

The Hamiltonian of the system is the following:

$$\mathcal{H} = -\sum_i (h\sigma_x^i + J\sigma_z^i\sigma_z^{i+1}) \tag{1}$$

where σ_αs are the Pauli spin operators. The spin operators satisfy the commutation relations given by (with $\hbar = 1$):

$$[\sigma_\alpha^i, \sigma_\beta^j] = 2i\delta_{ij}\epsilon_{\alpha\beta\gamma}\sigma_\gamma^k, \quad \alpha = x, y, z \tag{2}$$

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and also they satisfy the anti commutation relations given by:

$$\{\sigma_\alpha^i, \sigma_\beta^i\} = \sigma_\alpha^i \sigma_\beta^i = 0 \tag{3}$$

and

$$(\sigma_\alpha^i)^2 = 1 \tag{4}$$

on the same site.

This transverse field Ising chain Hamiltonian can be exactly diagonalized, and the entire eigenvalue spectrum and eigenfunctions can be calculated by Jordan-Wigner transformation.

Using a canonical transformation:

$$\sigma_x \to \sigma_z, \quad \sigma_z \to -\sigma_x \tag{5}$$

then we have

$$\mathcal{H} = -\left(h \sum_i \sigma_z^i + J \sum_i \sigma_x^i \sigma_x^{i+1}\right) \tag{6}$$

Also, we can rewrite the Hamiltonian in terms of the raising and lowering operators σ_+^i and σ_-^i where

$$\sigma_+^i = \frac{1}{2}(\sigma_x^i + i\sigma_y^i) \tag{7}$$

$$\sigma_-^i = \frac{1}{2}(\sigma_x^i - i\sigma_y^i) \tag{8}$$

By using Jordan-Wigner transformation, we define

$$c_i = \prod_{j=1}^{i-1} \exp\Big(i\pi \sigma_+^j \sigma_-^j\Big) \sigma_-^i \tag{9}$$

$$c_i^\dagger = \sigma_+^i \prod_{j=1}^{i-1} \exp\Big(-i\pi \sigma_-^j \sigma_+\Big) \tag{10}$$

These creation and annihilation operators, c_i and $c_i^\dagger$ satisfy:

$$\{c_i, c_i^\dagger\} = \delta_{ij} \tag{11}$$

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \tag{12}$$

The Pauli spin operators, σ_x^i and σ_z^i are then transformed as follows:

$$\sigma_x^i = 1 - 2c_i^\dagger c_i \tag{13}$$

$$\sigma_z^i = -\prod_{j=1}^{i-1}(1 - 2c_j^\dagger c_j)(c_i^\dagger + c_i) \tag{14}$$

Thus the Hamiltonian becomes:

$$\mathcal{H} = -J \sum_{i=1}^{N} (c^i c_{i+1} + \sigma + \sigma_{i+1}^\dagger c_i + \sigma_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i + \frac{h}{J}(1 - 2c_i^\dagger c_i)) \tag{15}$$

The above equation is already quadratic in the fermion operators and it is obviously diagonalizable. Therefore, let us consider fermions in momentum space (Fourier space):

$$c_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j \exp(ikR_j) \tag{16}$$

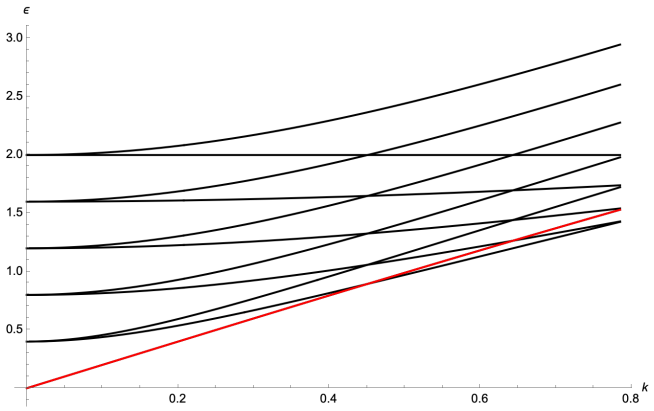


Figure 1: Elementary excitation energy as a function of k for different h. The red one is $h = 1$ and the other ones are the other h between 0 until 2

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} c_j^\dagger \exp(-ikR_j) \tag{17}$$

where $k = \frac{2\pi m}{N}$ and $m = \frac{-N-1}{2}, \cdots, 0, \cdots, \frac{N-1}{2}$ for even N and $m = \frac{-N}{2}, \cdots, 0, \cdots, \frac{N}{2}$ for odd N. The final Hamiltonian in momentum space is:

$$\mathcal{H} = J \sum_k (2(\frac{h}{J} - \cos(k) c_k^\dagger c_k - i \sin(k)(c_{-k}^\dagger c_k + c_{-k} c_k)) \tag{18}$$

to diagonalize this Hamiltonian, we should use the Bogoliubov transformation,

$$\gamma_k = u_k c_k - i v_k c_{-k}^\dagger \tag{19}$$

where γ_k is a new fermionic operator and u_k and v_k are real numbers which satisfy

$$u_{-k} = u_k, \quad v_{-k} = v_k \tag{20}$$

$$u_k^2 + v_k^2 = 1 \tag{21}$$

By this transformation, finally the Hamiltonian can be diagonalized:

$$\mathcal{H} = \sum_k \epsilon_k (\gamma_k^\dagger \gamma_k - \frac{1}{2}) + const. \tag{22}$$

$$\epsilon_k = 2J(1 + \frac{h^2}{J^2} - 2\frac{h}{J}\cos(k))^{\frac{1}{2}} \tag{23}$$

where the constant is the zero-point energy of the spinless fermion system, which is given by

$$E_0 = -\sum_k \epsilon_k \tag{24}$$

If we plot the elementary excitations as a function of wave vector k for different values of h (Figure 1), we can see there is an energy gap in the excitation spectrum of the system at $k = 0$ for $h_c = 1$.

3 Numerical Solution and Data generation

3.1 Exact diagonalization technique

Since our model is a finite system (chain of N atoms) and we need the most possible exact numerical solution to obtain our data, we decided to use Exact diagonalization (ED) technique. It's a common

numerical technique used in physics to determine the eigenstates and energy eigenvalues of a quantum Hamiltonian. In this technique we should express the Hamiltonian in a matrix form in order to diagonalize it by computer. First we need to construct pauli matrices to build the Hamiltonian, in this part we used sparse structure to minimize memory cost and speed up the code. Again, we write the Hamiltonian of the system which is

$$\mathcal{H} = -\sum_{i=1}^{N}(h\sigma_x^i + J\sigma_z^i\sigma_z^{i+1}) \tag{25}$$

where we choose $N = 12$, $J = 1$, and $h \in [0, 7]$. We want to find the phase transition point, called h_c and we expect it to be $h = 1$ as the analytical solution predicts. In our Hamiltonian, we have tensor products of Pauli matrices to find the spin operators for each site so

$$\sigma_z^i = \underbrace{I \otimes I \otimes \cdots \otimes I}_{\text{i-1}} \otimes \sigma_z \otimes \underbrace{I \otimes I \otimes \cdots \otimes I}_{\text{N-i}} \tag{26}$$

$$\sigma_x^i = \underbrace{I \otimes I \otimes \cdots \otimes I}_{\text{i-1}} \otimes \sigma_x \otimes \underbrace{I \otimes I \otimes \cdots \otimes I}_{\text{N-i}} \tag{27}$$

The next step is to diagonalize Hamiltonian by using *eig* function in MATLAB. This is the most important part of our numerical solution because we'll need the ground state wave function in order to calculate almost all of our features, as we know diagonalization means

$$\mathcal{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle \tag{28}$$

where $|\psi_n\rangle$ is the nth eigenvector (wave function) and E_n is the $n$the eigenvalue (energy). We seek to find the ground state. So we should find the minimum of E_n and call it E_{min} and the ground state $|\psi_{min}\rangle = |g\rangle$. We should mention that we have imposed periodic boundary conditions to our system.

3.2 Data

3.2.1 How the data is collected and what they physically mean?

Now that we have the ground state wave function, we begin to calculate physical quantities that will help us see the phase transition in our model. These quantities will be different features of our data. The most important feature is the spin - spin correlation functions (Figure 2):

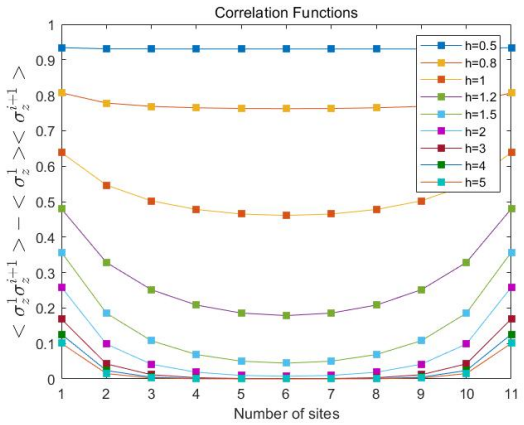
$$G(\sigma_z^i, \sigma_z^{i+1}) = \left\langle \sigma_z^i\sigma_z^{i+1} \right\rangle - \left\langle \sigma_z^i \right\rangle \left\langle \sigma_z^{i+1} \right\rangle \tag{29}$$

where $\langle C \rangle = \langle g|\, C\, |g\rangle$. As we can see in Figure 2.a , the visible gap between the $h = 1$ plot and other plots is a sign of phase transition in our model, also in Figure 2.b we can see that the $h = 1$ dashed line is like a vertical asymptote which is another sign to know that correlation function is a good feature. The next useful quantity is the mean of σ_x (Figure 3.a). In the other word, we try to find $\left\langle \sigma_x^i \right\rangle$. As we can see in Figure 3.a , again the $h = 1$ dashed line is like a vertical asymptote which is a sign for phase transition. The other helpful feature that we can calculate just by diagonalizing the Hamiltonian is the difference between the second excited state energy and the ground state energy (Figure 3.b). As it's shown in this Figure, this energy difference has it's minimum value at $h = 1$ which is the phase transition point.

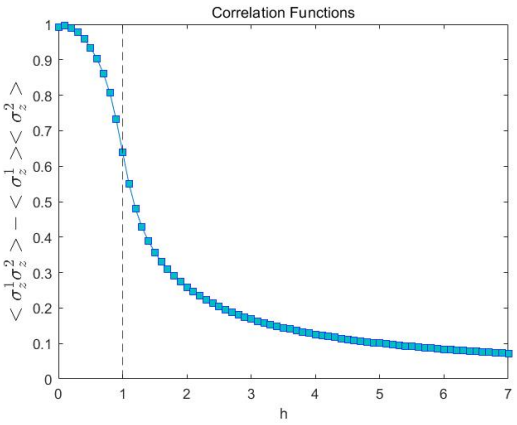
Considering that we have a transverse field applied to the system we guess that another good feature can be calculated by using σ_x . we'll call it μ_l (Figure 4) and again we calculate its expectation value which is defined by

$$\langle \mu_l \rangle = \left\langle \sigma_x^1\sigma_x^2 \cdots \sigma_x^l I^{l+1} \cdots I^N \right\rangle \tag{30}$$

Similar to the spin - spin correlation functions Figures, there's a gap between $h = 1$ plot and other plots in Figure 4.a and also in Figure 4.b the $h = 1$ dashed line is like a vertical asymptote which another sign for phase transition.

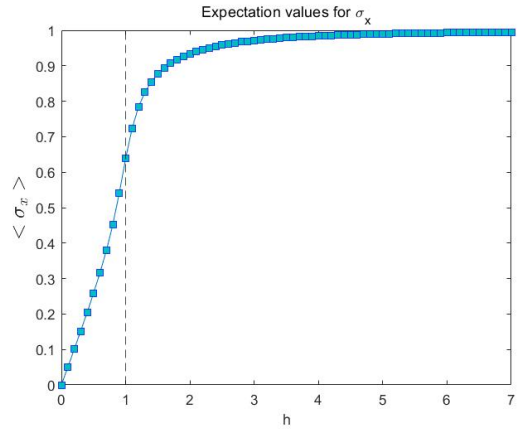


(a) Correlation functions of the first site as a function of its distance with others.

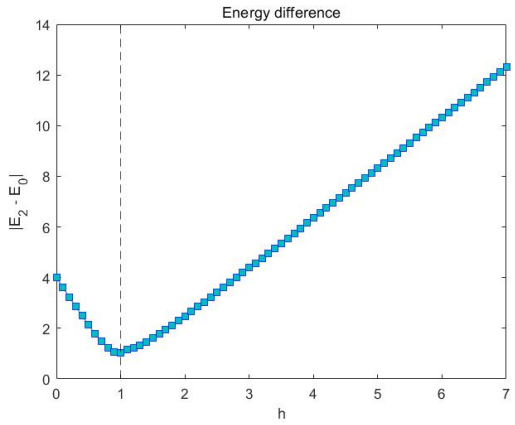


(b) Correlation function between the first and second site as a function of h

Figure 2: spin - spin Correlation functions

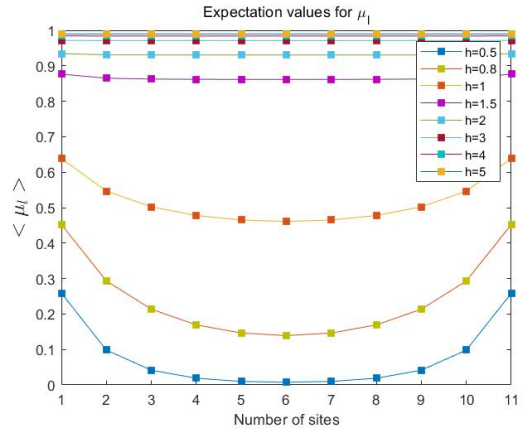


(a) $\langle \sigma_x \rangle$ as a function of h.

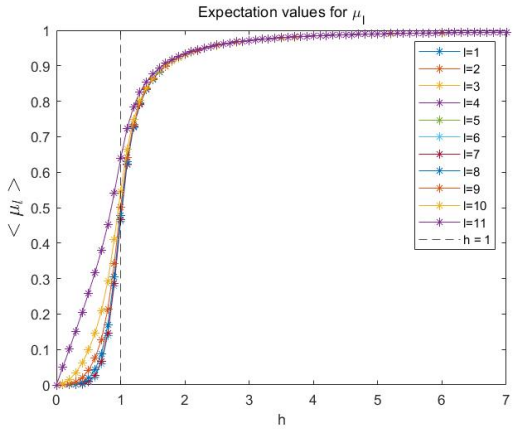


(b) E_2 - E_0 as a function of h.

Figure 3: Expectation value of σ_x and the Energy difference



(a) $\langle \mu_l \rangle$ as a function of number of sites



(b) $\langle \mu_l \rangle$ as a function of h

Figure 4: Expectation value of μ_l

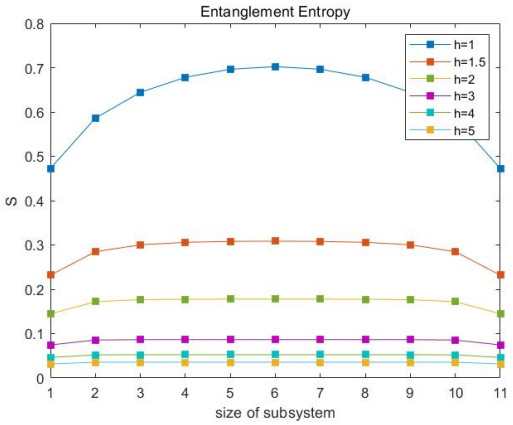
Other useful feature is Entanglement entropy for different subsystems in our chain (Figure 5). The first step is to find the Reduced Density Matrix (RDM) for $N-1$ possible subsystems. One easy method for this calculation is to reshape the ground state wave function in a form that is suitable for each subsystem. For example if we want to divide our chain to N_{left} spins and N_{right} spins ($N = N_{left} + N_{right}$) and then want to calculate reduced density matrix for N_{left} spins, our Hilbert space is $2^{N_{left}} \times 2^{N_{left}}$. So we reshape our $2^N \times 1$ ground state wave function to a $2^{N_{right}} \times 2^{N_{left}}$ matrix and call it $\tilde{\psi}_{left}$, hence we can calculate the reduced density matrix (ρ) by writing

$$\rho_{left} = \tilde{\psi}^{\dagger}_{left} \tilde{\psi}_{left} \tag{31}$$

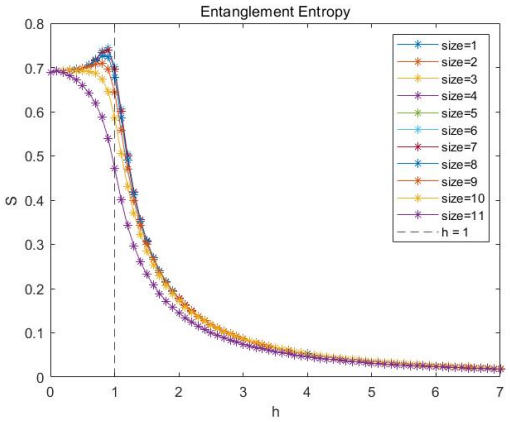
and we can easily see that it is a $2^{N_{left}} \times 2^{N_{left}}$ matrix. Then we diagonalize this ρ_{left} in order to find its eigenvalues (ω) and now we are able to calculate the Entanglement entropy using

$$S = -\sum_{k} \omega_{k,left} \log \omega_{k,left} \tag{32}$$

we repeat this procedure for all $N-1$ subsystems.



(a) Entanglement entropy as a function of size of subsystem.



(b) Entanglement entropy as a function of h.

Figure 5: Entanglement entropy

Apart from the gap for $h = 1$ plot in Figure 5.a, in Figure 5.b we see that the Entanglement entropy values drop at the phase transition point ($h = 1$) as it's shown with the dashed line, this is an evidence that the Entanglement entropy can also be cosidered a good feature. Now it seems that we have calculated many helpful features, but we know that the ultimate information about our system can be obtained from the ground state wave function and we haven't used it entirely unless we calculate all of the Higher order correlation functions and all other possible quantities, since it's not an efficient option due to the Computational cost that significantly increases the runtime, we decided to keep the ground state wavefunction (its 2^N numbers) so that we won't lose any substantial information about our model.

3.2.2 Cleaning up the data

As we mentioned before, we chose $h \in [0, 7]$. we covered this interval with small steps (0.01) and we calculated our features for different h's. So there're 701 samples in our data. Also we have 4186 features including spin - spin Correlation function, Expectation values for σ_x and μ_l, the Energy difference ($E_2 - E_0$), Entanglement entropy (S) and Wavefunction numbers. These are different labels in our data. Finally we cleaned up our data in form of a 701×4187 matrix. There are respectively 66 Correlation fuctions, one $\langle \sigma_x \rangle$, 11 $\langle \mu_l \rangle$, one Energy difference, 11 Entanglement entropy and 4096 ground state Wave function numbers. The last coloumn is y which is h in our model.

4 Data Analysis

In this part we want to inspect the data. We can see that there are 701 rows and 4187 columns . Consider that we don't know anything about these data sets and we want to discover some of their properties. So for this purpose, first of all it is a good idea to plot the heat map of the correlations. This will give a brief information about the columns (Figure 6). As we can see in Figure 6, there isn't any correlation between some blocks and it shows that we have to concentrate on different parts of the data, for instance maps of Figure 7, Figure 8 and Figure 9 are more specific and will give us better prospective to our data. As we know that there're periodic boundary conditions in our model we can expect the correlation heat map for the spin - spin correlation functions to have a symmetry.

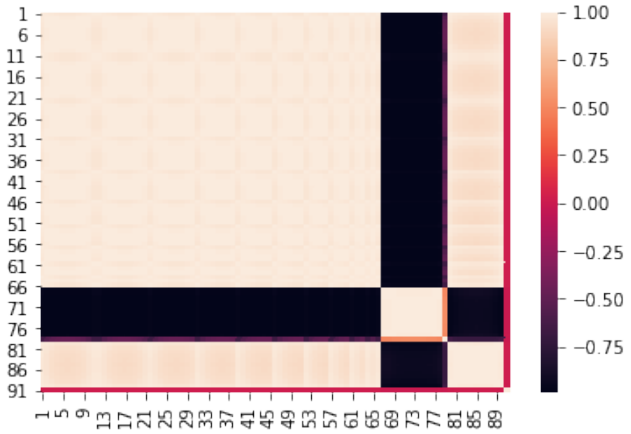
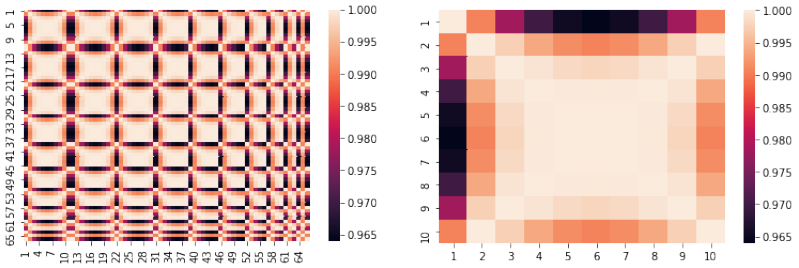
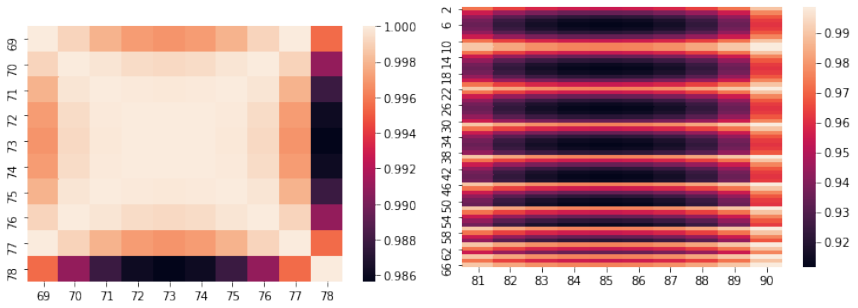


Figure 6: Correlation heat map of the data excluding wavefunctions



(a) All columns (b) The first 10 columns

Figure 7: Correlation heat map of the spin - spin correlation functions



(a) Expectation value of μ_l (b) Entanglement entropy and correlation function

Figure 8: Correlation heat map of the other features

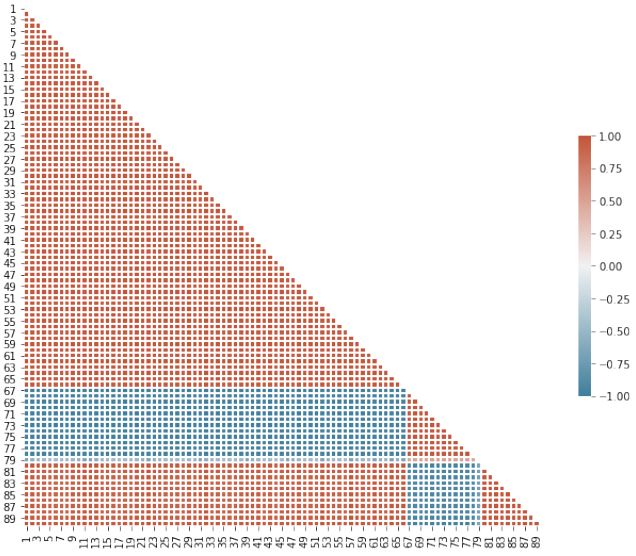


Figure 9: Correlations from the other view

Now we concern about the histogram of the data. Hence, we do some play with these columns and find out that if we break the data in some parts and plot the histogram for each part, then it will tell a good and brief description of the data. (Figure 10)

5 Related Articles

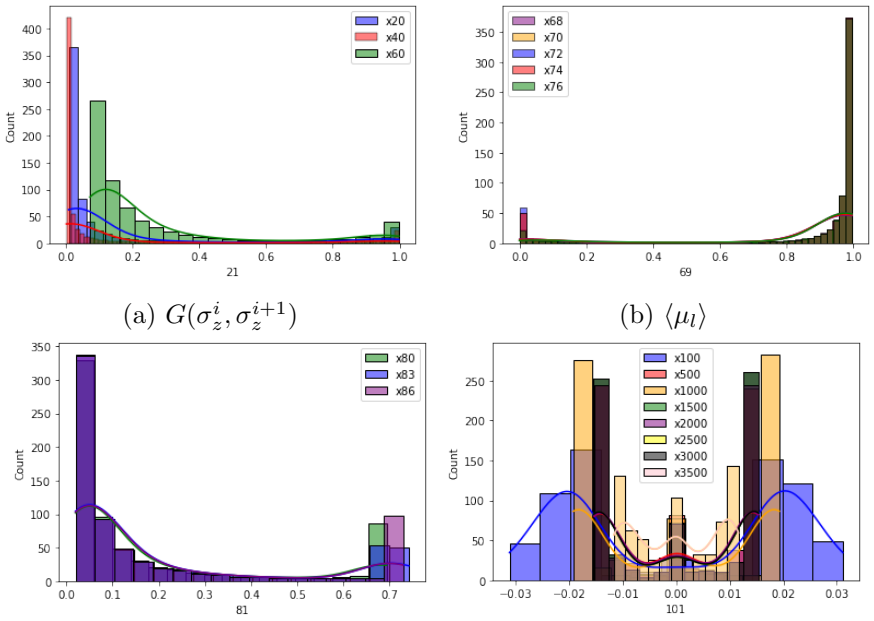
Now we try to mention some papers that are relevant to our project.

1. J. Carrasquilla and R. G. Melko "Machine learning phases of matter"
In this article the authors try to use Machine Learning techniques to detect phase transitions of matter, especially for quantum ising model for first time. They showed that the Classification of phases occurs within the neural network without knowledge of the Hamiltonian or even the general locality of interactions. This article is the basis of our project with the difference that they worked on 2D square-lattice but we are working at 1D chain of 12 atoms.

2. C. Bauer and K. Hyatt "Quantum Ising Phase Transition"
Bauer and Hayatt in this article try to find the transition of phase in Ising model numerically. By the exact diagonalization of the Hamiltonian at first, they found the ground state wave function and then they checked out the effect of transverse magnetic field on overall magnetization and tried to find phase transition. We did a similar process to obtain our data.

3. F. D'Angelo1 and L. Böttcher "Learning the Ising model with generative neural networks"
The authors of this article trained the Ising model to machine with the technique of neural networks. They used Restricted Boltzmann machine (RBM) which is particular type of stochastic neural networks to learn the distribution of Ising configurations at different temperatures. This enabled them to examine the ability of RBMs to capture the temperature dependence of physical features such as energy, magnetization, and spin-spin correlations.

4. A. V. Uvarov, A. S. Kardashin and J. D. Biamonte "Machine Learning Phase Transitions with a Quantum Processor"
The above article tries to use Machine Learning phase transition as a tool to classify phases of matter with Quantum Processor. This article proposed a nearest-neighbour quantum neural network. This quantum classifier is successfully trained to recognize phases of matter with %99 accuracy for



(a) $G(\sigma_z^i, \sigma_z^{i+1})$ (b) $\langle \mu_l \rangle$

(c) S (d) Eigenfunctions

Figure 10: Histogram of the data

the transverse field Ising model.

5. Han-qing Shi, Xiao-yue Sun and Ding-fang Zeng "Neural-network Quantum State of Transverse-field Ising Model"

In this article, they tried out neural-network quantum state (NQS) representation and machine learning method to reconstruct the ground state of the Transverse-field Ising Model (TFIM), both in one and two dimensions, and calculated its key observables, especially the entanglement entropy (EE). For the Stochastic Reconfiguration (SR method), they provided an understanding based on least action principle and information geometry.

6. Wei Zhang, Lei Wang and Ziqiang Wang "Interpretable Machine Learning Study of Many-Body Localization Transition in Disordered Quantum Ising Spin Chains"

They applied machine learning to the classification of two different phases, the eigenstate thermalization hypothesis (ETH) and the Many-body localization (MBL). They built and operated the support vector machine (SVM), designed for the random transverse field Ising chain. They demonstrated that the trained SVM with appropriate kernel choice is able to distinguish the two phases and determine the phase boundary. They trained data from two different energy densities to make the trained SVM work for the whole energy spectrum. This fact ensures that during the training process, the models are built on properties of the MBL phase itself which should not depend on energy. They studied and understood how the SVM makes the decision. They found evidence that the SVM has the ability to automatically choose 2 a decision function which is very closely related to the many-body inverse participation ratio (IPR) defined in the configuration space.

7. Remmy Zen, Long My, Ryan Tan, Frederic Hebert4, Mario Gattobigio, Christian Miniatura, Dario Poletti and Stephane Bressan "Finding Quantum Critical Points with Neural-Network Quantum States"

They had an approach to finding the quantum critical points of the quantum Ising model using innate restricted Boltzmann machines (RBMs), transfer learning and unsupervised learning for neural-network quantum states (NQS). They showed that their approach can significantly improve the efficiency and effectiveness of a simple network like RBM.

References

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