

Data Analysis and Machine Learning

Project 2

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FYS-STK 4155

December 29, 2018

Abstract

This project is devoted to study of Ising model using different statistical methods. We begin with linear regression then move to classification of spin configurations using either logistics regression and neural network. LASSO regression provide the best results among the regression methods with $R^2 = 1$ and $MSE = 10^{-6}$ for $\lambda = 10^{-3}$. Neural network and logistic regression (ADD).

1 Introduction

Data science is one of the most rapidly developing parts of information technologies nowadays. The increase of computer power allow us to analyze huge amounts of data and this require some specific methods and techniques to be studied. Some of them have been already under consideration in the previous project, for example simple regression methods - linear, Ridge and Lasso. In this project we aim to tackle a classification problem using logistics regression. After that our goal is to move towards the neural network. The problem we are going to use as a test bed is Ising model.

Structure of the report. The first part is a theoretical description of the 1D and 2D Ising model. Second part is a brief description of the methods. After this we move to the results and discussion part. The last part is conclusion where we present a brief summary of what have been done and also discuss some possibilities for further research.

2 Problem description

This project is mostly based on the work of Metha et al. [1] and that's why we are using the problem formulation provided in this article. However, Ising model is a well known model in physics and one may find many studies devoted to the model. For example, it's one of the natural choices to study Monte Carlo

simulations, as it have been done here (REF to project 4).

Ising model is a model that allows us to compute the energy of a system of spins. Each spin can take only two values ± 1 . The interaction is allowed only for closest neighbors. Generally speaking the Ising model provides us a simple approach to model the phase transitions of a ferromagnet. Phase transitions are transitions between ordered or disordered states. As soon as ordered state is more preferable for lower temperatures and disordered state is more preferred for higher temperature there shoud be some critical temperature when the switch is happening. In the project we will study 1D and 2D Ising models and the periodical boundary conditions are used. For the 1D Ising model there is no phase transition, while for the 2D the phase transition is happening at the critical temperature $T_c/J = 2/\log(1 + \sqrt{2}) \approx 2.26$.

2.1 1D Ising model

The Hamiltonian for the classical 1D Ising model is given by

$$H = -J \sum_i^N S_i S_{i+1}, \quad S_i \in \{\pm 1\}, \quad (1)$$

where N is number of particles in the system, and S_i is a spin pointing up or down.

2.2 2D Ising model

The Hamiltonian for the classical 2D Ising model is given by

$$H = -J \sum_{\langle ij \rangle}^N S_i S_j, \quad S_j \in \{\pm 1\}, \quad (2)$$

where the lattice site indices i, j run over all nearest neighbors of a 2D square lattice, and J is some arbitrary interaction energy scale. Onsager proved that this model undergoes a thermal phase transition in the thermodynamic limit from an ordered ferromagnet with all spins aligned to a disordered phase.

2.3 Ising model for statistical methods

In order to apply the regression methods to the Ising model we need to rewrite the equations in terms of so-called coupling coefficient J_{ij} as:

$$H = - \sum_{\langle ij \rangle}^N J_{ij} S_i S_j. \quad (3)$$

Now we can apply regression to determine the J_{ij} . In order to use classification methods, for example logistics regression, we use already prepared 2D spin configurations that have been prepared by Metha et al. in [1].

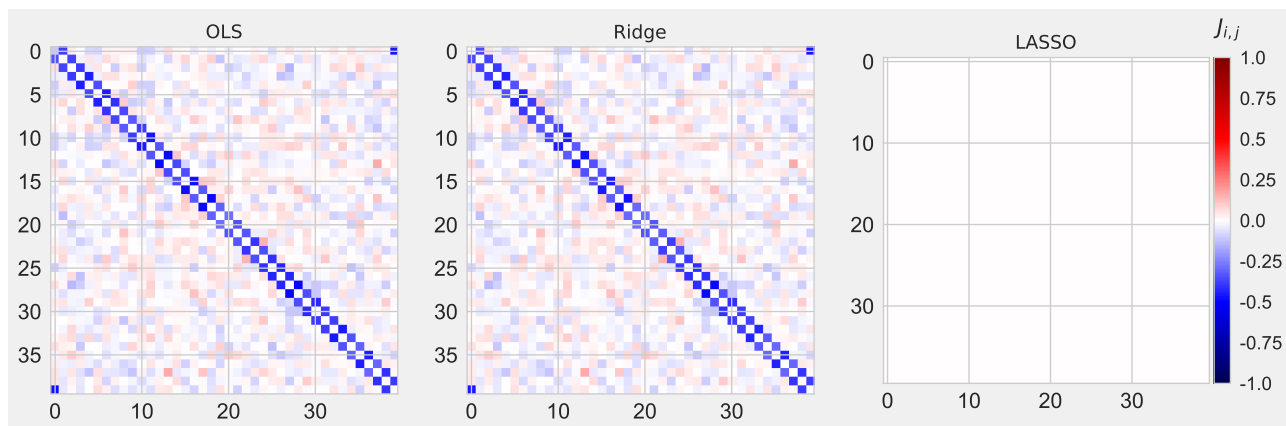


Figure 1: $\lambda=10.0$

3 Methods

3.1 Logistic Regression

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3.2 Neural networks

Neural networks are very popular in the field of machine learning. The name "neural" refer to the fact that such networks are supposed to mimic a biological system of communicating neurons. Neural network is a network of layers each of them containing an arbitrary number of neurons. The connection in this case is represented by a weight.

The artificially build neural network should be able to behave similarly to a real neural network in human brains.

4 Results and discussion

5 Conclusion

6 Further work

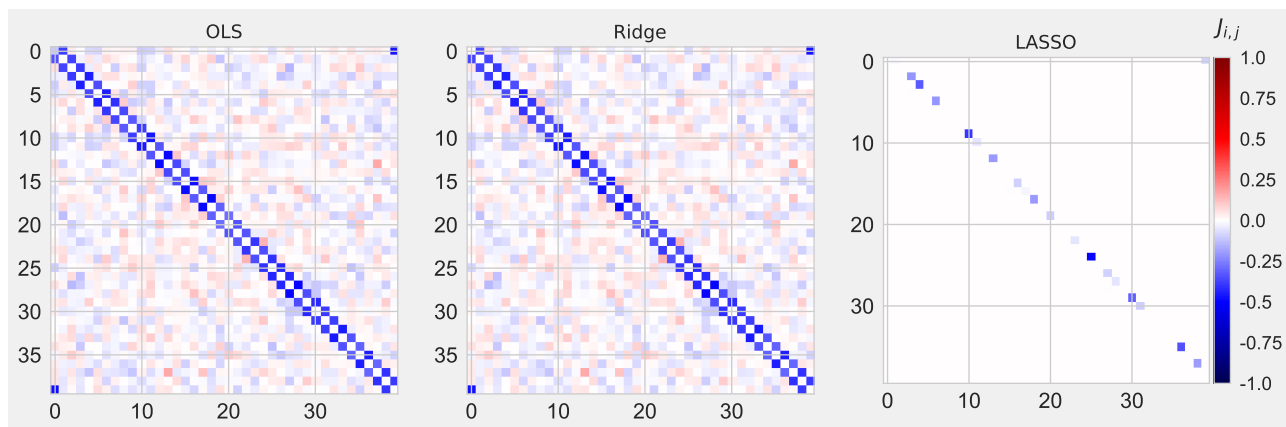


Figure 2: $\lambda=1.0$

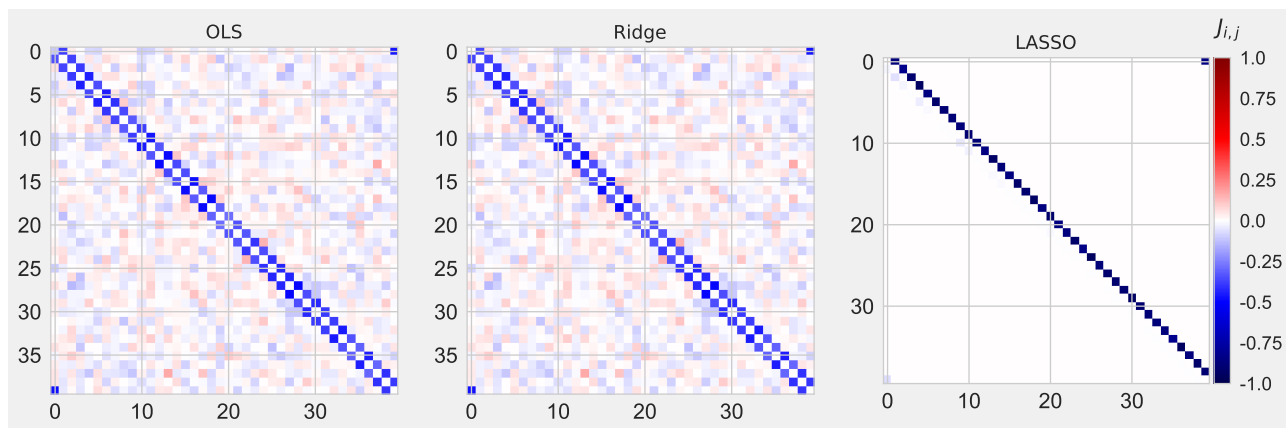


Figure 3: $\lambda=0.1$

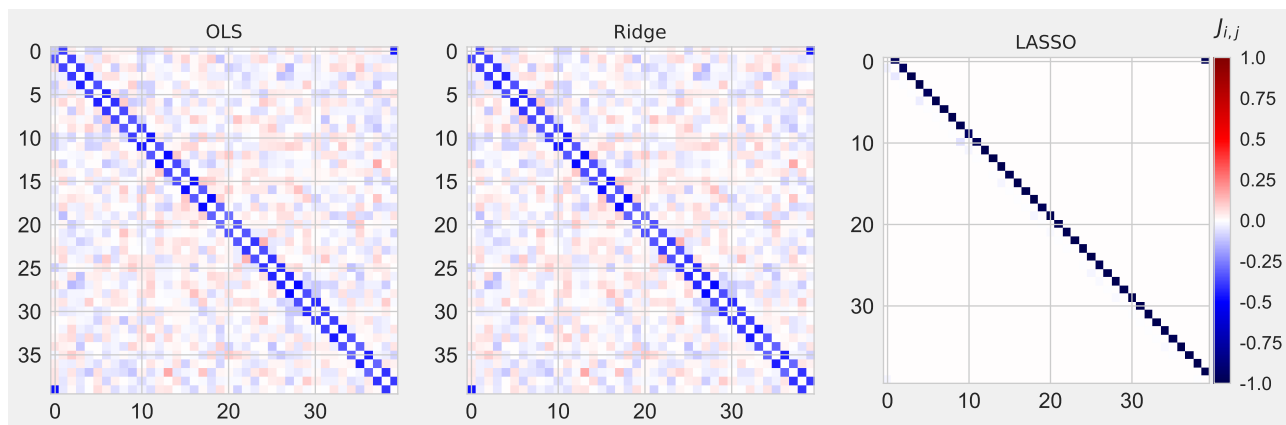


Figure 4: $\lambda=0.01$

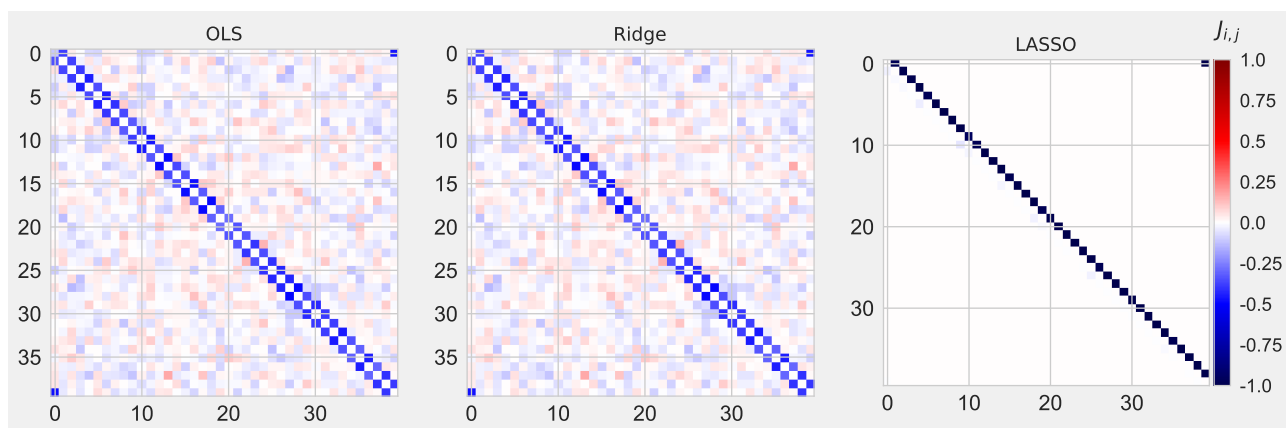


Figure 5: $\lambda=0.001$

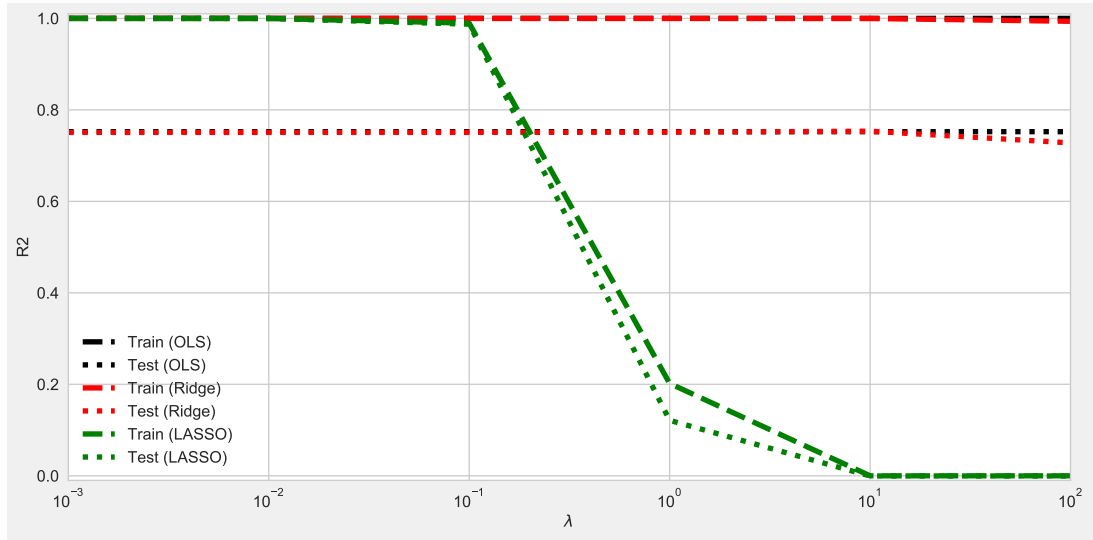


Figure 6: R^2

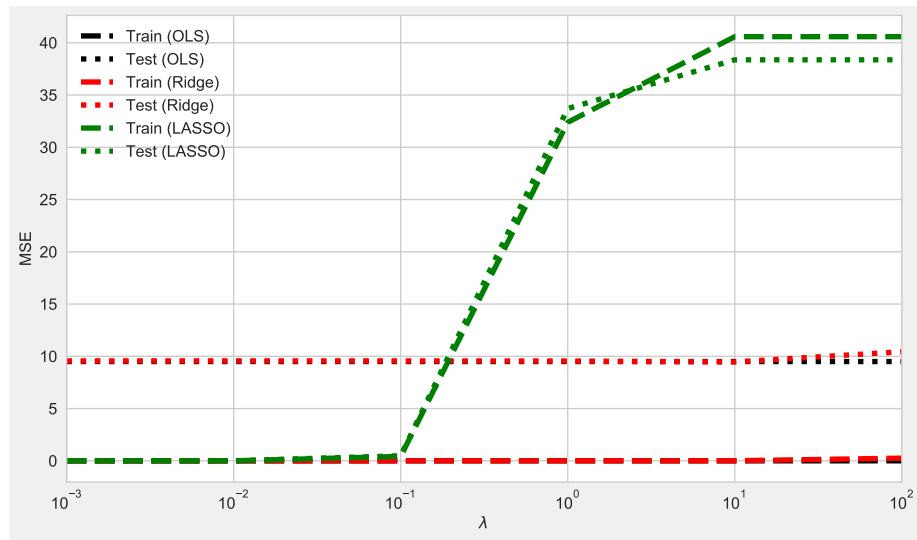


Figure 7: MSE

References

- [1] Pankaj Metha et al. *A high-bias, low-variance introduction to Machine Learning for physicists* ArXiv:1803.08823.