

Exploring the hyperspace of Machine Learning parameters

Eirik Ramsli Hauge, Joakim Kalsnes, Hans Mathias Mamen Vege

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Abstract

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1 Introduction

With the rapid expansion of computer power, data science is becoming an ever bigger part of modern society. Among the methods used to process data, some of the most popular are regression and classification. Through this paper we will look closely at the use of these methods when applied to data from the Ising model for spins. First of, we will use linear, ridge and lasso regression to estimate the coupling constant for the one-dimensional Ising model. Secondly, we move on to logistic regression and determining the phase of a spin matrix created by the two-dimensional Ising model. The latter problem is a classification problem and we will look further into it by creating a neural net. To learn more about the properties of a neural net, we will start by using the one-dimensional Ising model to find the optimal weights and biases in a regression case. Then we will apply what we learned by repeating the same classification as the logistic case, but this time we will train a neural net with a cross-entropy cost function to perform the task.

Our work is heavily inspired by the work of Metha et al. [6], and therefore it is only natural to compare our results to theirs. Lastly, we will give a detailed and in-depth analysis of the algorithms used and how our home-made algorithms compares to those of Metha et al. and similar calculations done by standard libraries such as scikit-learn or TensorFlow.

2 Theory

2.1 The Ising Model

The Ising model is a way of modeling phase transitions at finite temperatures of magnetic systems. When modeling, we set up a chain or a lattice of particles and allow them to have either spin up or spin down. From this, one can sample energy and magnetization, and measure several quantities such as the heat capacity or magnetic susceptibility. Our focus will be on prediction the energy coupling constant for a 1D lattice, and the phase of a 2D-lattice.

Periodic boundary conditions is given in both cases, such that $j = N = 0$, where j is the lattice site and N is the lattice size.

2.1.1 1-dimensional Ising model

Energy for a 1 dimensional Ising model is given as

$$E = -J \sum_{j=1}^N s_j s_{j+1} \quad (1)$$

where the N is number of particles(or lattice size). Our goal will be to predict J , but in order to do so, we must recast the problem as linear regression problem.

We begin by labeling each site as coupled with J .

$$E_{\text{model}}[\mathbf{s}^i] = - \sum_{j=1}^N \sum_{k=1}^N J_{j,k} s_j^i s_k^i, \quad (2)$$

where i is the index over lattice configurations. The coupling strength $J_{j,k}$ can now be cast as a matrix, and we end up with

$$E_{\text{model}}^i \equiv \mathbf{X}^i \cdot \mathbf{J}, \quad (3)$$

where \mathbf{X}^i is the design matrix consisting of all two-body interactions $\{s_j^i s_k^i\}_{j,k=1}^N$, and \mathbf{J} the weight matrix we wish to find later using machine learning techniques.

2.1.2 2-dimensional Ising model

The 2D Ising model has its energy stated as,

$$E = -J \sum_{\langle kl \rangle} s_k s_l, \quad (4)$$

where $\langle kl \rangle$ indicates a sum over the nearest neighbors. That is, written out,

$$E = -J \sum_{i,j}^N 2s_{i,j}(s_{i+1,j} + s_{i-1,j} + s_{i,j+1} + s_{i,j-1}), \quad (5)$$

where we have used the symmetry that $s_i s_{i+1,j} = s_{i+1,j} s_i$. J as as before a coupling constant, but will not be of our main focus when studying the 2D Ising model. This time, we will focus on its property of exhibiting phase transitions. Below a critical temperature of $T_C \approx 2.269$ found analytically by [8], the lattice will exhibit a ordered state, one in which the spins is *locked* or *frozen* into place. Above T_C the lattice exhibit a disordered phase, as the spins will be fluctuating randomly.

We will investigate the classification of states below $T < 2.0$ and $T > 2.5$. The phase for states between we will dub as being in a *critical phase*.

2.2 Logistic regression

In project 1 we used linear regression to predict a continuous output from a set of inputs [1, 10]. We used ordinary least squares regression (OLS), Ridge regression and Lasso regression, where the two latter impose a penalty to the OLS. In this project we will reuse the ideas and code of project 1, but we will also use neural networks to predict continuous variables. In addition we study situations where the outcome is discrete rather than continuous. This is a classification problem, and we will use logistic regression to model the probabilities of the classes.

2.3 Logistic regression

Just like a linear regression model, a logistic regression model computes a weighted sum of the predictor variables, written in matrix notation as $\mathbf{X}^T \beta$. However, the logistic regression returns the logistic of the this weighted sum as the probabilities. For a classification problem with K classes, the model has the following form [3, p.119],

$$\begin{aligned} \log \frac{Pr(G = 1|X = x)}{Pr(G = K|X = x)} &= \beta_{10} + \beta_1^T x \\ \log \frac{Pr(G = 2|X = x)}{Pr(G = K|X = x)} &= \beta_{20} + \beta_2^T x \\ &\vdots \\ \log \frac{Pr(G = K-1|X = x)}{Pr(G = K|X = x)} &= \beta_{(K-1)0} + \beta_{K-1}^T x \end{aligned} \quad (6)$$

It is arbitrary which class is used in the denominator for the log-odds above. Taking the exponential on both sides and solving for $Pr(G = k|X = x)$ gives the following probabilities,

$$\begin{aligned} Pr(G = k|X = x) &= \frac{\exp(\beta_{k0} + \beta_k^T x)}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)}, \quad k = 1, \dots, K-1, \\ Pr(G = K|X = x) &= \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)}, \end{aligned} \quad (7)$$

and the probabilities sum to one. The output is then classified as the class with the highest probability.

2.3.1 Fitting logistic regression model

The usual way of fitting logistic regression models is by maximum likelihood. The log-likelihood for N observations is defined as,

$$l(\theta) = \sum_{i=1}^N \log p_{g_i}(x_i; \theta), \quad (8)$$

where $p_k(x_i; \theta) = Pr(G = k|X = x_i; \theta)$ and $\theta = \{\beta_{10}, \beta_1^T, \dots, \beta_{(K-1)0}, \beta_{K-1}^T\}$.

One very common classification problem is a situation with binary outcomes, either it happens or it does not. As we see from Equation 6 above, setting $K=2$ simplifies the model considerable, since there will now be only a single linear function. θ in Equation 8 will also be simplified: $\theta = \beta = \{\beta_{10}, \beta_1^T\}$. The two-class case is what is used in this project, and the following discussion will assume the outcome has two classes.

We start by coding the two-class g_i with a 0/1 response y_i , where $y_i = 1$ when $g_i = 1$, and $y_i = 0$ when $g_i = 2$. Next, we let $p_1(x; \theta) = p(x; \beta)$, and $p_2(x; \theta) = 1 - p(x; \beta)$. The

log-likelihood can then be written

$$\begin{aligned}
l(\beta) &= \sum_{i=1}^N \{y_i \log p(x_i; \beta) + (1 - y_i) \log(1 - p(x_i; \beta))\} \\
&= \sum_{i=1}^N \{y_i \log \frac{p(x_i; \beta)}{1 - p(x_i; \beta)} + \log(1 - p(x_i; \beta))\} \\
&= \sum_{i=1}^N \{y_i \beta^T x_i + \log(1 - \frac{1}{1 + \exp(-\beta^T x_i)})\} \\
&= \sum_{i=1}^N \{y_i \beta^T x_i + \log(\frac{\exp(1)}{1 + \exp(\beta^T x_i)})\} \\
&= \sum_{i=1}^N \{y_i \beta^T x_i - \log(1 + \exp(\beta^T x_i))\}.
\end{aligned} \tag{9}$$

This is the equation we want to maximize to find the best fit. Following the approach in Géron’s book [2], we chose the equivalent approach of minimizing the following,

$$J(\beta) = -\frac{1}{N} \sum_{i=1}^N \{y_i \beta^T x_i - \log(1 + \exp(\beta^T x_i))\} \tag{10}$$

This is just the negative of Equation 9, divided by the number of samples. This is our cost function, and dividing by the number of training samples finds the mean cost.

As with all cost functions, the goal is to minimize it. This introduces it’s own potential pitfalls such as overfitting. In order to avoid that, we can introduce regularizations. Let us begin by looking the optimization problem.

2.4 Optimization

As well as in logistic regression as in neural networks, minimizing(or maximizing depending on your setup) the cost function is a central problem, and can to some extent be stated as *the* problem. Having a method which is both efficient and converges towards the minimum is, luckily, not a new problem in computer science. In the logistic regression optimization, three main methods will be utilized, while in the neural network we will focus on the stochastic conjugate gradient descent. For logistic regression we will use an learning rate optimized gradient descent method, and

For two of the four optimizers, we will use SciPy’s library[4] and simply refer the reader to their implementation.

2.4.1 Newton-Conjugate Gradient

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2.4.2 Conjugate gradient

2.4.3 Stochastic gradient descent

To minimize this cost function we use gradient descent. **Gradient descent measures the local gradient of the cost function, with regards to β in our case. Since the gradient goes in the**

direction of fastest increase, we will go in the opposite direction, i.e. negative gradient. We start by choosing random values for β (since our cost function is convex any choice should give correct results), calculate the gradient, update the β values, and do this iteratively until the algorithm converges to a minimum. The size of the steps is important, and is determined by the learning rate. If the learning rate is too small, we will need many iterations which is time consuming. However, if the learning rate is too high, we might overshoot and miss the minimum. One way to choose the learning rate is to let it depend on the size of the gradient. If the gradient is large, i.e. a steep slope, the learning rate can be relatively high. When the gradient is small, the learning rate is also small.

Returning to the logistic regression problem, the derivative of the cost function is

$$\begin{aligned}\frac{\partial J(\beta)}{\partial \beta} &= -\frac{1}{N} \mathbf{X}^T (\mathbf{y} - \mathbf{p}) \\ &= \frac{1}{N} \mathbf{X}^T (\mathbf{p} - \mathbf{y}),\end{aligned}\tag{11}$$

where \mathbf{X} is the $N \times (p+1)$ matrix of x_i values, \mathbf{p} is the vector of fitted probabilities with i th element $p(x_i; \beta)$ and \mathbf{y} is the vector of y_i values. The new β using gradient descent is then $\beta_{new} = \beta_{old} - \frac{\partial J(\beta)}{\partial \beta} lr$, where lr is the learning rate (step size). This is done iteratively until we reach the set max iterations or $\frac{\partial J(\beta)}{\partial \beta}$ is within a given tolerance of zero.

2.5 Regularization

Like we introduced Lasso and Ridge regression to avoid over fitting in Project 1, we can add a penalty term to the cost function in equation (10).

2.5.1 L^1 regularization

The L^1 regularization utilizes the Taxi-cab metric,

$$\|\mathbf{a}\|_1 = |a_0| + \dots + |a_{n-1}| = \sum_{i=0}^{n-1} |a_i|,$$

and is defined as

$$\lambda \|\mathbf{w}\|_1,\tag{12}$$

with \mathbf{w} being the weight matrix. This is equivalent with β as seen in the logistic regression. Its derivative is given as,

$$\lambda \text{sign}(\mathbf{w})\tag{13}$$

where sign is simple the sign of \mathbf{w} .

For logistic regression, this becomes in the gradient of the Geron cost function (10),

$$\frac{\partial J(\beta)}{\partial \beta} = \frac{1}{N} \mathbf{X}^T (\mathbf{p} - \mathbf{y}) + \lambda \cdot \text{sign}(\beta)\tag{14}$$

2.5.2 L^2 regularization

The L^2 regularization is given as the Euclidean norm of the weight matrix,

$$\|\mathbf{a}\|_2 = \left(\sum_{i=0}^{n-1} a_i^2 \right)^{1/2}, \quad (15)$$

and is given as

$$\lambda \|\mathbf{w}\|_2^2, \quad (16)$$

with its following derivative

$$\lambda \cdot 2\mathbf{w}. \quad (17)$$

The 2 in front is often offset by redefining the L^2 norm with a factor half, and will not affect the final outcome.

Implementing the L^2 norm in the gradient of the Geron cost function(10), we get

$$\frac{\partial J(\beta)}{\partial \beta} = \frac{1}{N} \mathbf{X}^T (\mathbf{p} - \mathbf{y}) + \lambda \cdot 2\beta \quad (18)$$

2.5.3 Elastic net regularization

Elastic net regularization utilizes a linear combination of L^1 and L^2 regularization, and consists of adding a term

$$\lambda_1 \|\mathbf{w}\|_1 + \lambda_2 \|\mathbf{w}\|_2^2 \quad (19)$$

The derivative of this w.r.t. \mathbf{w} is simply the combined derivatives of L^1 and L^2 . For our purposes we will set $\lambda_1 = \lambda_2$ in order to avoid having the hyper parameter space become too large.

2.6 Neural Networks

Among the many methods developed for machine learning, neural networks, and especially deep neural networks, are among the most popular. Neural networks were suggested already in 1943 [5] and have had many renaissances since. Currently we are experiencing such a renaissance, but in contrast to earlier periods of resurfaced interest, we now have the computer power to use neural nets efficiently.

A neural net bases itself loosely upon the biological model of neurons communicating together in the brain. A neuron cell contains most of what a normal cell contains, but it also has a long tail called an axon and some antenna like extension called dendrites. The axon of one cell can extend quite far and attach to some of the dendrites of another neural cell. Thus, the biological neural net consists of neural cells receiving input through their dendrites from many other cells and sending output through one output [2, p. 257].

The computed neural networks works in a similar way. We construct "neurons" or "nodes" which are ordered in different layers where each neuron in one layer is connected to all neurons in the next layer. Initially, we start with an input layer which we feed information. Following this initial layer we have one or many hidden layers before we reach the output layer. A

neural network with two or more hidden layers are called deep neural networks [2, p. 263]. Each neuron contains an activation function which determines the strength of the output. In the early days, a step function was used as the activation function. However, one has found that the use of a activation function with a gradient, such as the logistic function used in logistic regression, gives a better neural net. This is due to the fact that we now can apply gradient descent when optimizing the neural net which is discussed below.

To activate a neuron, it needs an input. This input is provided by all the neurons in previous layers through "wires" connecting the neurons (think of the axon to a dendrite). Each of these "wires" is weighted and all connections between one layer and the next is affected by a bias term. Thus, the output of a neuron is given as [2, p. 260]

$$a = \sigma(\vec{w}^T \cdot \vec{x} + b) \quad (20)$$

where a is the output, \vec{w} are the weights, \vec{x} are the inputs and b is the bias term. Note that if we had used a step function instead of the logit(sigmoid) function in the equation above, the neuron would either give an output of 1 or nothing, i.e. 0. When we instead use the sigmoid function, the output can be in the range of 0 to 1.

Once all neurons have been calculated in a layer, we can move on to the next and continue until we reach our output layer. Each layer can have as many neurons as the user wants. Optimizing the number of neurons in each layer is an art and requires both experience and a bit of luck. The output layer needs one neuron for each class we wish to identify.

After initial calculation of the outer layer, you will most likely have an answer that is completely rubbish. It is clear that we have to optimize the neural net. As each neurons activation function is calculated using equation (20), we can see that we can optimize the weights between the neurons and the bias between the layers. This is done through a method called backwards propagation where one uses the cost function to identify the magnitude of the error (the cost) of a neural net and then one goes backwards through the neural net to update the weights and biases.

The basic procedure of back propagation is this (heavily influenced by the work of Nielsen [7]):

- Compute the output error vector for the final layer (L) given by

$$\delta^L = \nabla_a C \odot \sigma'(\vec{w}^T \cdot \vec{x} + b)$$

where C is the cost function and ∇_a is a vector who has components that are the partial derivatives $\frac{\partial C}{\partial a_j^L}$ where a_j is the j'th output found by using equation (20) for a .

- Go back through all the previous layers $l = L-1, L-2, \dots, 2$ and compute

$$\delta^l((\vec{w}^{l+1})^T \delta^{l+1}) \odot \sigma'(\vec{w}^T \cdot \vec{x} + b)$$

this is where we back propagate the error.

- Finally, find the gradient of the cost function for the two parameters we want to change, \vec{w} and b by:

$$\begin{aligned} \frac{\partial C}{\partial \vec{w}_{jk}^l} &= a_k^{l-1} \delta_j^l \\ \frac{\partial C}{\partial b_j^l} &= \delta_j^l \end{aligned}$$

where k indicates the column of \vec{w}^l as j indicates the row.

Once all layers have been adjusted through back propagation, one can run through the whole network again and repeat the process. A common cost function may be the quadratic loss function given by:

$$C = \frac{1}{N} \sum_j (y_j - a_j^L)^2 \quad (21)$$

where N are the total numbers of outputs in j and y are the true answers.

3 Implementation

Code can be found on [9].

4 Results

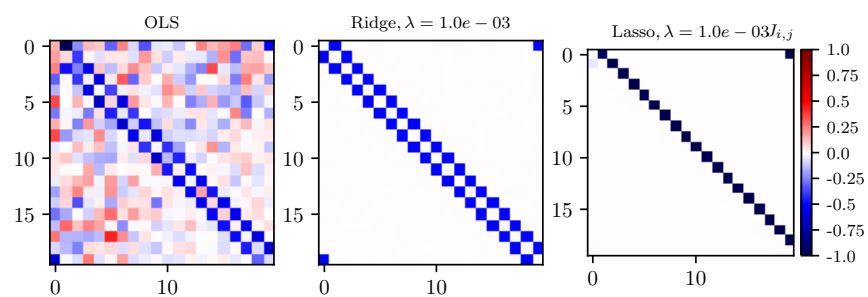
Results for two different cases are being presented, one the one-dimensional Ising Model and another for the the two-dimensional Ising model. We begin with looking at the. 1D Ising model.

4.1 1D Ising model

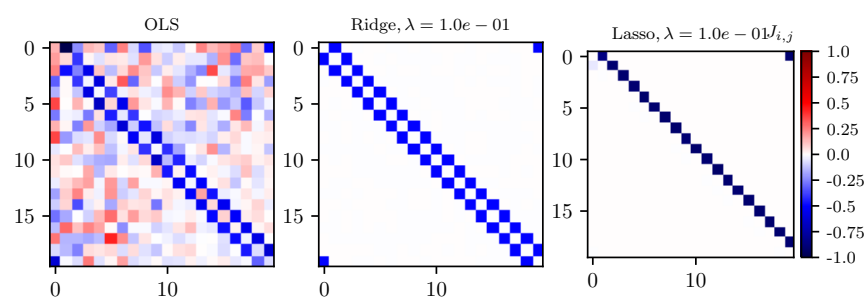
4.1.1 Fitting with linear regression

For linear regression we got coefficients of \mathbf{J} in (3) as the following,

The R^2 score of the OLS, Ridge and Lasso can be seen in figure 2,



(a) $\lambda = 10^{-3}$



(b) $\lambda = 10^{-1}$

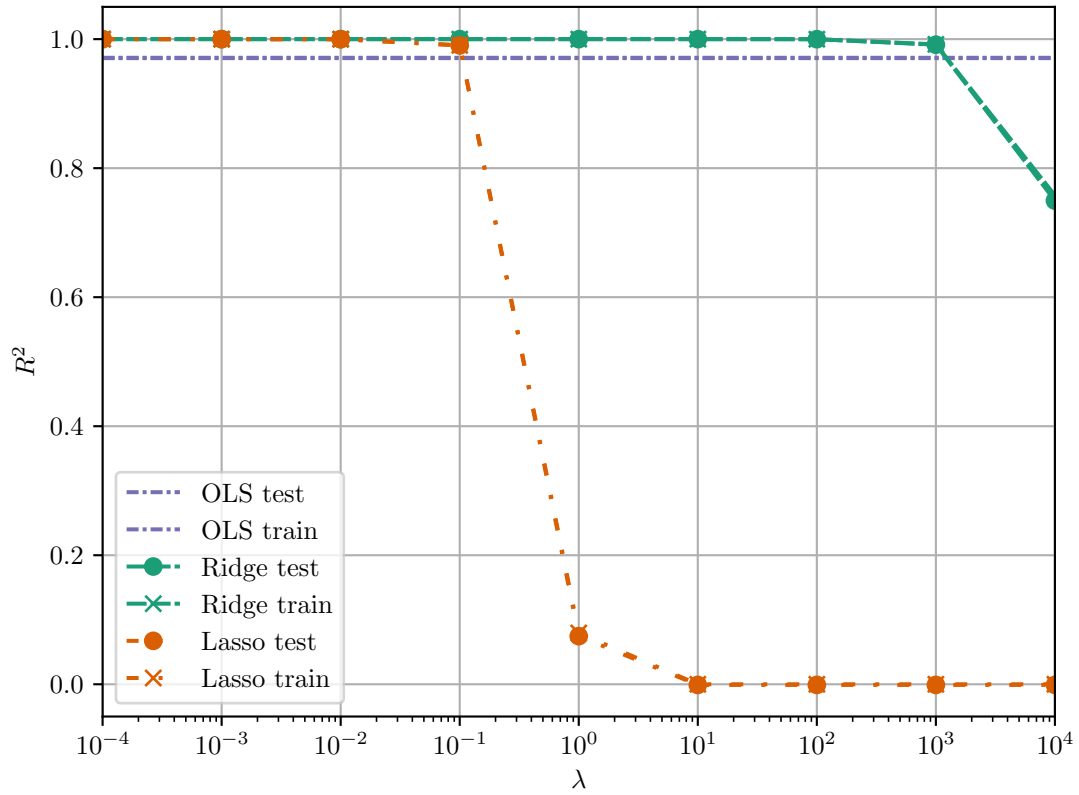
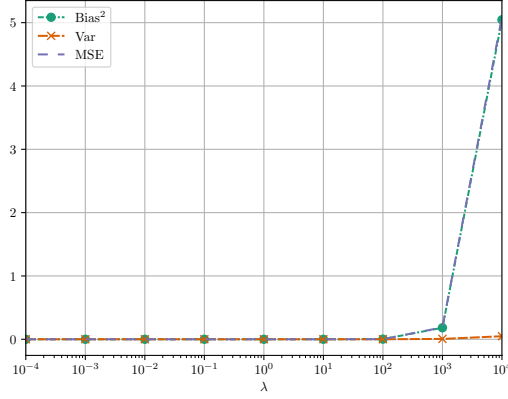
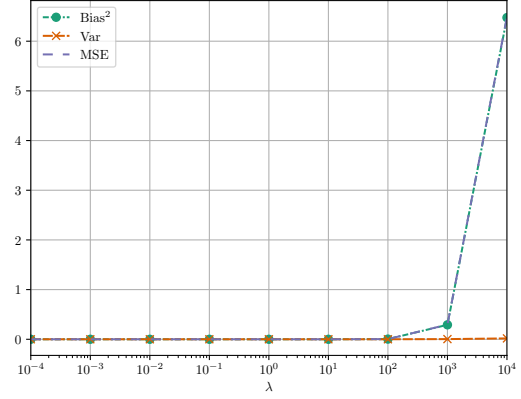


Figure 2: R^2 score for different Ordinary Least Squares(OLS), Ridge and Lasso regression. Retrieved $N_{\text{train}} = 5000$ on a 1D Ising model of size $L = 20$.

The bias-variance decomposition for Ridge and Lasso using bootstrap and cross validation can be viewed in figure 3 and 4.

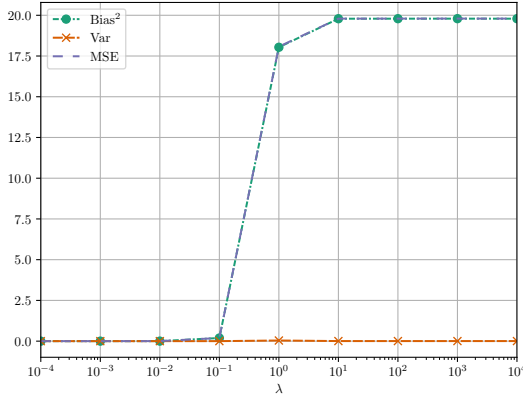


(a) Bootstrap.

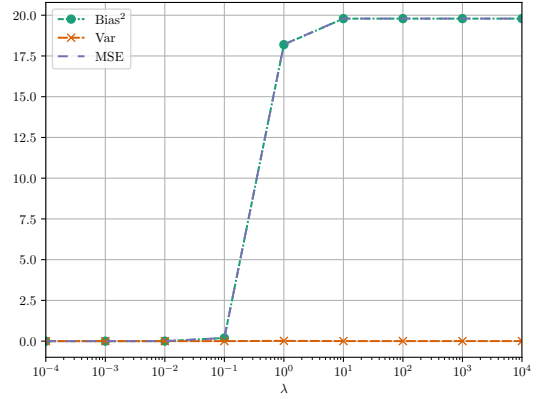


(b) k -fold Cross Validation.

Figure 3: A bias-variance decomposition of Ridge regression using bootstrapping3a and cross-validation3b.



(a) Bootstrap.

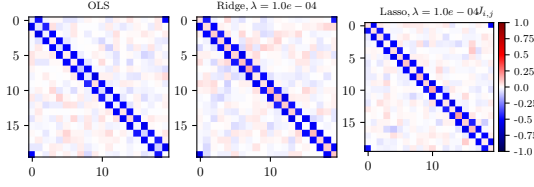


(b) k -fold Cross Validation.

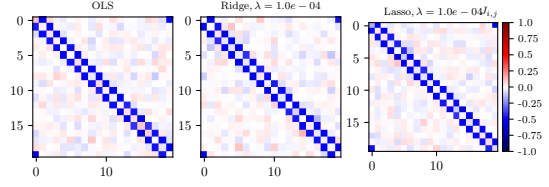
Figure 4: A bias-variance decomposition of Lasso regression using bootstrapping4a and cross-validation4b.

4.1.2 Fitting with a neural network

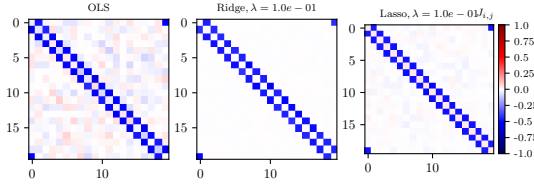
By setting the output activation function to the identity and by having zero hidden layers, we are essentially performing a regression analysis on the 1D Ising model. We generate the same amount of data by inputting the same RNG(random number generator) seed. A fit using $N_{\text{train}} = 400$ and $N_{\text{train}} = 5000$ for $\lambda = 10^{-3}, 10^{-1}, 10^1$ can be seen in figure ??.



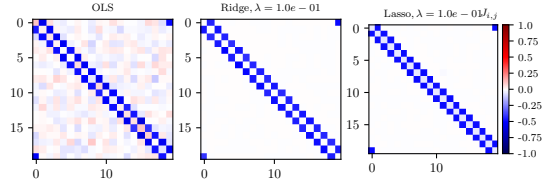
(a) $N_{\text{train}} = 400, \lambda = 10^{-3}$



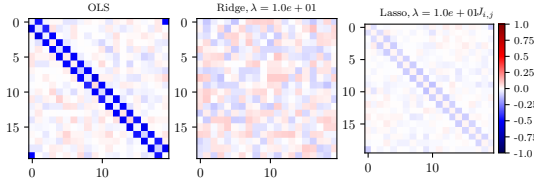
(b) $N_{\text{train}} = 5000, \lambda = 10^{-3}$



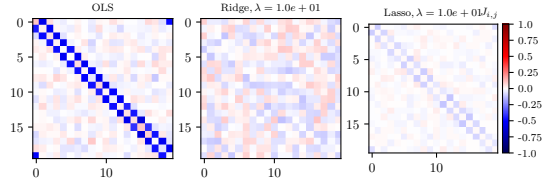
(c) $N_{\text{train}} = 400, \lambda = 10^{-1}$



(d) $N_{\text{train}} = 5000, \lambda = 10^{-1}$



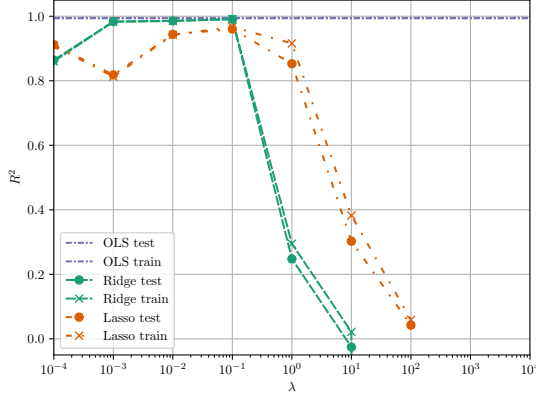
(e) $N_{\text{train}} = 400, \lambda = 10^1$



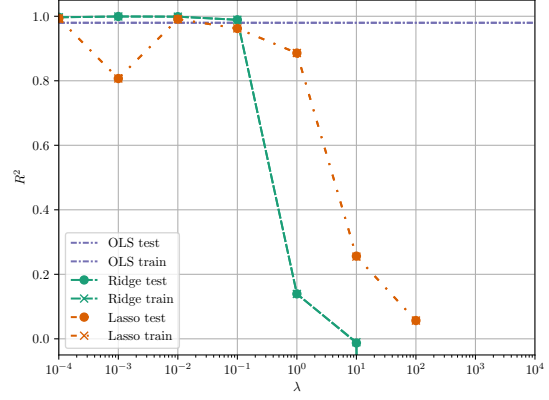
(f) $N_{\text{train}} = 5000, \lambda = 10^1$

Figure 5: Heat map plot of the coefficients of \mathbf{J} in (3) using neural networks with different regularizations for $\lambda = 10^{-3}, 10^{-1}, 10^1$.

The R^2 score of the neural network using L^1 , L^2 and no regularization can be seen in figure 6,



(a) $N_{\text{train}} = 400$



(b) $N_{\text{train}} = 5000$

Figure 6: R^2 score for the neural network using L^1 , L^2 and no regularization. Retrieved $N_{\text{train}} = 400$ on the left and $N_{\text{train}} = 5000$ on the right, for a 1D Ising model of size $L = 20$.

4.2 2D Ising model

As stated in the section about the 2D Ising model 2.1.2, the classification will focus on evaluating the phases of different lattice configurations, and whether or not it is below or above a critical temperature. We begin by listing the results from the logistic regression.

4.2.1 Classification through logistic regression

4.2.2 Classification through neural networks

5 Discussion

5.1 1D Ising model

5.1.1 Fitting with linear regression

5.1.2 Fitting with a neural network

5.2 2D Ising model

5.2.1 Classification through logistic regression

5.2.2 Classification through neural networks

6 Conclusion

Appendices

Put stuff like Bootstrapping, kfold CV, OLS/Ridge/Lasso regression here.

A Refreshing linear regression

A.1 Ridge regression

A.2 Lasso regression

B Bootstrapping

C k -fold Cross-Validation

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