Project 1: Regression and Resampling Methods

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Abstract

In this project we present a theoretical overview and practicum of linear regression. We first describe the theory behind the different regression methods - ordinary least squares, ridge, and lasso regression - and then describe data resampling methods - bootstrapping and cross validation - which provide information necessary for better model selection. These models and resampling techniques are then applied on data generated by a 2D analytical function (the Franke function). Our results demonstrate several important concepts, such as the negative influence of noisy data, and the bias variance tradeoff inherent to model selection. Finally we test our model development workflows on real topography data from Iowa and Pennsylvania.

Reproducibility

The code used for this report can be accessed at:
https://github.com/orhuff/FYS-STK-4155-Project1-Regression

Introduction

The goal of regression is to produce a model that can return accurate predictions of continuous function values, based on inputs of data from one or more explanatory variables. Regression is applied frequently in science, engineering, economics, and practically any analytical field because of its power with simplicity. As an example, suppose you wanted to build a model to predict someone's income based on variables such as their age, years of work experience, and other quantities. Because you want to predict a continuous value (income), and the relationship between the variables likely isn't exceedingly complex, linear or polynomial regression is probably the best approach.

Let's say you collect data on income based on P explanatory variables from N people. This data can be thought of as a vector $\boldsymbol{y}$ which is N entries long. In an ideal world there would be a function $f(x)$ that perfectly describes this data - however in actuality there will almost always be error. Thus we can think of the data as a sum of the ideal function and an irreducible error vector ϵ. For simplicity, we will consider error to follow a Gaussian distribution with zero mean and a variance of σ^2.

$$\boldsymbol{y} = f(\boldsymbol{x}) + \boldsymbol{\epsilon} \tag{1}$$

In linear (or polynomial) regression our goal is to build a model $\tilde{\boldsymbol{y}}$ that best approximates the data $\boldsymbol{y}$. To build such a model we set up a linear algebra problem in which the model is equal to the product of a design matrix $\boldsymbol{X}$ and adjustable model parameter values $\boldsymbol{\beta}$. The design matrix consists of all the observations for each explanatory variable, and is therefore of dimension NxP. The model parameters are the weights by which to adjust and multiply the data in order to yield predictions - the most familiar example of these are the slope and intercept of a linear equation.

$$\tilde{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\beta} \tag{2}$$

The optimization of the model parameters $\boldsymbol{\beta}$ is at the heart of regression (and machine learning in general) and requires selecting a metric by which to evaluate the quality of the model. This metric is called the cost function or loss function. Different cost functions define different regression models - ordinary least squares, ridge, and lasso - and are described next in the Theory section.

Theory

Ordinary Least Squares Regression

The most basic form of regression is that of ordinary least squares (OLS). In OLS the cost function by which to optimize the model parameters $\boldsymbol{\beta}$ is called the mean squared error (MSE). The MSE measures the mean difference in error between the data $\boldsymbol{y}$ and the model $\tilde{\boldsymbol{y}}$, and is defined as such:

$$MSE(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2 \tag{3}$$

We want to find the model parameters $\boldsymbol{\beta}$ that result in this quantity reaching a minimum value, because that will result in a model with the lowest possible error. Thus we can re-express the MSE cost function in matrix form (using the knowledge that $\tilde{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\beta}$):

$$C(\boldsymbol{X}, \boldsymbol{\beta}) = \frac{1}{n}[(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})] = \frac{1}{n}\left\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\right\|_2^2 \tag{4}$$

And then set its derivative with respect to $\boldsymbol{\beta}$ equal to zero:

$$\frac{\partial C}{\partial \beta} = \frac{\partial}{\partial \beta}(\frac{1}{n}[(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})]) = 0 \tag{5}$$

Solving this equation for β yields:

$$\boldsymbol{\beta} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{6}$$

Therefore the beauty of OLS is that we have an expression that can be solved analytically for the optimal parameters β. The only sometimes-problematic aspect of this expression is if the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is not analytically invertible, though this is not a large concern since pseudo-inverse methods such as singular value decomposition (SVD) can still be applied to return an inverse. Once β is calculated using this expression, the matrix multiplication of $\boldsymbol{X}\boldsymbol{\beta}$ then yields the predicted model values.

Because we have analytical expressions for the quantities in OLS, it is also relatively easy to derive analytical expressions for their statistical quantities, such as the expected value and variance. These following proofs assume again that our data is described by a function with added irreducible Gaussian noise of mean zero and variance σ^2:

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

Proof 1:

$$\mathbb{E}[y_i] = \boldsymbol{X_{i,*}}\beta,$$

$$\mathbb{E}[y_i] = \mathbb{E}[f(x_i) + \epsilon_i] = \mathbb{E}[\boldsymbol{X_{i,*}\beta} + \epsilon_i] = \mathbb{E}[\boldsymbol{X_{i,*}\beta}] + \mathbb{E}[\epsilon_i]$$
$$= \mathbb{E}[\sum_j x_{ij}\beta_j] + \mathbb{E}[\epsilon_i] = \sum_j x_{ij}\beta_j = \boldsymbol{X_{i,*}}\beta,$$

Proof 2:

$$Var(y_i) = \sigma^2$$

$$Var(y_i) = \mathbb{E}[(y_i - \mathbb{E}(y_i))^2] = \mathbb{E}[y_i^2] - \mathbb{E}[y_i]^2$$
$$= \mathbb{E}[(\boldsymbol{X_{i,*}}\beta + \epsilon_i)^2] - (\boldsymbol{X_{i,*}}\beta)^2$$
$$= \mathbb{E}[(\boldsymbol{X_{i,*}}\beta)^2 + 2\epsilon_i\boldsymbol{X_{i,*}}\beta + \epsilon_i^2] - (\boldsymbol{X_{i,*}}\beta)^2$$
$$= (\boldsymbol{X_{i,*}}\beta)^2 + 2\mathbb{E}[\epsilon_i]\boldsymbol{X_{i,*}}\beta + \mathbb{E}[\epsilon_i^2] - (\boldsymbol{X_{i,*}}\beta)^2$$
$$= \mathbb{E}[\epsilon_i^2] = Var(\epsilon_i) = \sigma^2$$

Proof 3:

$$\mathbb{E}[\hat{\boldsymbol{\beta}}] = \boldsymbol{\beta}$$

$$\mathbb{E}[\hat{\boldsymbol{\beta}}] = \mathbb{E}[(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}] = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\mathbb{E}[\boldsymbol{Y}]$$
$$= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{\beta}$$

Proof 4:

$$Var(\hat{\boldsymbol{\beta}}) = \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$$

$$Var(\hat{\boldsymbol{\beta}}) = \mathbb{E}[(\boldsymbol{\beta} - \mathbb{E}[\boldsymbol{\beta}])(\boldsymbol{\beta} - \mathbb{E}[\boldsymbol{\beta}])^T]$$
$$= \mathbb{E}[((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y} - \boldsymbol{\beta})((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y} - \boldsymbol{\beta})^T]$$
$$= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\mathbb{E}[\boldsymbol{Y}^T\boldsymbol{Y}]\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1} - \boldsymbol{\beta}\boldsymbol{\beta}^T$$
$$= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T(\boldsymbol{X}\boldsymbol{\beta}\boldsymbol{\beta}^T\boldsymbol{X}^T + \sigma^2)\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1} - \boldsymbol{\beta}\boldsymbol{\beta}^T$$
$$= \boldsymbol{\beta}\boldsymbol{\beta}^T + \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1} - \boldsymbol{\beta}\boldsymbol{\beta}^T$$
$$= \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$$

Ridge Regression

Ridge regression we use in a project is a technique for analyzing multiple regression data suffering from multicollinearity. When it occurs, least squares estimates are unbiased while variances are large so they may be inaccurate. Ridge regression doesn't require unbiased estimates and adds just enough bias to make the estimates reasonably reliable approximations to true values, it reduces the standard errors by adding a degree of bias to the regression estimates, thus they are getting to be more reliable.

If we have large number of features and test results are worse than the results of model training, it could be described as the problem of over-fitting. In case the score is poor for both training and test data it's a problem of under-fitting.

In ridge regression, called also as L2 regularization, the cost function is altered by adding a penalty equivalent to square of the magnitude of the coefficients. The penalty term (lambda) performs regularization in a way that if the coefficients take large values the function is penalized. When lambda tends to zero function becomes similar to the linear regression. So lower the constraint on the features, the model will approximate linear regression model.

$$C(\boldsymbol{X},\boldsymbol{\beta}) = \frac{1}{n}\left\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\right\|_2^2 + \lambda\left\|\boldsymbol{\beta}\right\|_2^2 \tag{7}$$

$$\hat{\boldsymbol{\beta}}_{Ridge} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} \tag{8}$$

Lasso Regression

Lasso regression is another regularization technique (L1 regularization) used to reduce model complexity and prevent over-fitting which may occur when simple linear regression is used. As for the Ridge regression when lambda tends to zero, in case of LASSO when lambda equal to zero the equation reduces to a linear regression. The difference is that instead of taking the square of the coefficients, true magnitude values are taken into consideration.

The Lasso regression has certain potential advantages over the OLS and Ridge regression schemes. The name is short for "least absolute shrinkage and selection operator". It thus not only helps in eliminating over-fitting but also in feature selection. LASSO is also robust to outliers unlike ridge regression.

$$C(\boldsymbol{X},\boldsymbol{\beta}) = \frac{1}{n}\left\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\right\|_2^2 + \lambda\left\|\boldsymbol{\beta}\right\|_1 \tag{9}$$

$$\hat{\boldsymbol{\beta}}_i^{\text{Lasso}} = \begin{cases} y_i - \frac{\lambda}{2} & \text{if} \quad y_i > \frac{\lambda}{2} \\ y_i + \frac{\lambda}{2} & \text{if} \quad y_i < -\frac{\lambda}{2} \\ 0 & \text{if} \quad |y_i| \leq \frac{\lambda}{2} \end{cases} \tag{10}$$

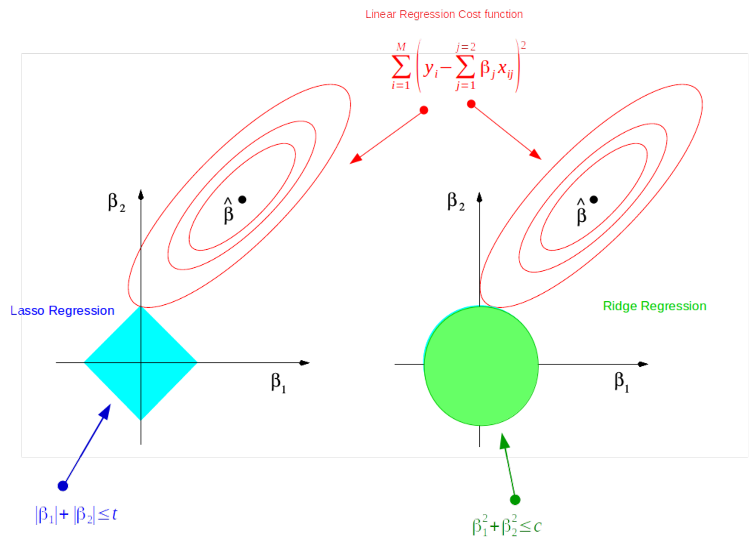

Linear Regression Cost function
$\sum_{i=1}^{M}\left(y_i - \sum_{j=1}^{j=2} \beta_j x_{ij}\right)^2$
β_2
$\hat{\beta}$
Lasso Regression
β_1
Ridge Regression
$|\beta_1| + |\beta_2| \leq t$
$\beta_1^2 + \beta_2^2 \leq c$

Figure 1: Dimension reduction of feature space with LASSO (figure from James et al., 2013; modified in Bhattacharyya, 2018

Data Splitting and Resampling

We have described the analytical expressions used to calculate model parameters $\boldsymbol{\beta}$ for different regression methods. However, it is also important to understand methods that help in selecting a good model. In practice when training a machine learning model, it is important to split the data into a training set and testing set. The testing set is usually between 20-30% of the entire dataset. The model is then trained using X and y values (in the case of linear regression) from the training set, and predictions are made using the product of the testing set X values and the determined parameters β. These predictions are compared with the true y values, using a metric such as the MSE or R^2 score (defined below) over all the points in order to evaluate the effectiveness of the model.

$$R^2(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = 1 - \frac{\sum_{i=0}^{n-1}(y_i - \tilde{y}_i)^2}{\sum_{i=0}^{n-1}(y_i - \bar{y})^2} \tag{11}$$

However, this practice of data splitting has limitations if it is done alone. For instance, what if an overabundance of outlier data is contained in either the training or testing set? In this case the testing of the model may yield different results than are actually the case, and this could hinder the selection of the best model. This motivates the need for resampling techniques, whereby models can be trained over multiple resamplings of the dataset in order to find the best overall model.

One of the most common resampling techniques is the bootstrap method. In this method, one extracts samples with replacement repeatedly from the whole dataset, and calculates desired quantities from the samples. Then statistical properties of the dataset, such as the mean and variance, can be more accurately determined by investigating the behavior across all the samples that were drawn. This is a directly related to the central limit theorem, which says that if you repeatedly resample from normally-distributed data with replacement, then the sample means themselves will be normally-distributed. In statistics, the bootstrap method is usually applied to make more accurate statistical inferences about a population.

However in machine learning, we can also apply the method towards achieving the optimal hyperparameter selection for a model. This is accomplished by bootstrapping the data splitting operation described earlier. Essentially, we can iterate over the model hyperparameter we want (such as the polynomial order for OLS or λ value for ridge regression) and then for each hyperparameter value perform bootstrapping. For each bootstrap iteration we resample (with replacement) the data in order to obtain a training dataset, and then use the remaining data as the testing dataset. The temporary model resulting from this bootstrap iteration and data sampling can then be evaluated using an accuracy metric of choice, like the MSE or R2 value. Then we can average across all accuracy results to find how well, on average, the model with the given hyperparameter values performs. Thus with bootstrapping you can be more confident that a particular model is superior, if it performs better than other model configurations over many resamplings.

Another popular resampling technique is called k-fold cross validation. This technique involves splitting the dataset into k equal groups (or folds) and then using one group as the testing dataset, and the other k-1 groups as the training dataset. After training a model with this configuration, the groups are cycled so that a different group is the testing dataset and the remaining groups are used for training. This repeats k-1 times so that each group gets a turn being the testing dataset. During each iteration, an evaluation of the model performance can be made and then averaged over all k folds following completion, to get a more accurate estimation of the strength of a particular model configuration. Typically the number of folds used is from 5-10, so as to have a reasonable relative size between the testing and training datasets.

The Bias Variance Tradeoff

In the model selection process, one of the overarching concepts that can be observed is the bias variance tradeoff. In order to understand this concept we go back to the mean squared error cost function for ordinary least squares. Through the following Proof 5, this cost function can be re-expressed as the sum of three terms: the (square of the) bias, the variance of the irreducible noise of the data, and the variance of the model.

Proof 5:

$$\frac{1}{n}\sum_{i=0}^{n-1}(y_i-\tilde{y}_i)^2 = Bias[\tilde{\boldsymbol{y}}]^2+\sigma^2+Var[\tilde{\boldsymbol{y}}]$$

$$\begin{aligned}
C(\boldsymbol{X},\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=0}^{n-1}(y_i-\tilde{y}_i)^2 = \mathbb{E}[(\boldsymbol{y}-\tilde{\boldsymbol{y}})^2] \\
= \mathbb{E}[(\boldsymbol{f}+\boldsymbol{\epsilon}-\tilde{\boldsymbol{y}})^2] = \mathbb{E}[(\boldsymbol{f}+\boldsymbol{\epsilon}-\tilde{\boldsymbol{y}}+\mathbb{E}[\tilde{\boldsymbol{y}}]-\mathbb{E}[\tilde{\boldsymbol{y}}])^2] \\
= \mathbb{E}[(\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}])^2]+\mathbb{E}[\epsilon^2]+\mathbb{E}[(\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})^2]+2\mathbb{E}[(\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}])\epsilon]+2\mathbb{E}[\epsilon(\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})]+2\mathbb{E}[(\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})(\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}]))] \\
= (\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}])^2+\mathbb{E}[\epsilon^2]+\mathbb{E}[(\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})^2]+2(\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}])\mathbb{E}[\epsilon]+2\mathbb{E}[\epsilon]\mathbb{E}[\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})]+2\mathbb{E}[\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}}](\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}]) \\
= (\boldsymbol{f}-\mathbb{E}[\tilde{\boldsymbol{y}}])^2+\mathbb{E}[\epsilon^2]+\mathbb{E}[(\mathbb{E}[\tilde{\boldsymbol{y}}]-\tilde{\boldsymbol{y}})^2] \\
= Bias[\tilde{\boldsymbol{y}}]^2+Var[\epsilon]+Var[\tilde{\boldsymbol{y}}] \\
= Bias[\tilde{\boldsymbol{y}}]^2+\sigma^2+Var[\tilde{\boldsymbol{y}}]
\end{aligned}$$

The bias is defined as the difference between the mean prediction of the model and the truth. The conceptual meaning of bias can be thought of in terms of throwing many darts at a dartboard. If the average distance of the darts from the bullseye is low, then the bias is low. And the variance has the intuitive meaning of the degree of spread of the darts. These meanings translate to real plots of data in terms of the concepts of underfitting and overfitting. Underfitting is when the model has lower variance (spread) but higher bias (far from the target) - thus it can be thought of as a very simple fit of a curve with low polynomial order that does not contain enough complexity to correctly model the data. Overfitting is the opposite, where the model has higher variance and lower bias - this can be thought of as a needlessly-complex fit of a curve with high polynomial order that follows every little variation. Underfitted models can usually be easily detected because they will just return incorrect prediction values. Overfitted models may perform well on the current training and testing dataset, but are not likely to generalize well to make predictions on unseen data.

The bias variance tradeoff is therefore the concept that you want to strike a balance between these two effects, selecting a model that has a low bias and low variance. One can plot the bias and variance of a model, along with its overall error, in order to see this concept. Figure 1 from James et al., 2013 demonstrates this, where they plot the bias, variance, and the MSE (the bias + variance + irreducible noise) as a function of the model flexibility/complexity. At low model complexity, the bias is high and the variance is low, while at high model complexity, the bias approaches zero and the variance increases significantly. The best model to select is therefore in the middle of these extremes, at a moderate model complexity, where the total error is minimized. This can be seen as the minima of the MSE curve. We will reproduce a similar curve to this in the Results section of the report.

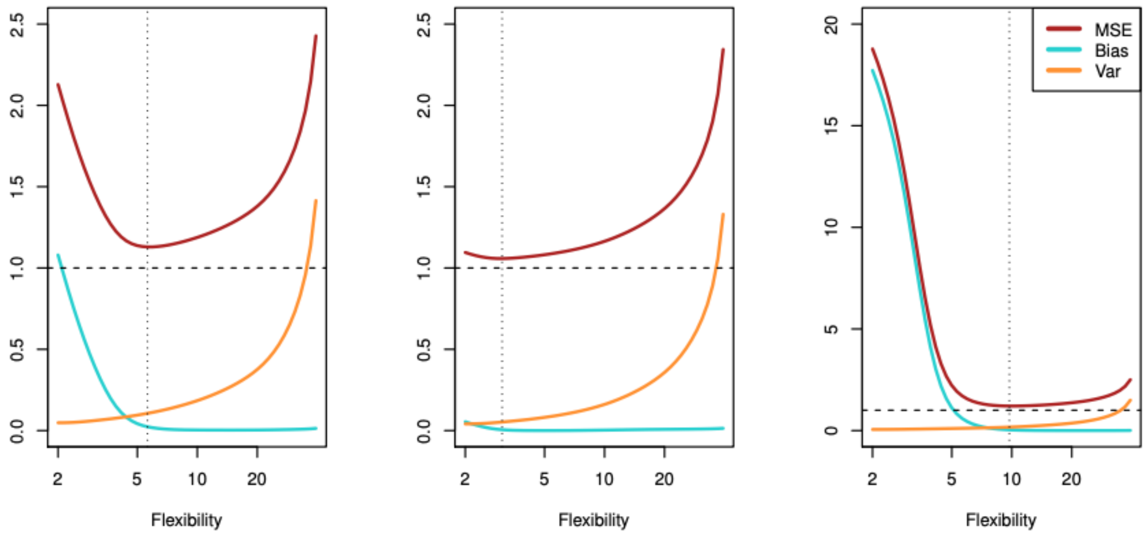


Figure 2: Model error, bias, and variance plotted as a function of model flexibility/complexity, illustrating the bias variance tradeoff (James et al., 2013)

The Franke Function

For our method of implementation to test the various regression methods and their properties, we will use a function called the Franke function (Franke, 1979). This function is two-dimensional and is frequently used to test spatial regression and interpolation problems. It is a weighted sum of four exponential terms and is defined below. An example surface plot of the Franke function calculated for 100 x and y points in the range [0,1] is shown in Figure 2. By having an analytical function with which to test, we can more easily see the influence of added noise and other factors before moving to real data.

$$\begin{aligned} f(x,y) &= \frac{3}{4}\exp\left(-\frac{(9x-2)^2}{4}-\frac{(9y-2)^2}{4}\right)+\frac{3}{4}\exp\left(-\frac{(9x+1)^2}{49}-\frac{(9y+1)}{10}\right) \\ &+\frac{1}{2}\exp\left(-\frac{(9x-7)^2}{4}-\frac{(9y-3)^2}{4}\right)-\frac{1}{5}\exp\left(-(9x-4)^2-(9y-7)^2\right) \end{aligned} \tag{12}$$

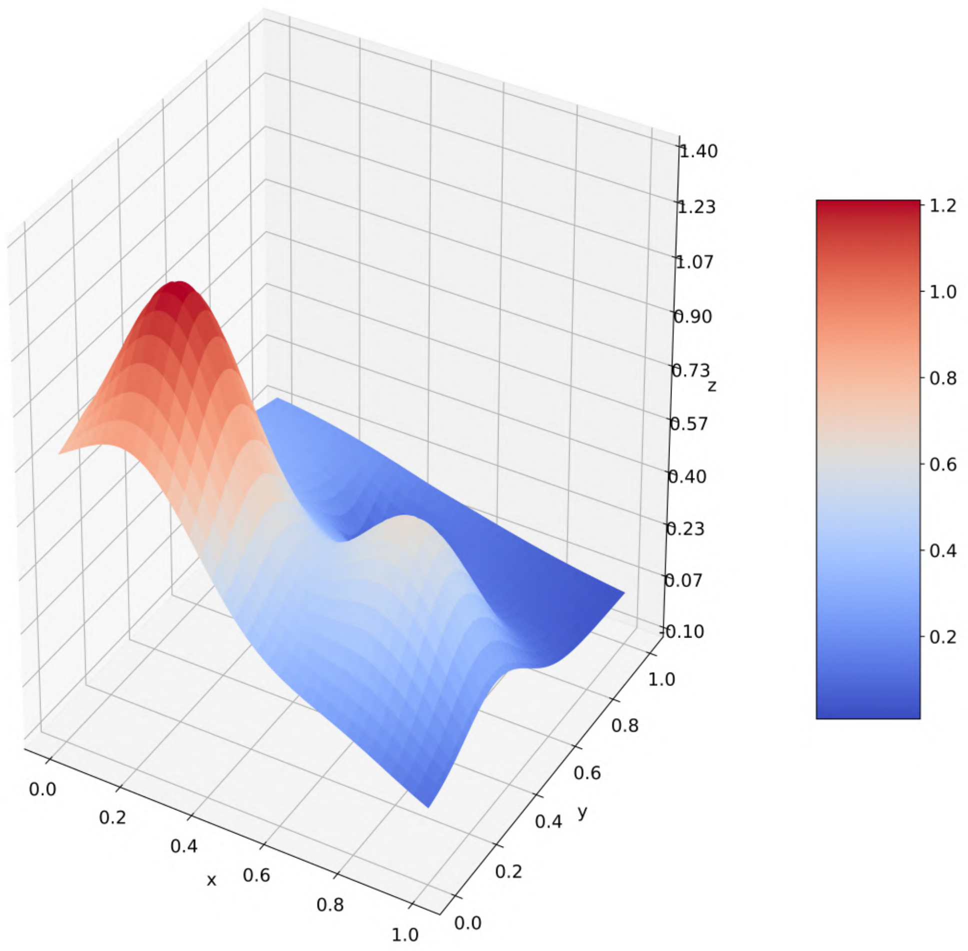


Figure 3: Surface plot of the Franke function calculated for 100 evenly-spaced x and y values in the range [0,1].

Therefore the formulation of the linear algebra problem we want to solve (similar to equation (2)) is as follows, where the model $\tilde{\boldsymbol{z}}$ is a multiplication of the design matrix for an mth degree polynomial of x and y, and the parameters $\boldsymbol{\beta}$:

$$
\begin{aligned}
\tilde{\boldsymbol{z}} &= \boldsymbol{X}\boldsymbol{\beta} \\
&\tilde{z}_0 = \beta_0 + \beta_1 x_0 + \beta_2 y_0 + \beta_3 x_0^2 + \beta_4 x_0 y_0 + \beta_5 y_0^2 + \ldots + \beta_{p-1} y_0^m, \\
&\tilde{z}_1 = \beta_0 + \beta_1 x_1 + \beta_2 y_1 + \beta_3 x_1^2 + \beta_4 x_1 y_1 + \beta_5 y_1^2 + \ldots + \beta_{p-1} y_1^m, \\
&\quad \vdots \\
&\tilde{z}_n = \beta_0 + \beta_1 x_n + \beta_2 y_n + \beta_3 x_n^2 + \beta_4 x_n y_n + \beta_5 y_n^2 + \ldots + \beta_{p-1} y_n^m,
\end{aligned}
\tag{13}
$$

Results and Discussion

OLS Regression on the Franke Function

We begin by implementing the ordinary least squares algorithm on the Franke function for different model complexities. The workflow consists of first generating an x,y grid of evenly-spaced points in the range [0,1], and calculating the Franke function values z from these x,y points. Optionally, we can include Gaussian noise by adding it to these z values. Then we iterate over polynomial order and do the following for each order:

1. generate the design matrix of the given order
2. perform a train-test split of X and z in the proportion 80-20
3. scale the data by subtracting the mean of the training datasets
4. calculate the beta parameters using equation 6
5. calculate the beta parameters variance using the relation in Proof 4
6. make the z predictions for train and test data
7. calculate the mean squared error (equation 3) and R2 values (equation 11) for the train and test data

This overall structure of this workflow is largely similar for the implementation of other regression algorithms later in this report, with the main change being a resampling loop.

Our first test consists of an iteration over polynomial order from 1 to 15, where we also investigate the impact of added Gaussian noise and data scaling. We use 100 data points (evenly-spaced in the range [0,1]) to calculate the Franke function z values, and then add Gaussian noise of mean 0 and standard deviation 0.1. The results are presented in Figure 4.

We can see that, as an overall trend, the mean squared error decreases and the R2 value increases with increasing polynomial order. However, there is a point of diminishing returns at around order 5, after which the error decreases almost insignificantly in an asymptotical fashion. Furthermore, we notice that the run with noise added results in higher error and lower R2 value, which is intuitive because the noise is making the data more difficult for the model to fit. In the case of noise added, the train error tends to be lower than the test error, which is a pattern we see consistently throughout these regression tests. This is because the model has been trained on this set of data, while it has not been previously exposed to the testing data.

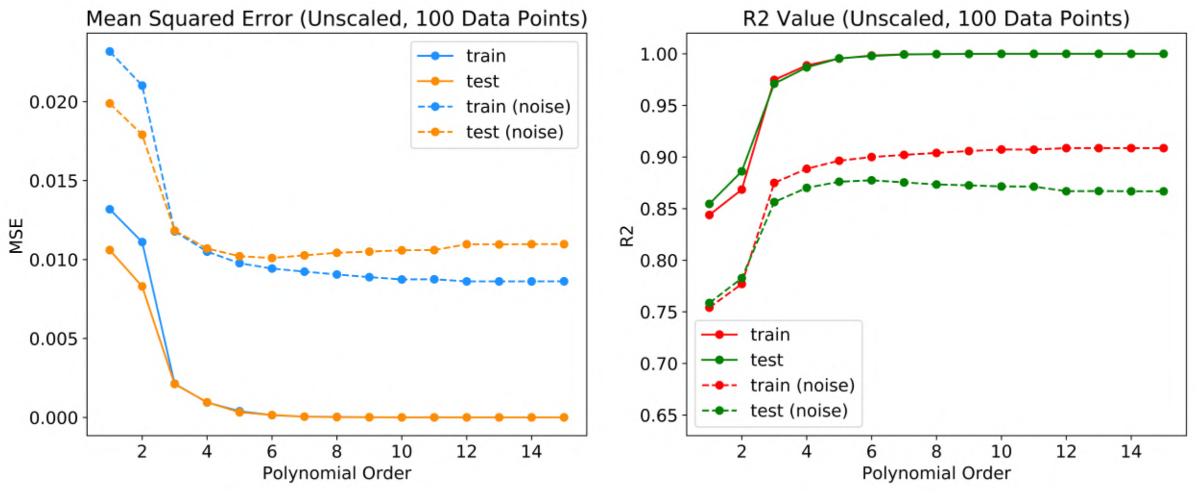


Figure 4: MSE and R2 values for OLS, unscaled data.

We also test the results of scaling our data in Figure 5. In our scaling we subtract the mean of the X train values from the X train and X test datasets, and subtract the mean of the z train values from the z train and z test datasets. The reason for this method (as opposed to scaling by the mean of the whole data) is to avoid biasing the training data towards the mean of the test dataset, which it should not see. The results in terms of the error using the scaled data are largely the same as for unscaled data, because our data values are all very similar (approximately from 0 to 1). However, we choose to use scaled data for future OLS tests (and for ridge and lasso regression) because of several benefits. First, in the case of features which are significantly different from each other, such as measurements of different quantities or different units, scaling will help make it so that features arenât inappropriately weighted. Secondly, scaling removes the intercept column from the data and design matrix, thus simplifying calculations and allowing easier comparisons between model performance.

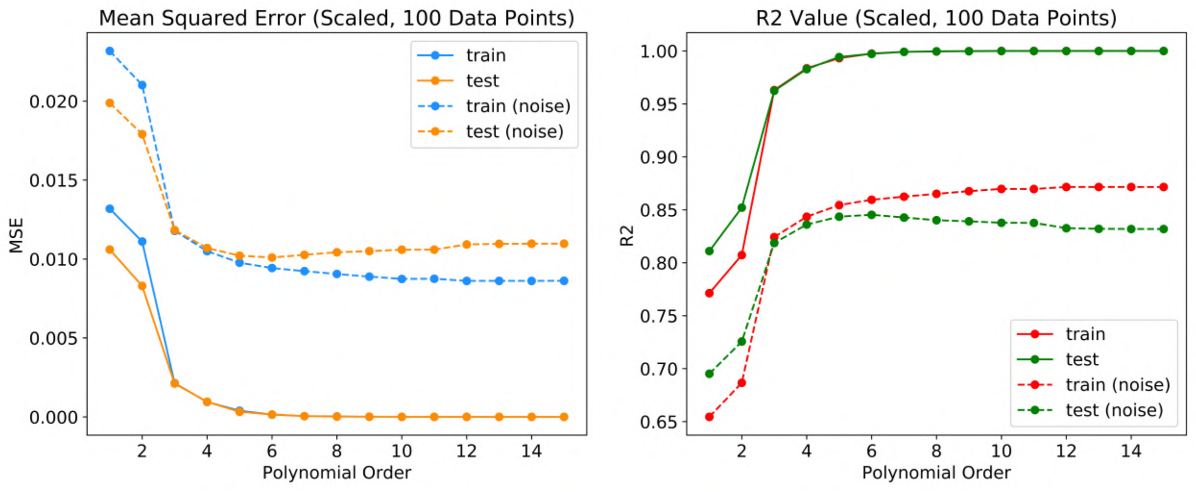


Figure 5: MSE and R2 values for OLS, scaled data.

While doing this OLS regression test over polynomial order, we also calculated the variance of the determined parameters beta using the equation in Proof 4. By taking the square root of these variances, we have standard deviations which can be plotted as error bars on the beta values in order to show their uncertainties. This is shown in Figure 6. As we can see, the variance of parameters for higher order polynomials tends to increase significantly, especially approaching order 5. This indicates that a lower polynomial order such as 4 is likely better suited for building a model, especially considering that the improvement in error reduction is negligible as was seen in Figure 5.

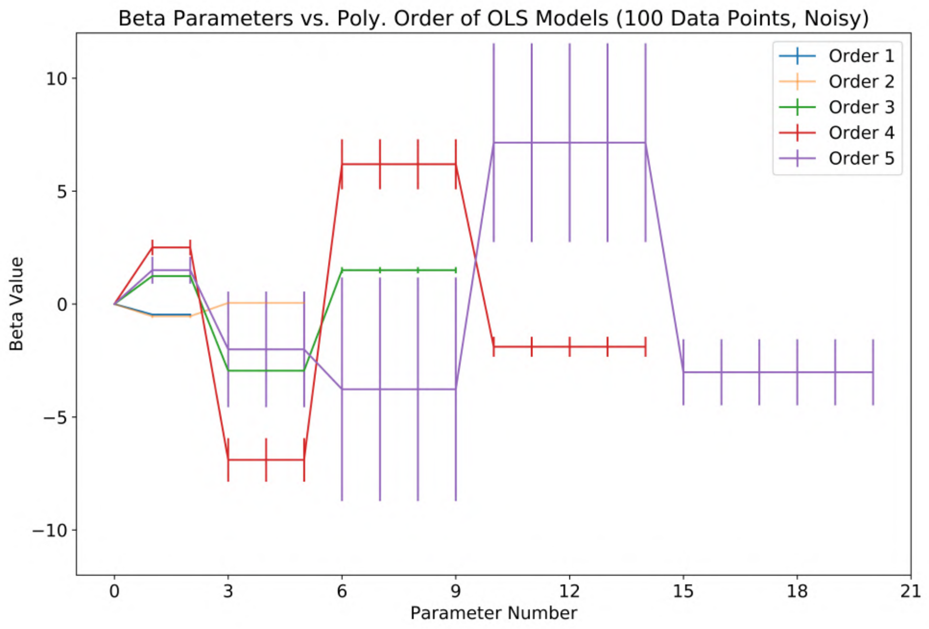


Figure 6: Beta parameter uncertainty.

Next we implement bootstrap resampling with OLS regression. The purpose of this resampling is to obtain more accurate overall behavior of the model. Using 100 bootstraps (re-samplings) we again calculate the mean squared error of OLS models with respect to polynomial degree, but now also calculate the bias and variance as defined in Proof 5. We can now see the bias variance tradeoff demonstrated in Figure 7. Note that we use 50 data points in the calculation in order to see a more pronounced effect of the bias variance tradeoff, as the normal 100 points results in models that are âtoo goodâ and donât show the effects we want to see, namely significant increases in error and variance. We also include Gaussian noise of mean 0 and standard deviation 1. At low polynomial order the MSE and bias are higher with a low variance, and the error decreases to a minimum around order 3 to 6. However as we go past that, the variance and error increase dramatically while the bias stays low. Thus this is the bias variance tradeoff, and the best model to select is in this minimum area from around order 3 to 6.

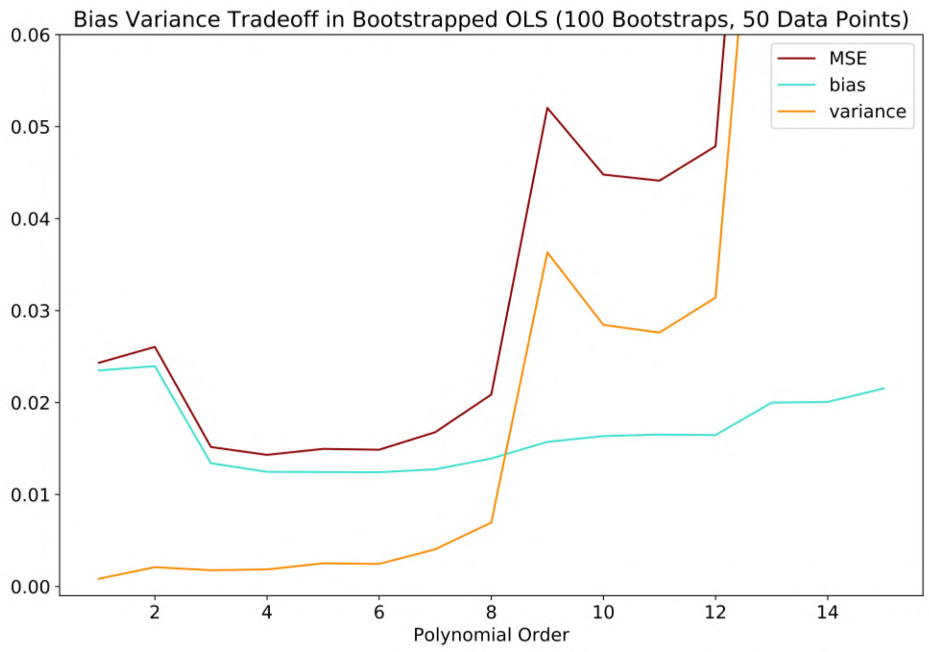


Figure 7: Bias variance tradeoff illustrated for OLS with bootstrap method.

In the next test we implement OLS with cross validation as the resampling technique. We again calculate the MSE as a function of polynomial order, but now also as a function of the number of folds in the cross validation resampling. Going from 5 to 10 folds, we find that the calculated error decreases significantly as the fold number increases, as can be seen in Figure 8. This is because as the number of folds in cross validation increases, the selected training folds are more representative of the entire dataset and thus the effect is to reduce the bias. However, going too high in fold number can increase the variance and would of course increase the computational time. Thus 10 folds is commonly used as a fold number, as it has empirically often yielded good results (Kohavi, 1995).

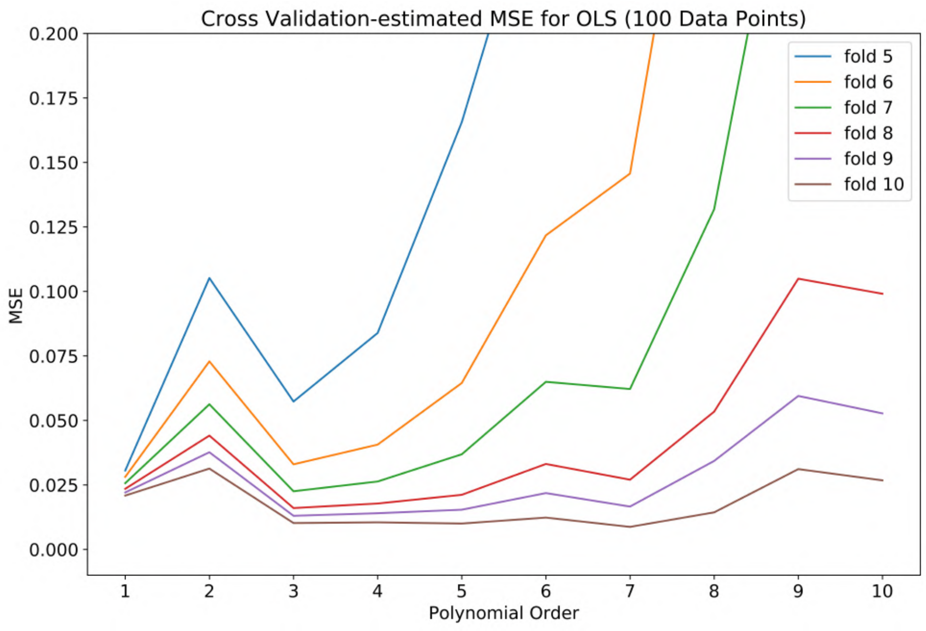
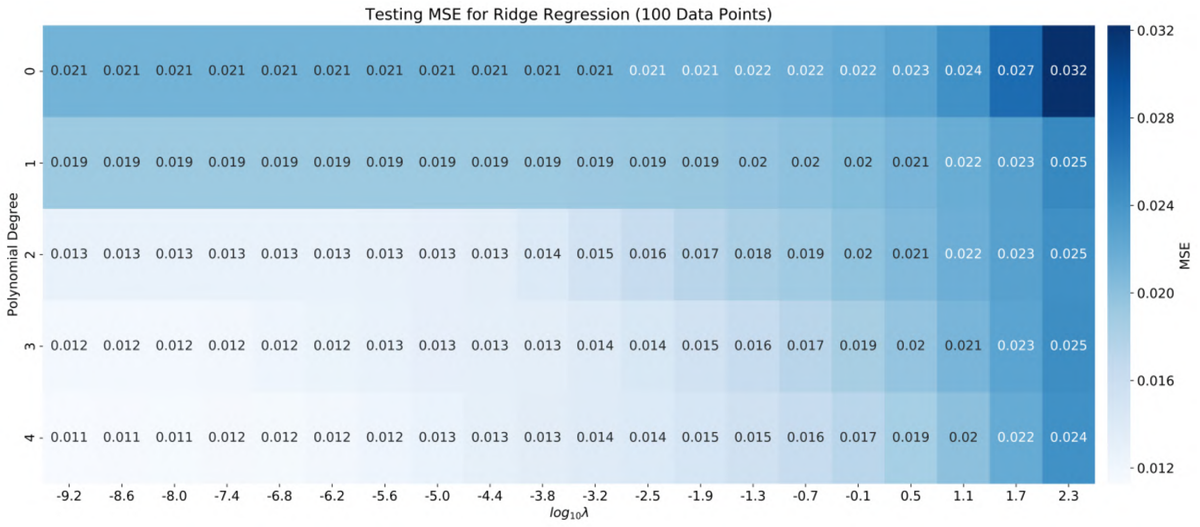


Figure 8: Cross validation for OLS.

Ridge Regression on the Franke Function

After analysis of OLS model behaviour, next we apply Ridge regression method. For Ridge regression Fig.9 represents the mean squared error in a prediction on the test data for 20 values of λ hyperparameter and different polynomial degrees. Lowest MSE achieved is 0.011 respective to 4th polynomial degree and λ equal to 1e-4



	-9.2	-8.6	-8.0	-7.4	-6.8	-6.2	-5.6	-5.0	-4.4	-3.8	-3.2	-2.5	-1.9	-1.3	-0.7	-0.1	0.5	1.1	1.7	2.3
0	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.021	0.022	0.022	0.022	0.023	0.024	0.027	0.032
1	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.019	0.02	0.02	0.02	0.021	0.022	0.023	0.025
2	0.013	0.013	0.013	0.013	0.013	0.013	0.013	0.013	0.013	0.014	0.015	0.016	0.017	0.018	0.019	0.02	0.021	0.022	0.023	0.025
3	0.012	0.012	0.012	0.012	0.012	0.012	0.013	0.013	0.013	0.013	0.014	0.014	0.015	0.016	0.017	0.019	0.02	0.021	0.023	0.025
4	0.011	0.011	0.011	0.012	0.012	0.012	0.012	0.013	0.013	0.013	0.014	0.014	0.015	0.015	0.016	0.017	0.019	0.02	0.022	0.024

Figure 9: Mean squared error for the Ridge regression for different values of λ and polynomial degree

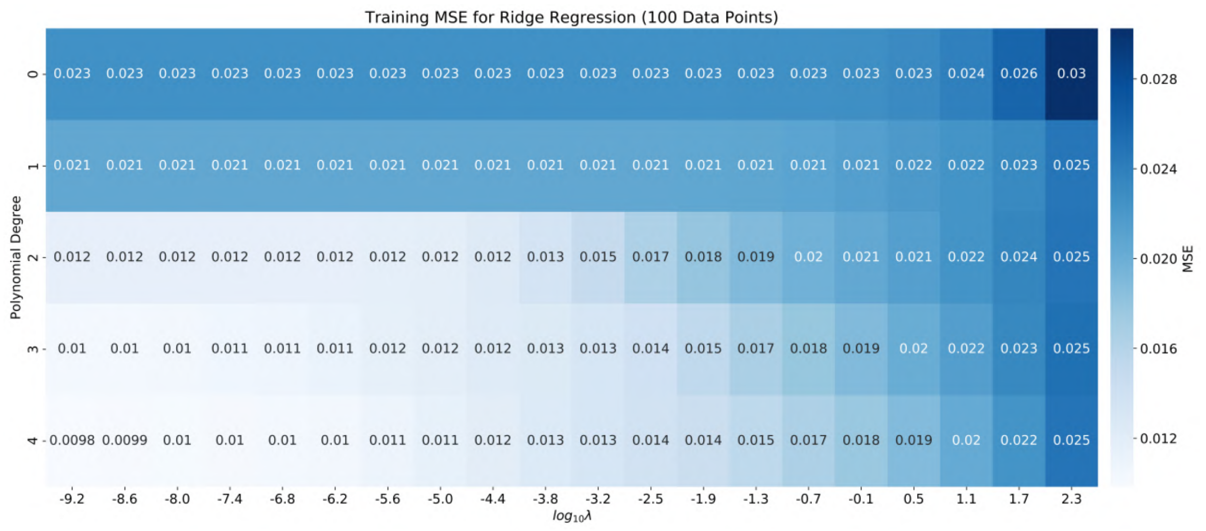


Figure 10: Ridge poly training.

Fig.11 represents MSE for the Ridge regression performed using bootstrap method and shows similar results with achieved for simple Ridge regression. Lowest MSE achieved is 0.012 respective to the 4th polynomial degree and λ equal to 1e-4

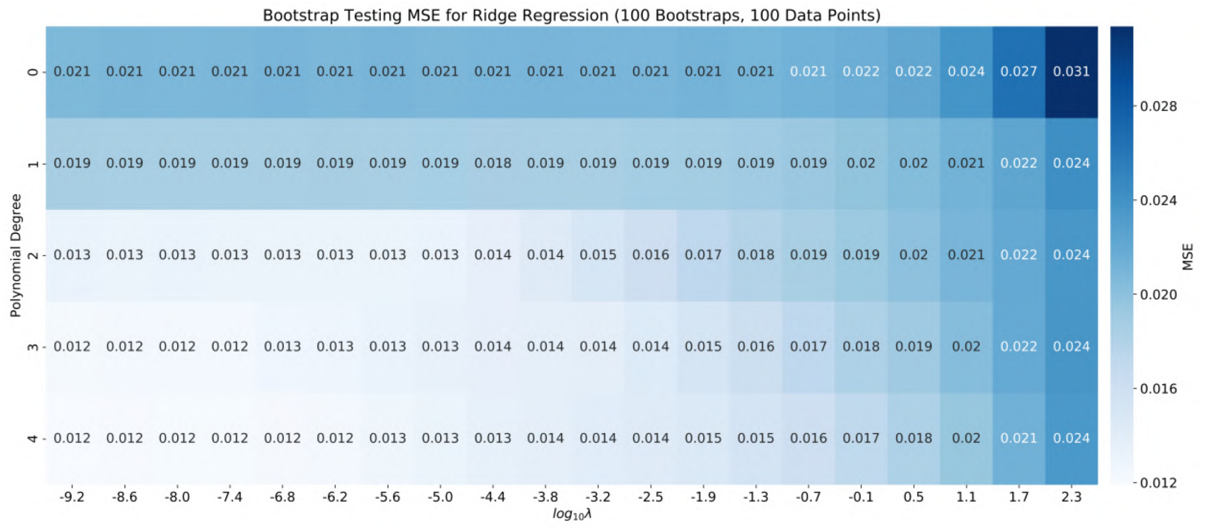


Figure 11: Mean squared error for the Ridge regression for different values of λ and polynomial degree using bootstrap method

Regularization works by reducing the variance at the cost of adding some bias to the model. Bias-variance tradeoff is then required. As MSE can be written as the sum of the variance and the squared bias, with increasing the model complexity increases the variance and bias tend to drop quickly, faster than the variance can increase and there we can achieve a drop in MSE.

Fig.12 illustrates MSE, bias and variance in respect to the polynomial degree for predefined λ

= 1e-4, providing lowest MSE respective to the 4th polynomial order where bias tend to drop.

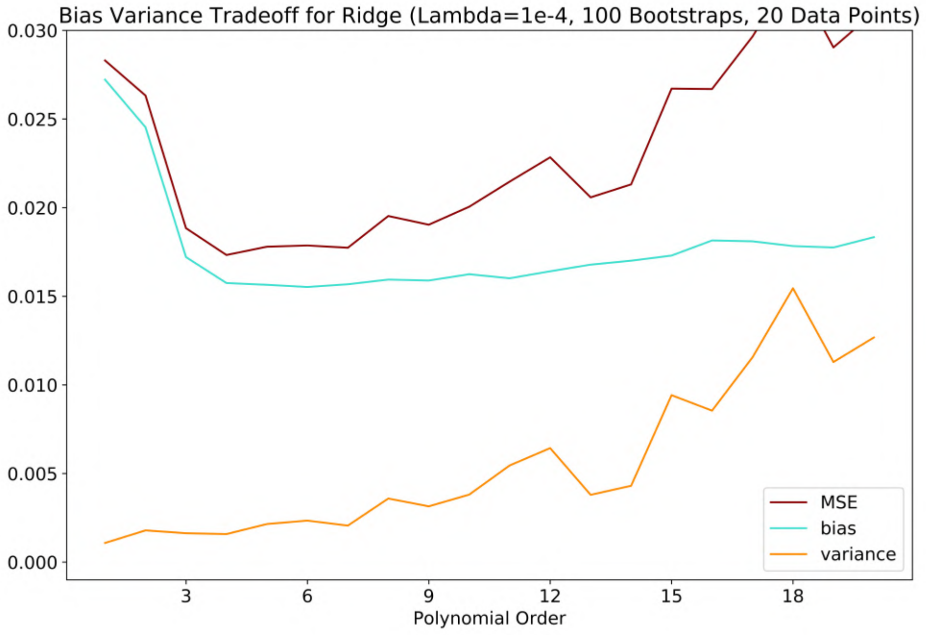


Figure 12: Bias-variance tradeoff and MSE of Ridge regression for different polynomial degree

The other method we used in our research is k-fold cross validation, where k = 10, σ = 1e-1 and number of data points is 100.

Fig.13 illustrates MSE for the Ridge regression for different values of λ and polynomial degree using this technique. Lowest MSE achieved is 0.0055 respective to the 4th polynomial degree and λ equal to 1e-4

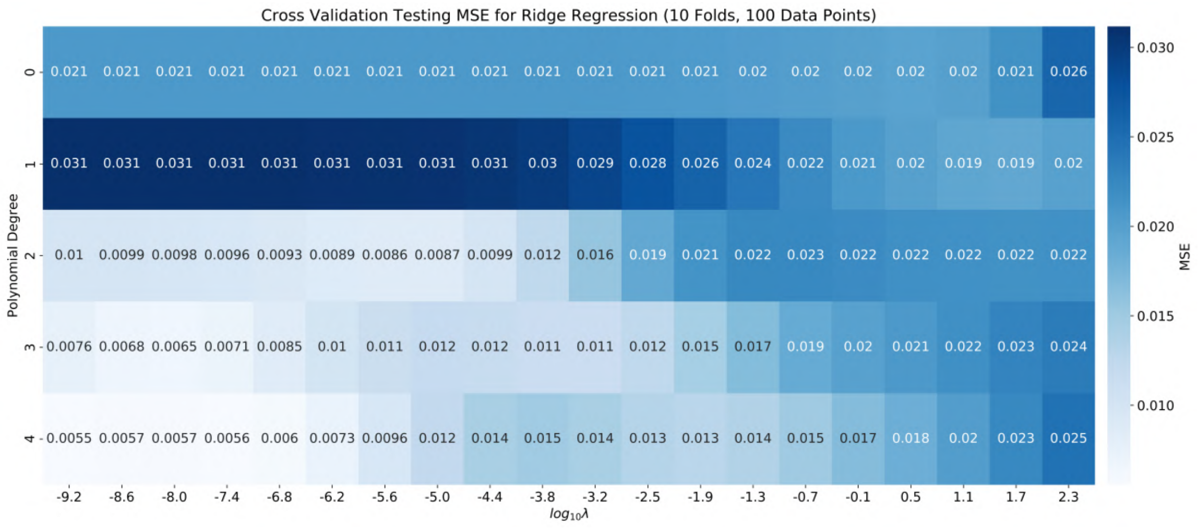


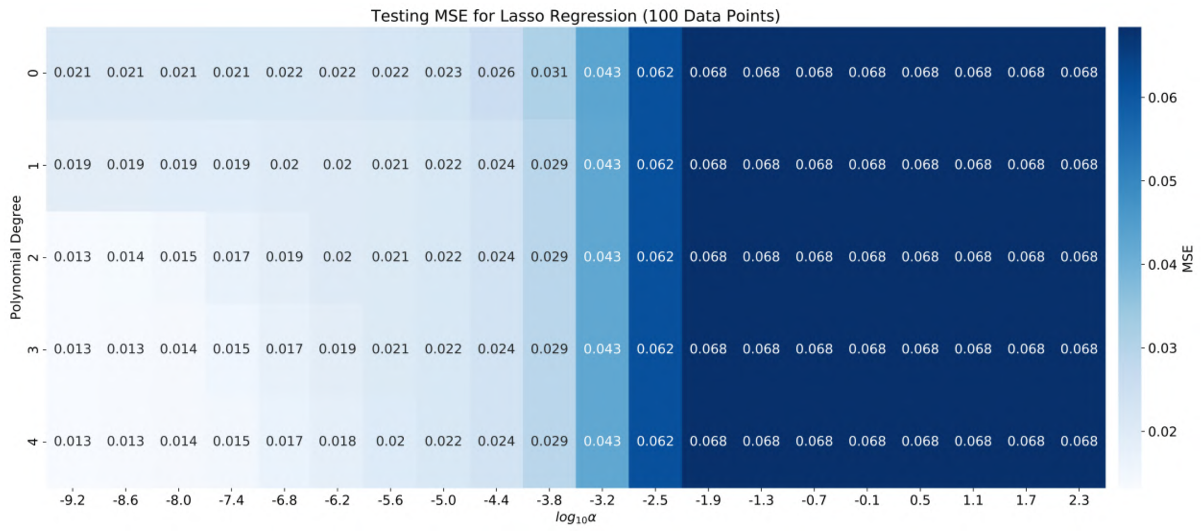
Figure 13: MSE for the Ridge regression for different values of λ and polynomial degree using cross validation technique

Comparing achieved results for the Ridge regression on the Franke function, we can acknowledge that used bootstrap method provides us with better results, then the standard and cross validation, with MSE of 0.0012 for the 4th polynomial degree and λ equal to 1e-4

Lasso Regression on the Franke Function

The name Lasso is short for "least absolute shrinkage and selection operator". The shrinkage λ parameter represents an adjustable penalty for large β values, we can therefore explore whether the MSE is dependant on it.

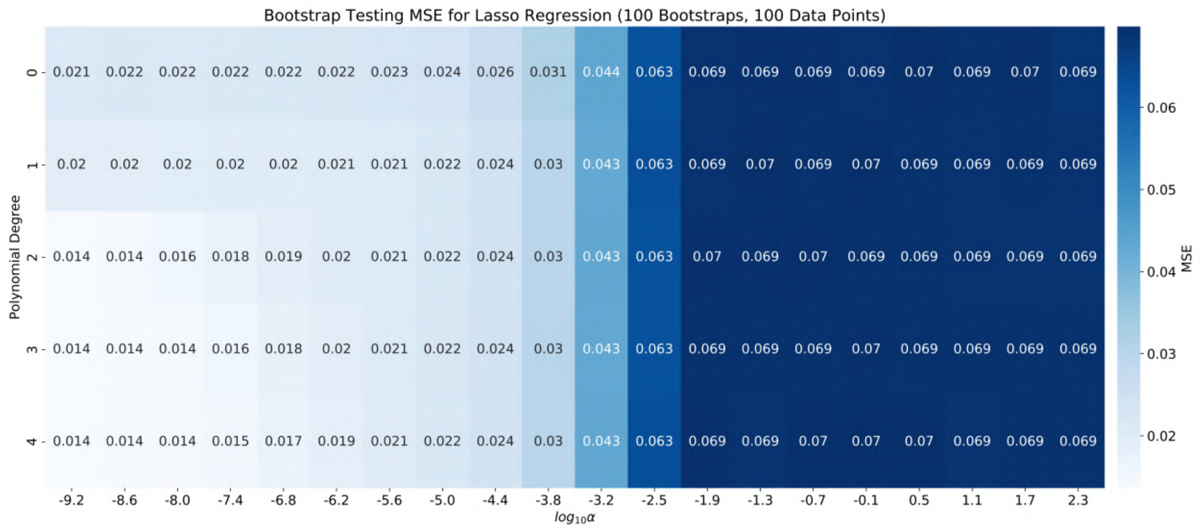
Fig.14 illustrates MSE for the LASSO regression on the Franke function for different values of λ and polynomial degree using 100 data points. Lowest reasonable MSE achieved is 0.013 respective to the 2nd polynomial degree and λ equal to 1e-4



	-9.2	-8.6	-8.0	-7.4	-6.8	-6.2	-5.6	-5.0	-4.4	-3.8	-3.2	-2.5	-1.9	-1.3	-0.7	-0.1	0.5	1.1	1.7	2.3
0	0.021	0.021	0.021	0.021	0.022	0.022	0.022	0.023	0.026	0.031	0.043	0.062	0.068	0.068	0.068	0.068	0.068	0.068	0.068	0.068
1	0.019	0.019	0.019	0.019	0.02	0.02	0.021	0.022	0.024	0.029	0.043	0.062	0.068	0.068	0.068	0.068	0.068	0.068	0.068	0.068
2	0.013	0.014	0.015	0.017	0.019	0.02	0.021	0.022	0.024	0.029	0.043	0.062	0.068	0.068	0.068	0.068	0.068	0.068	0.068	0.068
3	0.013	0.013	0.014	0.015	0.017	0.019	0.021	0.022	0.024	0.029	0.043	0.062	0.068	0.068	0.068	0.068	0.068	0.068	0.068	0.068
4	0.013	0.013	0.014	0.015	0.017	0.018	0.02	0.022	0.024	0.029	0.043	0.062	0.068	0.068	0.068	0.068	0.068	0.068	0.068	0.068

Figure 14: Mean squared error for the LASSO regression for different values of λ and polynomial degree

Fig.15 illustrates MSE for the LASSO regression on the Franke function for different values of λ and polynomial degree. Lowest MSE achieved is 0.013 respective to the 2nd polynomial degree and λ equal to 1e-4 using bootstrap method with 100 bootstraps and 100 data points



Polynomial Degree	-9.2	-8.6	-8.0	-7.4	-6.8	-6.2	-5.6	-5.0	-4.4	-3.8	-3.2	-2.5	-1.9	-1.3	-0.7	-0.1	0.5	1.1	1.7	2.3
0	0.021	0.022	0.022	0.022	0.022	0.022	0.023	0.024	0.026	0.031	0.044	0.063	0.069	0.069	0.069	0.069	0.07	0.069	0.07	0.069
1	0.02	0.02	0.02	0.02	0.02	0.021	0.021	0.022	0.024	0.03	0.043	0.063	0.069	0.07	0.069	0.07	0.069	0.069	0.069	0.069
2	0.014	0.014	0.016	0.018	0.019	0.02	0.021	0.022	0.024	0.03	0.043	0.063	0.07	0.069	0.07	0.069	0.069	0.069	0.069	0.069
3	0.014	0.014	0.014	0.016	0.018	0.02	0.021	0.022	0.024	0.03	0.043	0.063	0.069	0.069	0.069	0.07	0.069	0.069	0.069	0.069
4	0.014	0.014	0.014	0.015	0.017	0.019	0.021	0.022	0.024	0.03	0.043	0.063	0.069	0.069	0.07	0.07	0.07	0.069	0.069	0.069

Figure 15: Mean squared error for the LASSO regression for different values of λ and polynomial degree using bootstrap method

Fig.16 illustrates MSE, bias and variance in respect to the polynomial degree for predefined λ = 1e-4, providing lowest MSE respective from the 3rd to the 6th polynomial order. However, as 3rd polynomial order gives us a fairly similar MSE, thus there is no need to increase the model complexity.

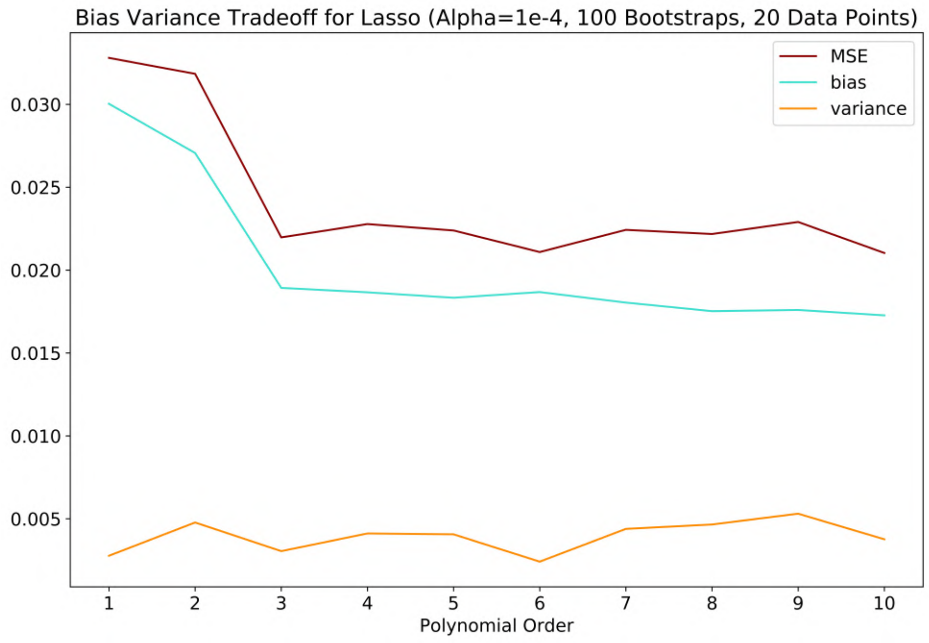


Figure 16: Lasso bias variance.

The other method we used in our research is k-fold cross validation, where k = 10, σ = 1e-1 and number of data points is 100. Fig.17 illustrates MSE for the LASSO regression on the

Franke function for different values of λ and polynomial order using this technique. Lowest MSE achieved is 0.022 respective to the 2nd polynomial degree and λ equal to 1e-4

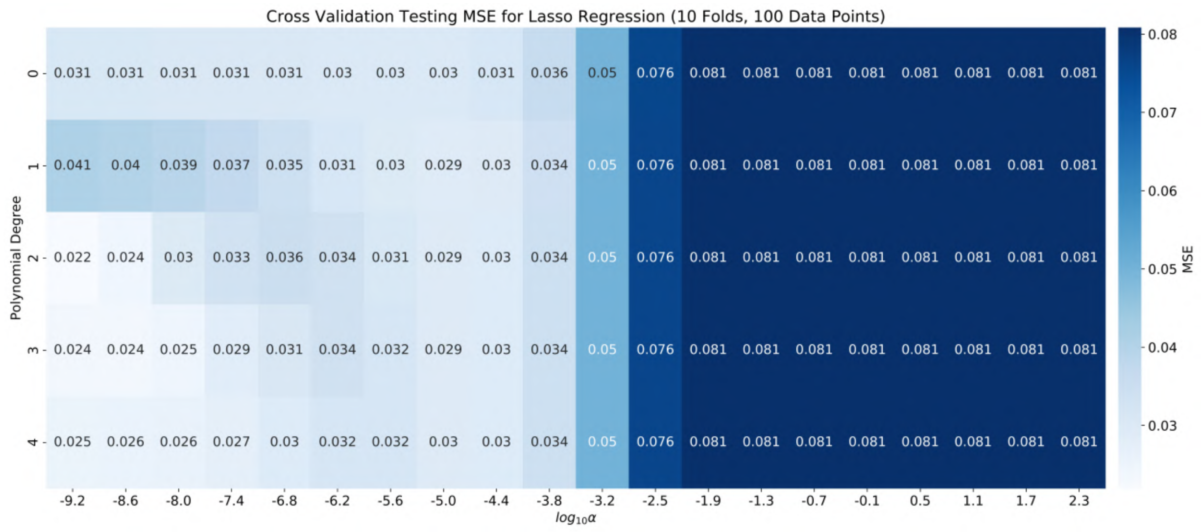


Figure 17: Mean squared error for the LASSO regression on the Franke function for different values of λ and polynomial degree using cross validation technique

Comparing achieved results for the LASSO regression on the Franke function, we can acknowledge that used technique provides us with better results for lower polynomial degrees then tested previously Ridge regression. However cross validation method gives almost twice as higher mean squared error then the standard LASSO and the bootstrap technique.

Regression on Real Topography Data

Using the knowledge we have gained from testing regression models on the Franke function, we now test our model workflows on real topography data. This data is from the Shuttle Radar Topography Mission (SRTM) and is provided by the U.S. Geological Survey (USGS, 2022). The first real dataset we select is from Iowa, which is a U.S. state that has mostly flat farmland. The second dataset we select is from Rothrock State Forest in the state of Pennsylvania, which is part of the Appalachian mountain range area and has significant variations in topography. We chose these two datasets in order to see how models would perform on a flat dataset that is easier to fit (Iowa) and a varying dataset that is harder to fit (Pennsylvania). The two datasets are shown in map view in Figure 18 and 3D view in Figure 19.

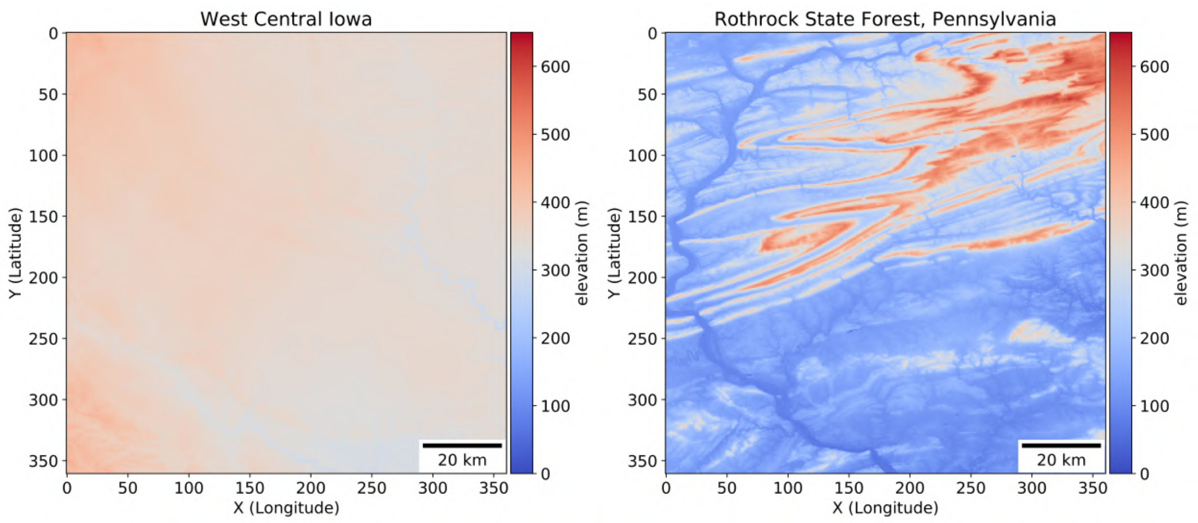


Figure 18: Topographic maps for two different locations in the United States.

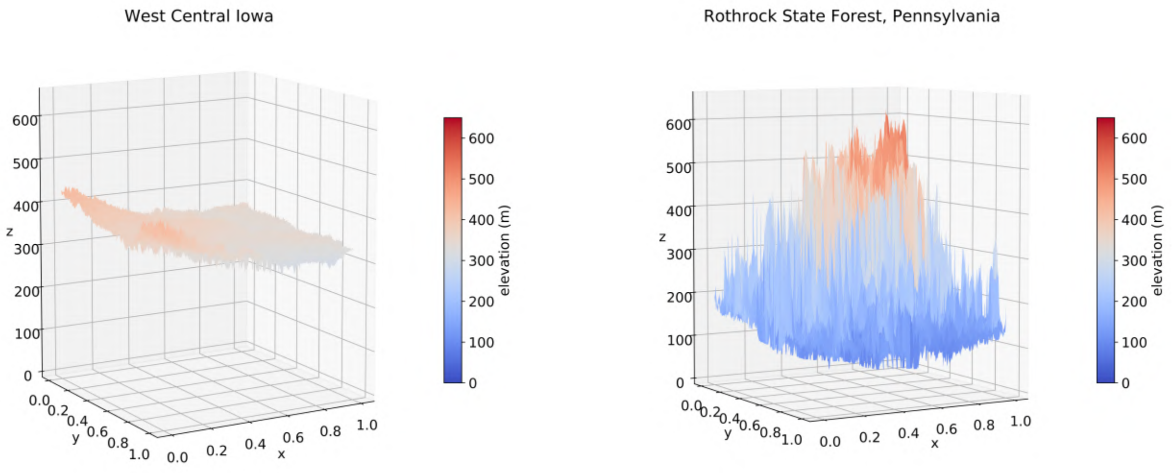


Figure 19: Topographic maps for two different locations in the United States.

We first conduct a test for OLS error as a function of polynomial order from 1-10, using 10-fold cross validation resampling. The results are presented in Figure 20. For the Iowa example, the errors are much lower because the data is flatter and easier to fit. However past order 8, the test error increases dramatically while the training error continues to decrease, indicating overfitting. In contrast the Pennsylvania data has significantly higher error since the topography is more varied and it is harder to fit a model. Furthermore the test error increases dramatically at only polynomial order 5, indicating extreme overfitting of the data.

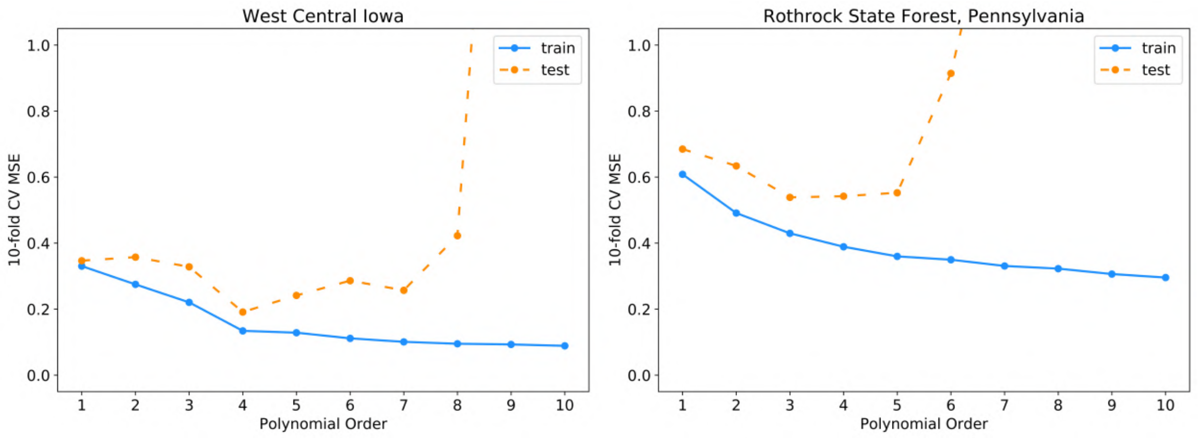


Figure 20: Real OLS CV.

Next we test ridge regression on the two real datasets, again with 10-fold cross validation resampling. We conduct a similar grid search to that used on the Franke function, going over polynomial degree 1-5 and lambdas in log space from -9.2 to 2.3. The lowest test MSE for the Iowa dataset is 0.17, and is at a somewhat-unexpected location near the bottom center in Figure 21.

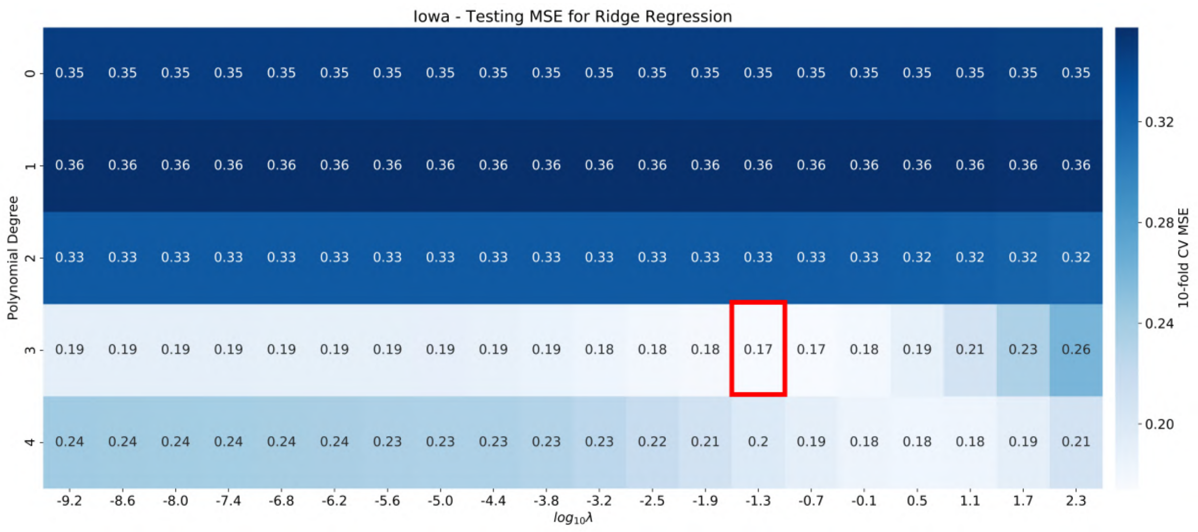


Figure 21: Iowa ridge test.

In the test on the Pennsylvania dataset, the MSEs are significantly higher, with the lowest being 0.5 and corresponding to order 5.

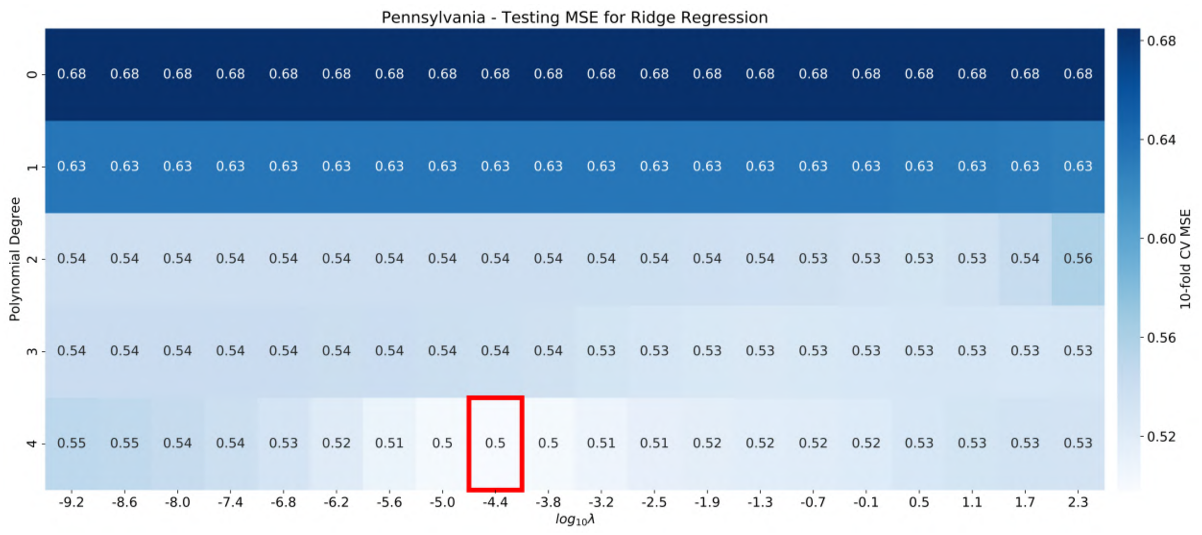


Figure 22: Pennsylvania ridge test.

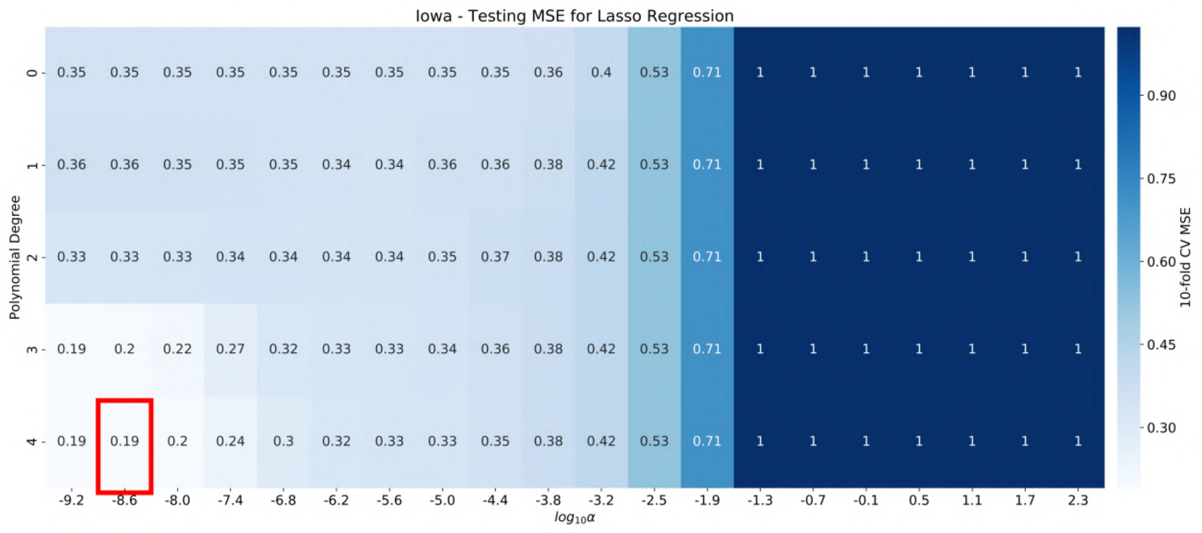


Figure 23: Iowa lasso test.

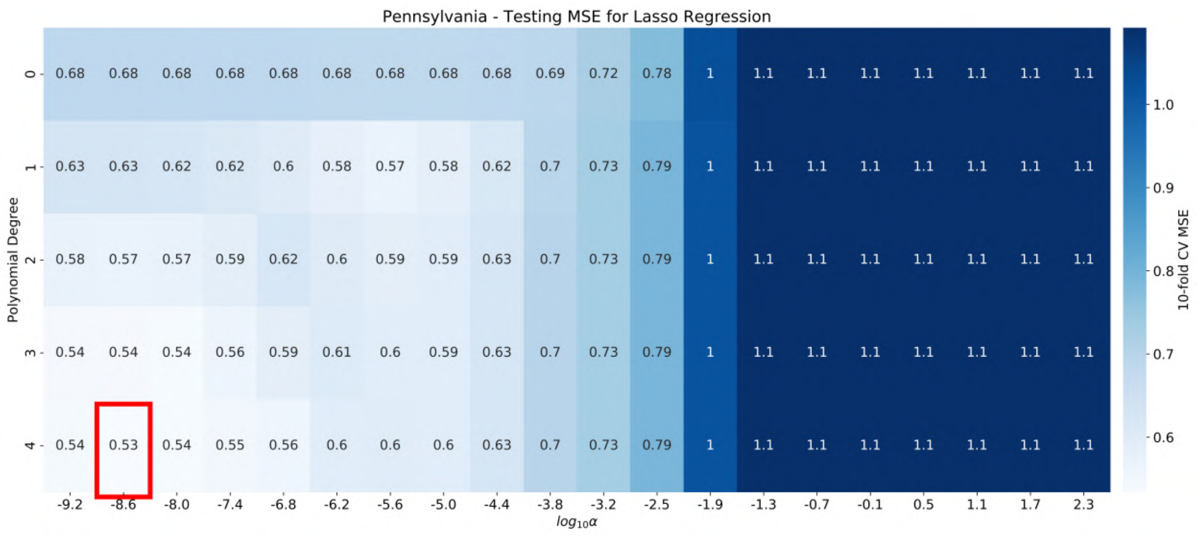


Figure 24: Pennsylvania lasso test.

	Iowa			Pennsylvania		
	OLS	Ridge	Lasso	OLS	Ridge	Lasso
Best Model Params	4th order	4th order, lambda = 2.6e-1	4th order, alpha = 1.8e-4	4th order	4th order, lambda = 1.3e-2	4th order, alpha = 1.8e-4
Best Test MSE	0.19	0.17	0.19	0.54	0.50	0.53

Table 1: Best models for real datasets.

Conclusions

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