Regression analysis and resampling methods

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In this paper we aim to explore the application of three distinct regression methods to both a sampling of the Franke function, as well as a set of terrain data. We utilize the ordinary-least-square (OLS) regression, Ridge regression and LASSO regression along with bootstrap and k-fold cross-validation re-sampling techniques in order to create and assess predictive polynomial models. We analyze the performance of the different regression models on the two data sets, with the ultimate goal of determining the best regression method and the best predictive polynomial model for each data set. We found that OLS was generally able to better capture the finer details in the data prior to over-fitting; whilst Ridge and LASSO were more stable past this point at the cost of recreating less details. Ultimately, we conclude that the best choice of model depends on the problem at hand.

I. INTRODUCTION

In essence, Linear Regression is the process of taking points from a function, or a set of measurements, and mapping them linearly to coordinates in a chosen basis in order to create an approximation, or model, explaining the original dataset and estimating unseen points in the domain spanned by the original data set. That is, from a limited set of data try to infer a linear functional relationship between some chosen prediction variables and the measured/sampled responses, and use this functional relationship to predict new data points in the domain. Typically, one is either interested in extracting the functional relationship between the measured responses and the prediction variables in order to say something about the relative importance of the conjectured predictors; or one wants to create a "best possible" predictive map of the (mostly unmeasured) response variables as a function of the (mostly unmeasured) prediction variables. In both cases what one really wants is some form of optimal mapping from prediction variables to response variables, and that mapping can be estimated by the use of linear regression methods.

Obviously, this way of doing predictions and inferences has an enormous range of possible applications; in basically every instance where one expects some linear relationship between selected prediction variables and a response variable one can, if one has a data set containing measurements of the variables, try to use regression methods to create an optimal model. Examples might be the construction of a model for housing prices as a function of distance from city center, living area, building year and whatever else one could imagine might affect the prices. Or one may wish to determine the best coefficients in a model for nuclear binding energy as a function of nucleon numbers.

In this paper we investigate two illustrative and similar applications: The reconstruction of the Franke function from sampled values, and the (re-)construction of an elevation map from a down-sampled set of terrain data. In a way, our data sets are "low-resolution images" of the Franke function and the terrain. Our goal is then to find the best possible "high-resolution images" by using different regression methods and re-sampling techniques on the sampled data, using two-dimensional polynomials as basis functions. In other words, we want to find the most faithful recreation of the original terrain data and the Franke function expressed in a basis of two-dimensional polynomials.

We begin with a theoretical discussion of the regression and re-sampling methods that will be used, as well as some comments on the significance of the so-called Bias-Variance-Tradeoff in the context of linear regression. We then proceed to investigate the application of ordinary-least-squares (OLS), Ridge regression and LASSO regression to samplings of the Franke function. We use k-fold cross-validation to assess the mean-squared-error (MSE) of our different models, and we use bootstrap re-sampling in order to estimate the bias and variance of our models. We discuss the influence of the number of points sampled, the polynomial degree we try to fit, the values of the hyper-parameter lambda for the Ridge and LASSO regressions and the presence/absence of noise in our samplings. Afterwards we will move on to the terrain data, where we perform much of the same analysis as for the Franke function. We then try to evaluate which regression methods perform the best for different use cases, and which resulting models might be considered the 'best'.

II. THEORY

A. Linear Regression

Consider a set of data points $\{(x_1, y_i), \dots, (x_N, y_N)\}$ which we wish to fit to some linear model $\tilde{\boldsymbol{y}}(\boldsymbol{\beta})$ where $\boldsymbol{\beta}$ is a vector containing the free parameters of the model. The model $\tilde{\boldsymbol{y}}$ will then be related to the true data points $\boldsymbol{y}$ by

$$\boldsymbol{y} = \tilde{\boldsymbol{y}}(\boldsymbol{\beta}) + \boldsymbol{\varepsilon} \tag{1}$$

where $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_N)$ represents the error of the model. The aim of Linear regression models is thus to find the optimal parameters $\boldsymbol{\beta}$ such that not only the error of the model on some particular dataset is minimized, but also

the error of the model applied to different data sets sampled in the same domain is minimized such that we may use our model to make predictions about new datasets.

1. The Design Matrix

When constructing a model, we first have to chose a set of basis functions. A popular choice for which is $\mathbb{P}_n$, which is capable of modeling a wide range of different phenomena and is also the choice we will make for this paper. But in principle, any set of linear basis functions may be chosen. For a single variate polynomial, a model would then take the form

$$\tilde{y}(x) = \beta_0 + \beta_1 x + \cdots + \beta_n x^n \tag{2}$$

When trying to find the optimal $\boldsymbol{\beta}$, a useful construct is the so-called Design Matrix, which for a polynomial basis takes the form

$$\mathrm{X} = \begin{bmatrix} 1 & x_1 & \dots & x_1^n \\ 1 & x_2 & \dots & x_2^n \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & \dots & x_N^n \end{bmatrix} \tag{3}$$

where we see that entry X_{ij} contains the x_i data point evaluated in the j-th basis function. This matrix has the particularly useful property that we may then multiply it with $\boldsymbol{\beta}$ to obtain the corresponding set of predictions $\tilde{\boldsymbol{y}}$ like

$$\tilde{\boldsymbol{y}} = \mathrm{X}\boldsymbol{\beta} \tag{4}$$

leaving us with a linear algebra problem to solve in finding the $\boldsymbol{\beta}$ which optimizes $\tilde{\boldsymbol{y}}$.

This also extends directly to multivariate cases where we have more than one independent variable. In particular for two dimensional polynomials, our choice of basis for this article, we have that an n-th degree polynomial is constructed by all permutations of $x^p y^q$ where $p + q \leq n$ which means that the total number of predictors for degree n is given by

$$\binom{2+n}{n} = \frac{(2+n)!}{n!(2+n-n)!} = \frac{(n+1)(n+2)}{2} \tag{5}$$

2. Model assessment

Once we have constructed a model, we a also need a way to quantitatively evaluate its performance. Here, we will focus on two statistical measures; First, we have the *mean squared error* (MSE) defined as

$$\mathrm{MSE}(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = \frac{1}{n} \sum_i (y_i - \tilde{y}_i)^2 \tag{6}$$

which as the name suggests is a measure of the mean square distance the model $\tilde{\boldsymbol{y}}$ has from the data set $\boldsymbol{y}$. We also have the *coefficient of determination*, defined as

$$\mathrm{R}^2(\boldsymbol{y}, \tilde{\boldsymbol{y}}) = 1 - \frac{\sum_i (y_i - \tilde{y}_i)^2}{\sum_i (y_i - \mathbb{E}[\boldsymbol{y}])^2} \tag{7}$$

which loosely speaking is a measure of well the proposed model predicts the data, where $\mathrm{R}^2 = 1$ corresponds to a perfect fit and $\mathrm{R}^2 < 1$ an increasingly worse fit. It is worth to note that the MSE and R^2 are essentially equivalent when measuring the performance of a model on a particular sample, which is ultimately determined by the $\sum_i (y_i - \tilde{y}_i)^2$ term in both cases. Thus they differ mainly in scaling & centering. However, R^2 will notably yield results which translates somewhat more directly across different models.

A particularly important point to make when considering these measures is that they will both generally favor increasingly higher degree polynomials when looking at some particular data set. Whilst yielding good MSE & R^2 scores this leads to over-fitting, where the model becomes too specialized to one particular sample which means that the overall predictive capabilities of the model actually decreases. We will look closer at the details of this in a later section. For now, we simply note that this problem motivates us to split our data sets into training and test sets. Where we train our model using the training set, and subsequently validate the model by computing the MSE & R^2 scores on the test sets. Thus, if our model becomes too specialized to the training set, this will lower MSE & R^2 scores in the test set, giving us a much better indication on the predictive capabilities of our model.

3. Ordinary Least Squares

In ordinary least squares (OLS), we aim to find an optimal set of parameters $\hat{\boldsymbol{\beta}} = [\hat{\beta}_0, \dots, \hat{\beta}_n]^T$ such that the L^2 norm $\|\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}\|_2$ is minimal, with the L^2 norm being induced by the inner product

$$\|\boldsymbol{u}\|_2^2 = \sum_i u_i^2 = \boldsymbol{u}^T \boldsymbol{u} \tag{8}$$

This defines the cost function for OLS, which may be written as

$$C_{OLS}(\boldsymbol{\beta}) = (\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta})^T (\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}) \tag{9}$$

In order to find the minima, we differentiate wrt to $\boldsymbol{\beta}$ and assert that $\partial_{\boldsymbol{\beta}} C_{OLS} = 0$ for the optimal predictor. Taking the partial derivative yields

$$\frac{\partial}{\partial \boldsymbol{\beta}} C_{OLS}(\boldsymbol{\beta}) = -2\mathrm{X}^T (\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}) \tag{10}$$

We assert this is zero at the minima, which yields

$$\mathrm{X}^T \boldsymbol{y} = \mathrm{X}^T \mathrm{X}\boldsymbol{\beta} \tag{11}$$

then taking the inverse of $\mathrm{X}^T\mathrm{X}$ on both sides then gives the optimal $\boldsymbol{\beta}$ as

$$\hat{\boldsymbol{\beta}}_{\mathrm{OLS}} = (\mathrm{X}^T\mathrm{X})^{-1}\mathrm{X}^T\boldsymbol{y} \tag{12}$$

which mathematically is the best projection of the datapoints to our model. It can also be shown that the variance of these optimal predictors are given by [1]

$$\mathrm{Var}\left(\hat{\boldsymbol{\beta}}_{\mathrm{OLS}}\right) = \sigma^2\left(\mathrm{X}^T\mathrm{X}\right)^{-1} \tag{13}$$

Where σ^2 denotes the variance of the underlying noise of the sample.

While OLS yields the mathematically best model for some particular sample, it does not necessarily yield the best predictive model. OLS may suffer from over-fitting to the particular sample, and will therefore not always perform very well on new data points for which the model has not been trained. As such, we instead look at alternate regression methods with additional tuning parameters which allow us to account for the variance between different sets of data as to yield a model with better predictive abilities compared to the OLS.

4. Ridge Regression

One such method is the Ridge regression where we instead try to minimize $\|\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}\|_2 + \lambda\|\boldsymbol{\beta}\|_2$, from which we define our cost function as

$$C_R(\boldsymbol{\beta}) = (\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta})^T(\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}) + \lambda\boldsymbol{\beta}^T\boldsymbol{\beta} \tag{14}$$

Similar for what we did for OLS, we take the partial derivative wrt. $\boldsymbol{\beta}$, where the only difference in finding the minima resides in the additional term

$$\frac{\partial}{\partial\boldsymbol{\beta}}\lambda\boldsymbol{\beta}^T\boldsymbol{\beta} = 2\lambda\boldsymbol{\beta} \tag{15}$$

if we again assert that the optimal $\boldsymbol{\beta}$ is given by $\partial_{\boldsymbol{\beta}}C_R(\boldsymbol{\beta})$ and rearrange we get

$$\hat{\boldsymbol{\beta}}_R = \left(\mathrm{X}^T\mathrm{X} + \lambda\right)^{-1}\mathrm{X}^T\tilde{\boldsymbol{y}} \tag{16}$$

As the optimal β for Ridge regression. So we see that the only difference between OLS and Ridge regression is the addition of the "penalty" parameter λ to the L^2 norm of the coefficients $\boldsymbol{\beta}$. The main point of introducing this parameter is to reduce the variance of the regression coefficients $\boldsymbol{\beta}$. It introduces a constraint on the allowable values of $\boldsymbol{\beta}$, which means that the method no longer is unbiased. The aim is that the reduction of the variance outweighs the increase of the method's bias, leading to an overall lower test error, cf. the later discussion of the Bias-Variance Trade-off. As a technical note, during our computations we center our response-variable and scale plus center our predictors. This has the effect of removing the constant column in the design matrix, so that penalty term doesn't apply to β_0.

5. LASSO Regression

The cost function for the *least absolute shrinkage and selection operator* (LASSO) method is defined as

$$C_L(\boldsymbol{\beta}) = \|\boldsymbol{y} - \mathrm{X}\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1 \tag{17}$$

Which as opposed to OLS and Ridge has no analytical solution for finding the optimal $\boldsymbol{\beta}$, which is instead found by optimization methods such as gradient descent. The specifics of this is beyond the scope of this article, and we will simply use the existing libraries provided by scikit-learn [2] to perform the regression.

Qualitatively the LASSO method is distinguished from the Ridge regression by how the norm of $\boldsymbol{\beta}$ is penalized. While the Ridge regression applies the penalty to the L^2 norm, the Lasso aims to shrink the L^1 norm. Two important consequences arise from this: firstly, it is no longer possible to obtain a closed-form solution to the minimization problem; secondly, the regression coefficients may be shrunk far more unevenly. In contrast to the Ridge regression, LASSO regression may shrink individual β_i to zero. This is an extremely useful property of the method, since it allows unimportant predictors to be identified and discarded. The drawback, of course, is that the bias of the Lasso method is expected to exceed the bias of the Ridge method. Furthermore, for highly correlated prediction variables, like our two-dimensional polynomials, the LASSO method might struggle with which of those prediction variables to keep. Once again a technical note; by centering we remove the constant column from the design matrix to avoid penalizing the constant term through β_0.

B. Singular Value Decomposition

Consider an $m \times n$ matrix X of rank r. The singular values of X are then defined as the root of the eigenvalues of the diagonal matrix $\mathrm{X}^T\mathrm{X}$. We may also express X in the so-called singular value decomposition (SVD)

$$\mathrm{X} = \mathrm{U}\Sigma\mathrm{V}^T \tag{18}$$

where U, V are unitary matrices and

$$\Sigma = \begin{bmatrix} D & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} \tag{19}$$

an $m \times n$ matrix, where the matrix D is a diagonal $r \times r$ matrix containing the singular values of $\mathrm{X}^T\mathrm{X}$

$$D = \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n \end{bmatrix} \tag{20}$$

which by convention is ordered such that $\sigma_1 \geq \cdots \geq \sigma_n$.

1. Application to OLS

We may use the SVD to re-express the expression for $\hat{\boldsymbol{\beta}}$ in OLS given by Eqn. 12 by writing

$$\mathrm{X}^T\mathrm{X} = \left(\mathrm{U}\Sigma\mathrm{V}^T\right)^T\left(\mathrm{U}\Sigma\mathrm{V}^T\right) = \mathrm{V}\Sigma^T\mathrm{U}^T\mathrm{U}\Sigma\mathrm{V}^T \tag{21}$$

Since U is unitary, it follows that $\mathrm{U}^T\mathrm{U} = \mathbb{I}$, further we have that $\Sigma^T = \Sigma$ since it is a diagonal matrix. We therefore end up with

$$\mathrm{X}^T\mathrm{X} = \mathrm{V}\Sigma^2\mathrm{V}^T \tag{22}$$

inserting this into Eqn. 12 gives us

$$\hat{\boldsymbol{\beta}}_{\mathrm{OLS}} = \left(\mathrm{V}\Sigma^2\mathrm{V}^T\right)^{-1}\mathrm{V}\Sigma\mathrm{U}^T\boldsymbol{y} \tag{23}$$

This gives an alternate way of solving the OLS problem, which becomes particularly useful in situations where we have a large amount of data sampled from a relatively small domain, increasing the chance of X having linearly dependent columns which in turns leads to X, and by extension $\mathrm{X}^T\mathrm{X}$ no longer being invertible.

C. Re-sampling

Re-sampling methods are ways in which we can generate new statistics from our existing data, which as the name suggests implies sampling new data sets from our already existing data. By doing so, we may gain new insights about our data which may not be available through regular analysis, particularly in situations where we are limited by the number of data points.

Here, we will focus on two of many such techniques.

1. k-fold Cross Validation

In the k-fold cross-validation re-sampling method, we split our data set S into k equally sized subsets $s_1, \ldots, s_k$. We then for each $i = 1, \ldots, k$ assign the i-th subset as the test set and the remaining $k-1$ subsets as the training set and compute the statistics in the usual way. Then at the end, we compute the mean value of the k sets of statistics. A visual representation of this process can be seen in Fig. 1. When doing cross-validation, typical choices of k are 5 and 10 [1]. Which one is better will depend on how the error scales with the size of the training set, as such, choosing a suitable k requires some analysis[1]. However, for the present paper we will stick to 5-fold cross validation on the basis that we are mainly concerned with small data sets and increasingly larger complexities.

2. Bootstrap

In the bootstrap re-sampling method, we sample our data set $S = \{s_1, \ldots s_N\}$ N-number of times, in particular,

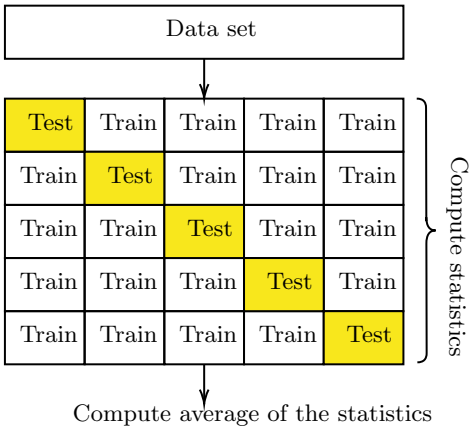


FIG. 1: Visual representation of k-fold cross-sampling for $k = 5$

we allow sampling the same s_i multiple times. In this way, we generate new datasets in which some points are under-weighted and others overweighted with respect to the original dataset S. Loosely speaking, the concept corresponds to evenly sampling the ensemble of all possible input data sets to our regression method, in order to estimate the variance and expectation values of our model predictions over the ensemble. The idea is that if our training set representatively covers the domain of inputs, each re-sampled regression computation will give a certain prediction $\tilde{\boldsymbol{y}}_{\boldsymbol{B}}$ and these $\tilde{\boldsymbol{y}}_{\boldsymbol{B}}$ will appear with a frequency corresponding to their underlying probability distribution. When we later try to compute statistics of the predictions, we will then be able to use point-estimators on the computed $\tilde{\boldsymbol{y}}_{\boldsymbol{B}}$ to obtain estimates of, for instance, the variance of the predictions or the mean value of the predictions over the ensemble of all possible inputs in the domain spanned by our data.

D. The Bias-Variance Trade-off

A key concept in much of machine learning is the so-called Bias-Variance Trade-off. Simply put the test error of a learned prediction method can be viewed as being partly the sum of two distinct quantities, the bias of the method and the variance of the method. The bias can be thought of as errors due to inflexible assumptions and constraints on the model, while the variance, quite opposingly, is the actual statistical variance of the procedure. Crucially, the variance is connected with the model having too much flexibility, over-fitting on the training data while giving very spread results on the test data. Naturally, the relative sizes of the errors due to bias and the errors due to variance change with the flexibility/-complexity of the model. For an inflexible model, e.g. a polynomial regression model of low degree, the bias is expected to be the dominant contribution to the test er-

ror. On the other side of the spectrum, for a very flexible model, e.g. a polynomial regression model of high degree, the variance would be anticipated to be the dominating source of the test error. Importantly, the relative effects of the bias and the variance won't necessarily change at the same rate. Thus, one could hope to find an optimally flexible model which minimizes the combined error due to variance and bias. This is the essence of the Bias-Variance Trade-off; one could, for instance, try to slightly increase the bias of a method in the hopes of reducing the variance far more.

Concretely for the problem at hand in this article, we use the expected MSE of our models on the test data to assess our models. This expected MSE can be explicitly decomposed into a bias term, a variance term and an irreducible error [1]. We assume that our response values $\boldsymbol{y}$ are given by a "true" function $\boldsymbol{f}$ with the addition of normally distributed noise $\boldsymbol{\varepsilon}$ with zero mean:

$$\boldsymbol{y} = \boldsymbol{f} + \boldsymbol{\varepsilon} \tag{24}$$

Denoting our model predictions by $\tilde{\boldsymbol{y}}$ and keeping our "true" test values $\boldsymbol{f}$ fixed, we can then decompose the expected squared test error, the expectations being taken over the ensemble of possible predictions and noise values, as:

$$\begin{aligned}
&\mathbb{E}[(\boldsymbol{y} - \tilde{\boldsymbol{y}})^2] \\
&= \mathbb{E}[((\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}]) - (\tilde{\boldsymbol{y}} - \mathbb{E}[\tilde{\boldsymbol{y}}]))^2] \\
&= \mathbb{E}[(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathbb{E}[(\tilde{\boldsymbol{y}} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] \\
&\quad - \mathbb{E}[2((\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])(\tilde{\boldsymbol{y}} - \mathbb{E}[\tilde{\boldsymbol{y}}]))] \\
&= \mathbb{E}[(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathrm{Var}[\tilde{\boldsymbol{y}}] - 2(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])\mathbb{E}[(\tilde{\boldsymbol{y}} - \mathbb{E}[\tilde{\boldsymbol{y}}])] \\
&= \mathbb{E}[(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathrm{Var}[\tilde{\boldsymbol{y}}] - 2(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])(\mathbb{E}[\tilde{\boldsymbol{y}}] - \mathbb{E}[\tilde{\boldsymbol{y}}]) \\
&= \mathbb{E}[(\boldsymbol{y} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathrm{Var}[\tilde{\boldsymbol{y}}] = \mathrm{Bias}^2[\boldsymbol{y}, \tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}] \\
&= \mathbb{E}[(\boldsymbol{f} + \boldsymbol{\varepsilon} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathrm{Var}[\tilde{\boldsymbol{y}}] \\
&= \mathbb{E}[(\boldsymbol{f} - \mathbb{E}[\tilde{\boldsymbol{y}}])^2] + \mathrm{Var}[\tilde{\boldsymbol{y}}] + \mathrm{Var}[\boldsymbol{\varepsilon}] \\
&= \mathrm{Bias}^2[\boldsymbol{f}, \tilde{\boldsymbol{y}}] + \mathrm{Var}[\tilde{\boldsymbol{y}}] + \boldsymbol{\sigma}^2
\end{aligned} \tag{25}$$

In a convenient abuse of notation, the above calculation is meant to be performed element-wise. What has been computed above is the expected squared test error for each data point in the test set separately; for notational convenience stacked up as vectors. To get a total MSE for the whole test set, one simply must take the mean over the vector elements afterwards. This yields:

$$\begin{aligned}
\mathrm{MSE} &= \frac{1}{n}\sum_i^n \mathbb{E}[(y_i - \tilde{y}_i)^2] \\
&= \frac{1}{n}\sum_i^n (\mathbb{E}[(y_i - \mathbb{E}[\tilde{y}_i])^2] + \mathrm{Var}[\tilde{y}_i]) \\
&= \frac{1}{n}\sum_i^n (\mathbb{E}[(f_i + e_i - \mathbb{E}[\tilde{y}_i])^2] + \mathrm{Var}[\tilde{y}_i]) \\
&= \frac{1}{n}\sum_i^n (\mathbb{E}[(f_i - \mathbb{E}[\tilde{y}_i])^2] + \mathrm{Var}[\tilde{y}_i] + \mathrm{Var}[e_i] \\
&= \frac{1}{n}\sum_i^n ((\mathbb{E}[(f_i - \mathbb{E}[\tilde{y}_i])^2] + \mathrm{Var}[\tilde{y}_i] + \sigma_i^2) \\
&= \frac{1}{n}\sum_i^n (\mathrm{Bias}^2[f_i, \tilde{y}_i] + \mathrm{Var}[\tilde{y}_i]) + \sigma^2
\end{aligned} \tag{26}$$

Here σ_i^2 is the variance of the noise for each test point. Since all test points are assumed to have the same noise distribution, their variances will be equal. To be perfectly clear, the random variables for both of the preceding calculations are the model predictions $\tilde{y}_i$ and the test point noises ε_i, which are considered to be independent of each other. As an annotation aside; similar derivations may be found in most, if indeed not all, textbooks on machine learning, though they are often less than explicit in defining what domains the expectation values are taken over. For a refreshingly clear presentation, complete with pointing arrows and text-boxes, the reader is referred to the set of lecture notes by Professor W. Cohen [3].

In practical terms, we use the bootstrap re-sampling to estimate the bias and variance of the model. This is achieved by replacing $\tilde{y}_i$ with $\tilde{y}_{i,B}$ in Eqn. 26. The expectation values will then be computed over all the bootstrap iterations. Furthermore, we are not able to extract the noise from the response values, and must then use the bias estimate $\mathrm{Bias}^2[y_i, \tilde{y}_{i,B}]$. Explicitly, the MSE, the bias and the variance estimates obtained from the bootstrap re-sampling become, for a test set with size n and a number M bootstrap iterations:

$$\mathrm{MSE}_B = \frac{1}{n}\sum_i^n \left(\frac{1}{M}\sum_B^M (y_i - \tilde{y}_{i,B})^2\right) \tag{27}$$

$$\mathrm{Bias}_B^2 = \frac{1}{n}\sum_i^n \left(y_i - \frac{1}{M}\sum_B^M \tilde{y}_{i,B}\right)^2 \tag{28}$$

$$\mathrm{Var}_B = \frac{1}{n}\sum_i^n \left(\frac{1}{M}\sum_B^M \left(\tilde{y}_{i,B} - \frac{1}{M}\sum_B^M \tilde{y}_{i,B}\right)^2\right) \tag{29}$$

E. The Franke Function

The Franke function is defined as

$$\begin{aligned} f(x,y) = &\frac{3}{4}\exp\left(-\frac{(9x-2)^2}{4} - \frac{(9y-2)}{4}\right) \\ &+ \frac{3}{4}\exp\left(-\frac{(9x+1)^2}{49} - \frac{(9y-21}{10}\right) \\ &+ \frac{1}{2}\exp\left(-\frac{(9x-7)^2}{4} - \frac{(9y-3)}{4}\right) \\ &- \frac{1}{5}\exp\left(-(9x-2)^2 - (9y-2)\right) \end{aligned} \tag{30}$$

and will serve as function on which we test the performance of our models and build an understanding before we tackle the real terrain data, which we do not have direct control over in the same way. For reference sake, we have plotted the Franke function for values $[0,1] \times [0,1]$ which can be seen in Fig. 2.

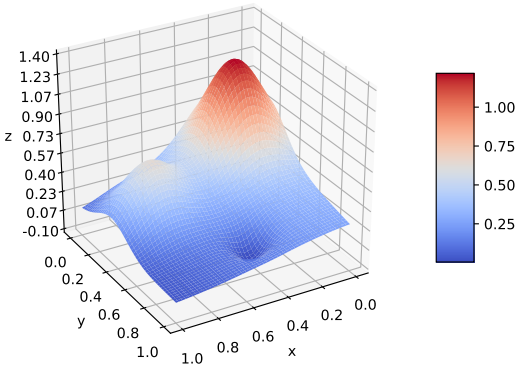


FIG. 2: The Franke Function

III. RESULTS & DISCUSSION

We aim to model both the Franke function and a set of terrain data as sums of polynomials in x and y. Our overarching goal is to determine which regression method performs the best (i.e. most faithfully reproduces the full data-set on which they are sampled) in both cases, and for which degree of the polynomial model and which value of the penalty parameter λ.

The terrain data, which has been downloaded from [4], is a collection of measured elevation heights at a discrete set of 3601×1801 pixel coordinates. For ease of interpretation and computation, we parameterize the pixel indices as uniformly spaced $x, y \in [0,1]$, and restrict ourselves to the first square of the terrain map, i.e. the first $[1801, 1801]$ pixels.

We first consider random samples of the Franke function where we analyze the performance of the different regression methods for various models (polynomial degrees) and penalty parameters. We then investigate the bias-variance behaviour of the methods, and the effect of the sampling size. Finally we compare various 'best predictions' for the different regression methods, in order to visualize the significance of their different approaches. These predictions are all trained on the same randomly sampled set of points in $x, y \in [0,1]$, and applied to a grid of 2000 points in each direction, with their resulting predictions being compared amongst the methods and with the ground truth of the Franke function evaluated on that grid.

Armed with insights from the investigation of the Franke function, we will subsequently do much of the same analysis for the terrain data. Ultimately we will compare the best predictions for each method (learned on the same down-sampled data set) with each other and with the ground truth of the full $[1801, 1801]$ terrain map we down-sampled from.

In order to ensure the reproducibility of our results, we used fixed seeds in the random number generators when producing the final results that were used in this report, and thus everything can be reproduced by running the notebooks in our Github repository [5]. The repository also contains various test cases & some unit tests to ensure that our codes work as expected. For further information, see the README files in the repository.

A. The Franke function

Throughout our analysis of the Franke function our focus was primarily on a data set consisting of $N = 500$ uniformly distributed random points, though we also made a brief analysis of the effects of varying the sample size. In particular, we present a limited analysis of a $N = 200$ sample in order to infer about the effects on which N has on the various regression methods.

1. *Noise & confidence intervals*

We start by looking at the behaviour of OLS limited to relatively modest complexities of polynomials up to the 5^{th} order modeled from data sets consisting of $N = 500$ random samples of the Franke function with added random noise in the form $0.2\mathcal{N}(0,1)$. We also chose our confidence interval for the predictors as $\beta_i \pm 2\sigma_i$ in adherence with the literature as a standard choice [1], which corresponds to 95% of similarly sampled models falling within our range of uncertainty. Here, σ_i denotes the standard deviation of β_i computed as the root of the variance given by Eqn. 13. Furthermore, we also scale this and all subsequent datasets by utilizing the StandardScaler() functionality provided by sci-kit learn on our design matrix.

In Fig. 7 we see the size of each predictor β_i for a 5^{th} order polynomial. Further, we also see the full size of the confidence interval for each term for all the polynomial degrees $p = 1, \ldots, 5$.

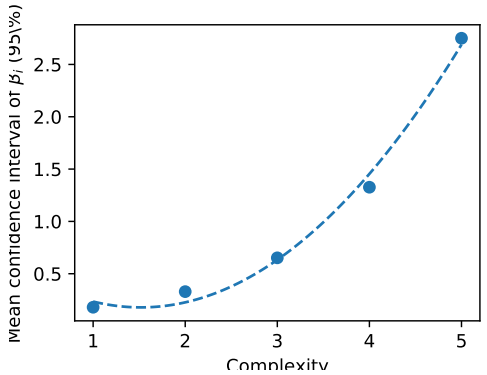


FIG. 3: Mean size of the 4σ (95%) confidence interval across all the predictors for polynomials up to the 5^{th} order with OLS for $N = 500$ random samples of the Franke Function. Where the dashed line indicates 2^{nd} order polynomial regression of the points

We observe that the confidence intervals markedly increases as a function of the models complexity, as shown more explicitly in Fig. 3, which seems to suggest a $\sim$ quadratic trend. This implies that as we try to model our data on higher order polynomials, we will at some point run into the issue of the confidence interval of our predictors becoming an increasingly significant problem for the regression. We observe the manifestation of this problem more concretely as the complexity of our model grows larger in Fig.4, where we observe a rather significant rise in the MSE of the test set compared to the training set.

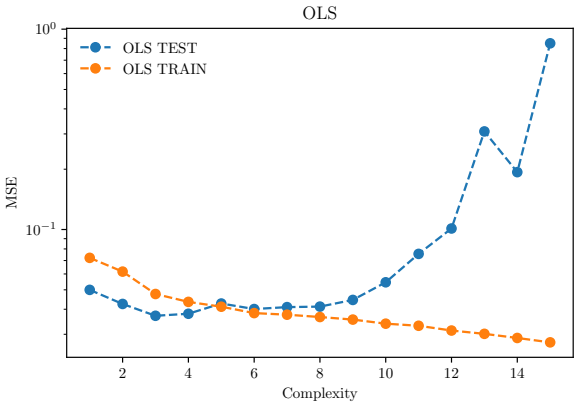


FIG. 4: The MSE for both the testing and the training data performed with OLS regression on $N = 500$ random samples of the Franke Function

We then investigated the effects that different magnitudes of noise had on OLS. In particular, we added random noise sampled from a weighted normal distribution $\delta \cdot \mathcal{N}(0, 1)$ for different weights δ. We also split our data set into a training and testing set with an 80/20 split using Sci-kit learn, where the R^2 score for each of the test sets over the different complexities are shown in Fig 5. We observe here that the regression becomes increasingly worse as δ approaches 0.5, and the noise begins to dominate.

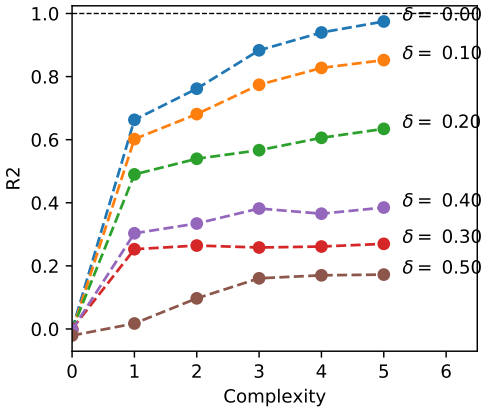


FIG. 5: R^2 measured for $N = 500$ random samples of the Franke function with added noise in the form $\delta \cdot \mathcal{N}(0, 1)$ modeled with complexities 0 to 5.

2. *Resampling*

We then move on to our comparison of the various regression methods; OLS, Ridge and LASSO. In order to infer about their relative performance, we first computed their MSE using standard[1] 5-fold cross-validation for complexities $p = 1, \ldots 15$ and in the case of Ridge & LASSO, 30 evenly spaced $\lambda \in [10^{-5}, 10^{0}]$. Then, for the optimal λ in each case we performed $M = 200$ bootstrap re-samplings for each of the models over all the complexities which we used to compute the MSE, as well as the MSE decomposed into the squared bias and variance. To specify, we performed the bootstrap with a 80/20 train/test split, where the re-samplings where performed on the training data and tested against the test data. Furthermore, in addition to scaling our design matrix, we will in these subsequent analyses also center the response variable in our datasets by subtracting the mean response.

Here, we present the above analysis performed for two datasets consisting of $N = 200$ and $N = 500$ random samples of the Franke function. Additionally, we again

[1] As in; we did **not** utilize a separate test/validation set in addition to the k-fold split

added Gaussian noise sampled from $0.2 \cdot \mathcal{N}(0,1)$ in both of the data sets.

As we saw in Fig. 4, once the complexity of our model reaches approximately the 8^{th} order, the MSE of our test set begins to grow rapidly. Looking then at Fig. 9d, we observe at the same complexity that the variance overtakes the square bias, and thus becomes the dominating term. Hence, the rapid growth of the MSE that we observed in Fig. 4 is an indication of the model being over-fitted to the data sample. This problem motivates the usage of Ridge and LASSO regression, which as we can see in Fig. 9d and Fig. 9f successfully suppresses the variance from becoming dominant for higher complexities. Furthermore, in both cases this is accomplished without affecting the bias of the model to a significant extent thus keeping the MSE relatively stable.

We turn then to Fig. 9a, 9b, 9c for the same analysis performed in a situation where the number of data samples has been limited to $N = 200$. Here, we observe the same problem but shifted to an lower complexity and to a much greater extent. Furthermore, the problem of over-fitting is apparently much greater in this case. We may explain this by considering how the number of data points in our sample relates to the total number of predictors in our model for each complexity. Using Eqn. 5, we may compute easily the number of predictors, which for convenience we list here in Table I for a range of complexities

TABLE I: Relationship between polynomial complexity and number of predictors for a 2D polynomial.

Complexity	3	4	5	6	7	8	9	10	11	12	13	14	15
No. Predictors	10	15	21	28	36	45	55	66	78	91	105	120	136

Looking at Fig. 9a, we observe the variance becoming problematic at around the $5^{\text{th}} - 7^{\text{th}}$ order. Corresponding to 21-36 predictors respectively. Similarly, in the case of $N = 500$ the same problem begins to occur at the around the 8^{th} order. Common to both of these cases are that the variance begins to increase rapidly once the number of predictors starts to approach $\sim 10\%$ the number of data points. This observation is supported by Harrell [6], in which limiting the complexity to $20\% - 10\%$ is proposed as a safe limit for the number of predictors compared to the number of data points, depending on the situation at hand.

We then move on to the $5-$fold cross-validation (CV), which is summarized for all the regression methods and both of the datasets in Fig. 8. Here, we note in particular for OLS that the CV yields a relatively low estimate of the MSE compared to the bootstrap. It is not completely clear why this is so, but a potential explanation is that the bootstrap estimates are more susceptible to variance. Since each individual bootstrap iteration is sampled with replacement they will contain on average only about 63.2% of the unique points from the original sample when the original sample is large [1]. For the highest degrees in our computations, 63.2% of our 400 training points (from the train-test-split of the original 500 points) will be cutting it dangerously close to the number of predictors, which might give rise to serious variance/over-fitting issues. For the lower degrees, the CV and bootstrap estimates seem to be more in line with each other, making this explanation at the very least plausible. Looking more closely at the CV plots in Fig. 8, we observe the same phenomenon as we did with the bootstrap, where the MSE grows rapidly for OLS past a certain complexity. However, in this case we also get a much better insight of how Ridge and LASSO behaves wrt. λ. We observe that there is little change in the MSE for Ridge and Lasso over a wide range of λ values and polynomial degrees. Though not shown here[2], we have investigated and found that, with the exception of for very high λ-values, the bias and variance versus complexity for both ridge and lambda does not vary appreciably with λ, nor do the actual predictions resulting from those methods trained on our 500-point data set.

3. *Fitting the Franke Function*

Just looking at the MSE-scores one might be tempted to simply pick the method and complexity with the lowest MSE-score. This is not always a good idea. As we will see, a low CV-estimate for the MSE-score does not guarantee that predictions will be good. In fact, low complexity models, while having small MSE-scores, fail to reproduce more than the main peak of the Franke function. They simply do not have the necessary degrees of freedom to incorporate the finer qualitative details. In Fig. 12 we show the Franke function and the predictions trained on $N = 500$ points for OLS, Ridge and Lasso, for polynomial degree 7. This seems, for our particular case, to be the highest complexity OLS manages before the variance becomes large enough to really ruin it. This is notedly NOT the highest degree that still keeps a low CV-estimate for the MSE-score, but rather the highest degree before the variance becomes appreciable in our bootstrap plots. We do see that already here the variance has started to affect the OLS prediction substantially, while the Ridge and Lasso predictions are much smoother and unbothered. All in all, for the current degree and sample Ridge seems to produce the closest fit to the actual Franke function. But one marked disadvantage of the regularized methods is that they struggle to capture actual variations in the Franke function, like the valley between the two peaks; in their attempts to stave off variance, they also stave off real variations.

In a preview of what we find for the terrain data, we might suspect that the "best" fit to this kind of "terrain"

[2] To see this, we refer the reader to the test folder in our Github repository; Specifically test_franke_analysis .ipynb

data, if the "terrain" is rapidly varying, is the highest degree of OLS that is not overpowered by variance. As might be imagined after our earlier discussion regarding the effect of the sample size, a larger sample size allows for the use of higher degrees before OLS meets a variance barrier; conversely, with fewer data points the highest "safe" complexity decreases. In the unfortunate case that one has so few data-points that variance becomes an issue for OLS even at uselessly low polynomial degrees, the Ridge and LASSO methods can still reliably reproduce the main features at higher degrees. Finally, the Ridge method seems to perform slightly better than the LASSO; possibly because the Lasso might struggle with our highly correlated basis functions.

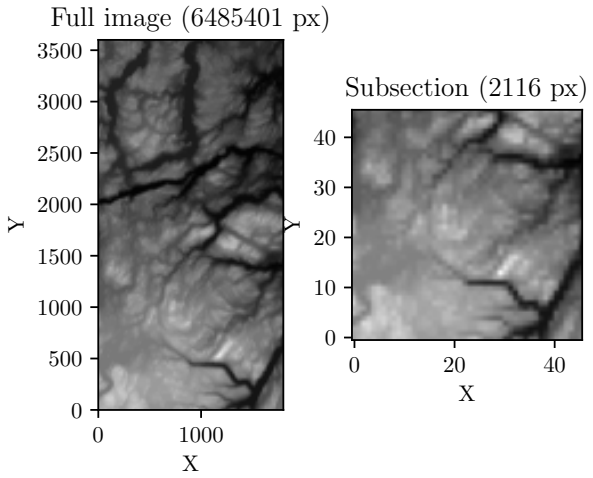


FIG. 6: The full terrain data as well as the down-sampled subsection which was used as the data set for our model.

B. The terrain data

Following our analysis of the Franke function, we performed a similar analysis of Terrain data found in [4]. In order to reduce the computational time required to process and analyze the data, we limited ourselves to a subsection of the full data set which was further down-sampled by only sampling every 40^{th} pixel of the subsection. The full data set, as well as the down-sampled subset are both shown in Fig. 6.

Once again using k-fold cross-validation with $k = 5$ on our complete data set, we try to estimate what the optimal complexities and penalty parameters might be for the three methods. The results are shown in Fig. 11. We see once again that the MSE-scores remains quite consistent for Ridge and Lasso, and that there is little dependence on λ outside the very largest values. Here, the MSE for OLS is actually decreasing with complexity, until it blows up past a certain point.

A bootstrapped bias-variance analysis of a train-test split, with test/train ratio 0.2, is then performed, in order to see whether the exploding OLS MSE is due to variance and whether Ridge and Lasso manage to keep the variance down. Fig. 10 shows this to be the case. Ridge and LASSO do keep the variance in check, so that most of their errors are due to bias. For OLS we see that it performs quite well according to MSE, until the variance kicks in and leads to a rapid growth similar to what we observed for the Franke function.

Keeping in mind our previous lesson about the CV-estimated MSE-scores not being the whole picture, we try to recreate our original terrain data with predictions trained on 2116 points. We try the highest polynomial degree possible before the OLS solution blows up. In this particular instance it seems that even though the CV-estimates for the MSE starts to increase, the highest degree in our calculation, polynomial degree 25, still remains stable. This is shown in Fig. 13. We see that only the OLS method really manages to capture the variability of the terrain, the other two mainly identify a peak and bottom then smooths out the paths between; with Ridge seemingly more capable of retaining some terrain variations. Though not shown here[3], we have tried the same procedure for a much smaller data sample (sampling every 100 pixel), and found the same trend, with the notable exception that at a certain complexity the OLS solution does blow up due to variance while the Ridge and Lasso solutions are able to keep stable.

IV. CONCLUSION

We have analyzed the performance of OLS, Ridge and LASSO regression on 'terrain-like' types of data, where the regression model was two-dimensional polynomials of varying degrees. We find that in order to qualitatively predict finer variations of the terrain, OLS with high complexity is the best suited method; the other two methods tend to smooth out the actual terrain variations in an effort to be stable against variance, with Ridge still capturing the main features reasonably while LASSO is rather more aggressive in its reductions. However, OLS can be quite unstable depending on the complexity and number of data points used. At what point the balance tips in favor either OLS or Ridge seems to need a case-by-case evaluation. For our computations, the Ridge method applied to high polynomial degrees seems to be the best of the bunch for the Franke function, while high degree OLS is superior on the terrain data. For the terrain data we have tested, but not shown here[4], that with fewer samples the higher degree OLS solutions hit a variance wall. In those cases, depending on at which complexity

[3] To see this, we refer the reader to the test folder in our Github repository; Specifically test_terrain_analysis .ipynb

[4] See again; test_terrain_analysis .ipynb in the test folder of our Github repository

the variance wall hits, lower degree OLS solutions may still be better than higher degree Ridge solutions. But at some point, when one has so few sample points that even low degree OLS solutions are unstable, the higher degree Ridge solutions will perform best and quite successfully reproduce the larger scale variations in the terrain.

As a concluding observation, the authors conjecture that the use of a different type of basis functions might be appropriate for these kind of 'terrain-like' data sets. For instance orthogonal polynomials, or a Fourier-type basis set, could be global basis sets that allow Ridge and Lasso to be more discerning in their regularizations, than with the highly correlated polynomials that have been used in the present study. Or basis functions with compact support, which are only non-zero on limited domains, such as B-splines could provide more freedom to adapt to the actual variations in the terrains, without having over-fitting ramifications outside their support.

[1] T. Hastie, R. Tibshirani, and J. Friedman, *The Elements of Statistical Learning*, 2nd ed. (2009).
[2] F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Prettenhofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and E. Duchesnay, Scikit-learn: Machine learning in Python, Journal of Machine Learning Research **12**, 2825 (2011).
[3] W. W. Cohen, Bias-variance in machine learning.
[4] Source of terrain data.
[5] T. E. Moe and N. Karlsen, Project 1: Regression analysis and resampling methods, https://github.com/nicholaskarlsen/FYS-STK4155/tree/master/project_1 (2020).
[6] F. Harrell, *Regression Modeling Strategies*, 2nd ed. (2015).

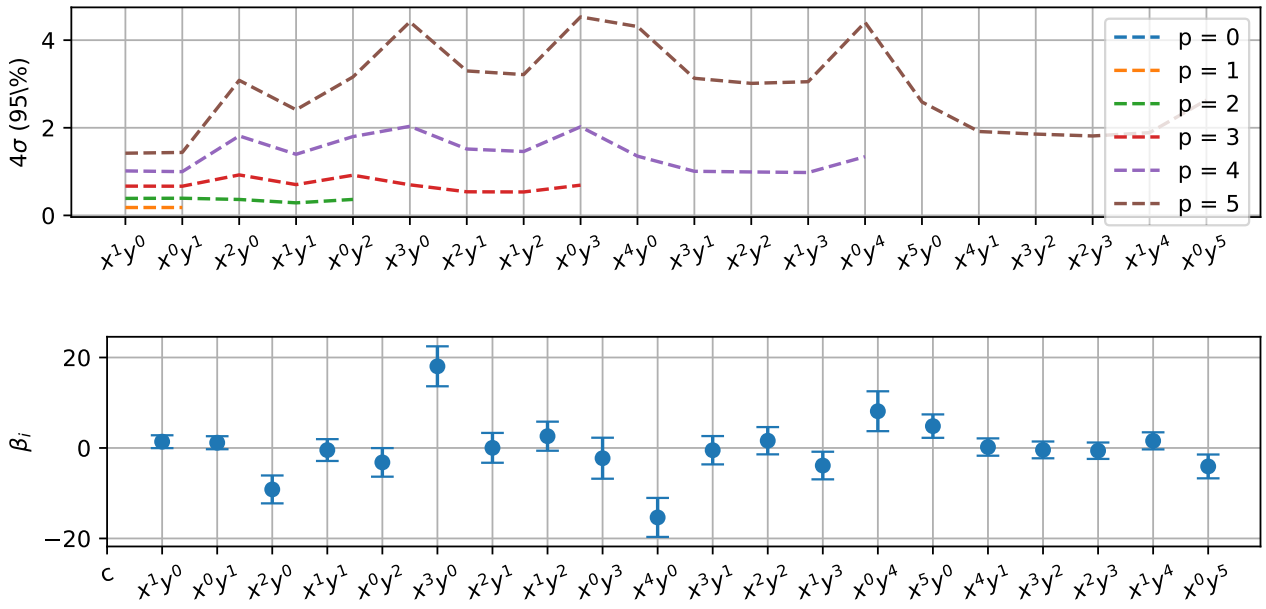
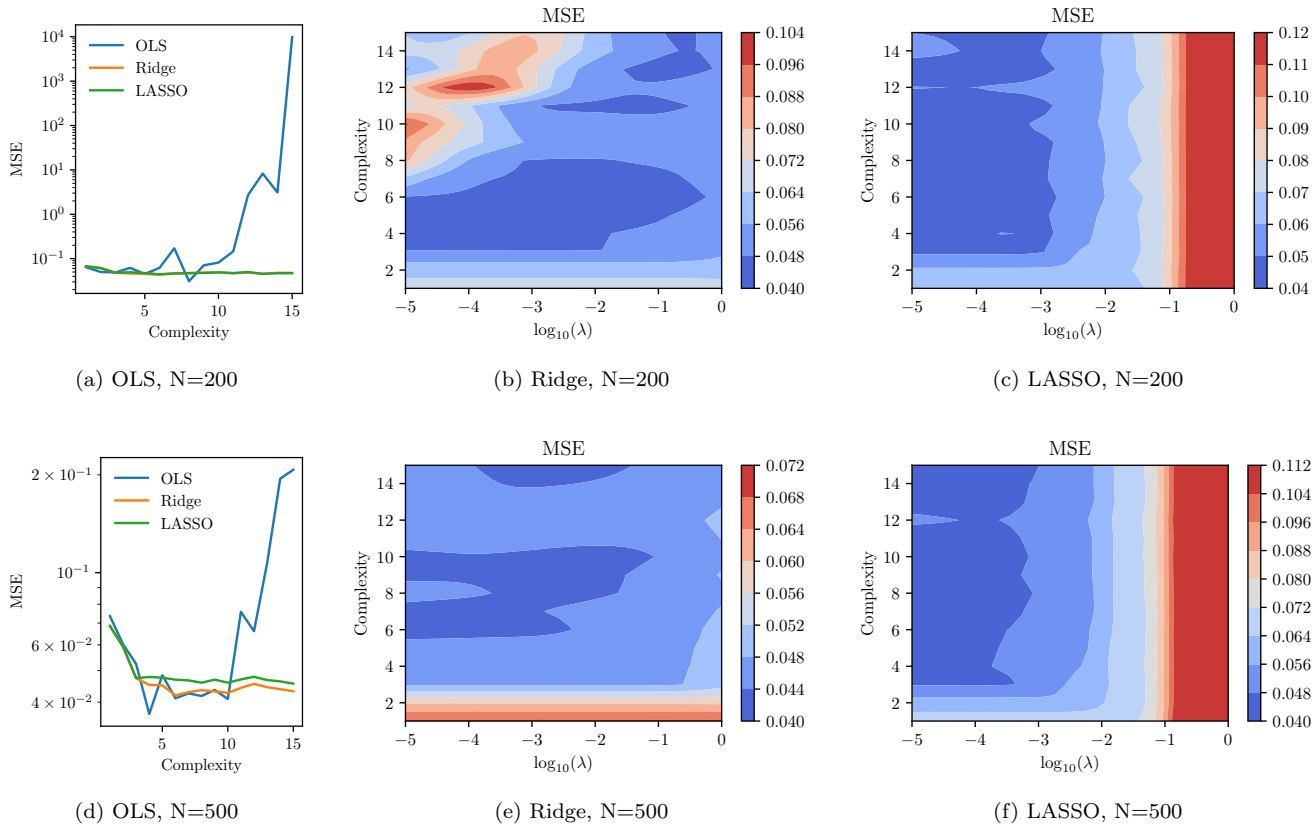


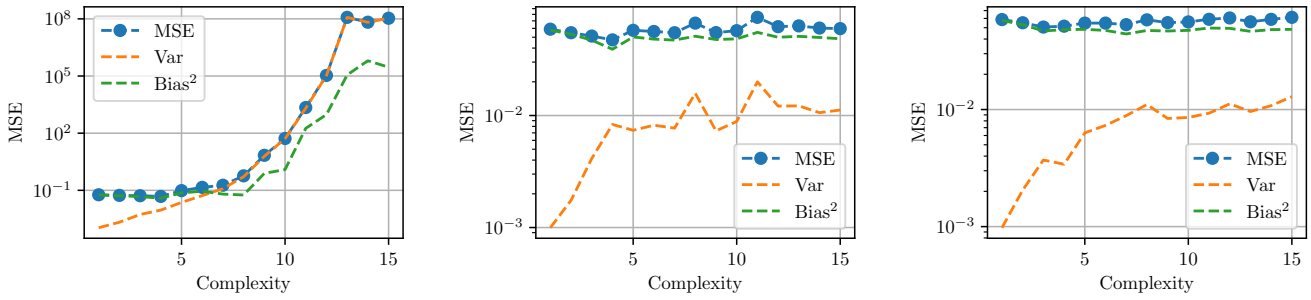
FIG. 7: (Bottom figure) Predictors βi for a 5^{th} degree polynomial modeled with OLS on random samples of the Franke Function with noise $0.2 \cdot \mathcal{N}(0,1)$ where the error bars indicate the confidence interval of $\pm 2\sigma$ (Top figure) as well as the size of the confidence intervals for the preceding complexities.



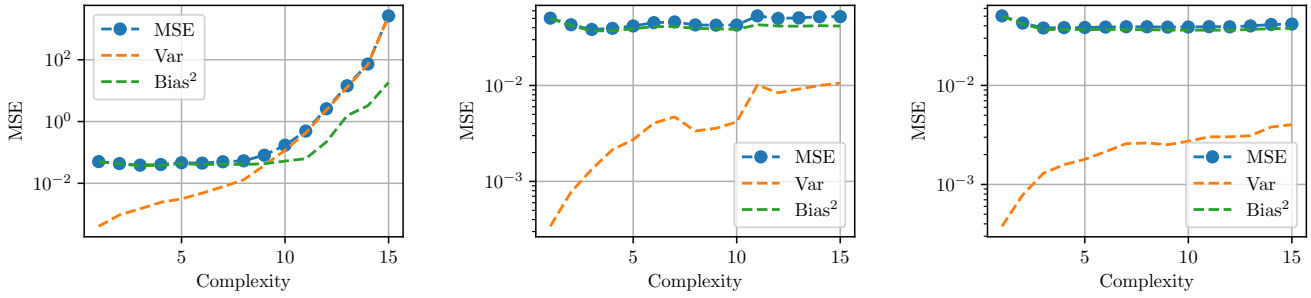
(a) OLS, N=200 (b) Ridge, N=200 (c) LASSO, N=200

(d) OLS, N=500 (e) Ridge, N=500 (f) LASSO, N=500

FIG. 8: MSE for $k = 5$ cross-validated Ridge & LASSO regression performed on N samples of the Franke Function with added random noise in the form $0.2 \cdot \mathcal{N}(0,1)$

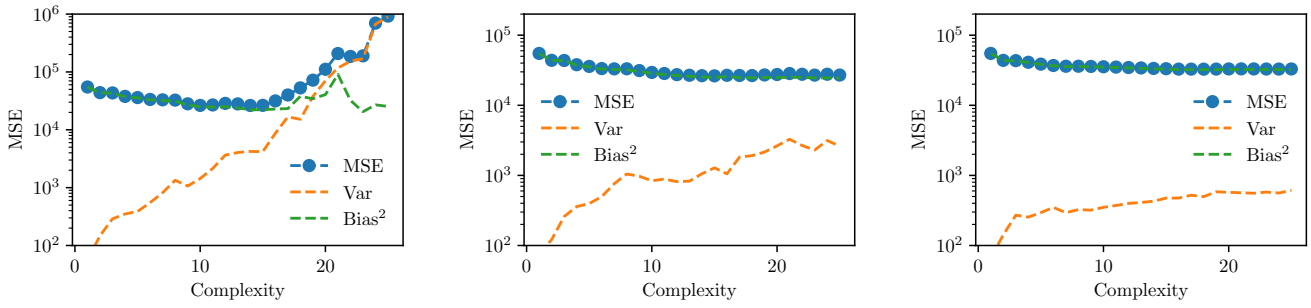


(a) OLS, N=200 (b) Ridge, N=200 (c) LASSO, N=200



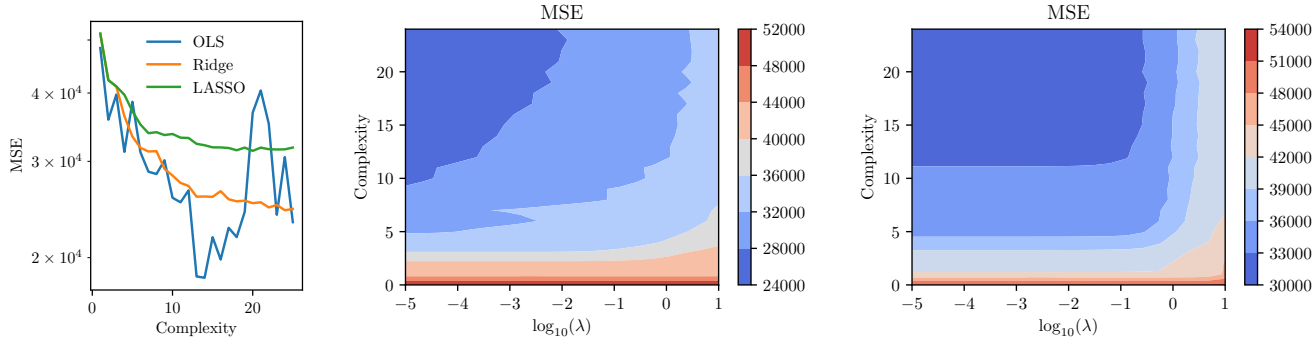
(d) OLS, N=500 (e) Ridge, N=500 (f) LASSO, N=500

FIG. 9: $M = 200$ Bootstrapped MSE, Bias^2 and Variance for OLS, Ridge and LASSO regression on N random samples of the Franke Function.



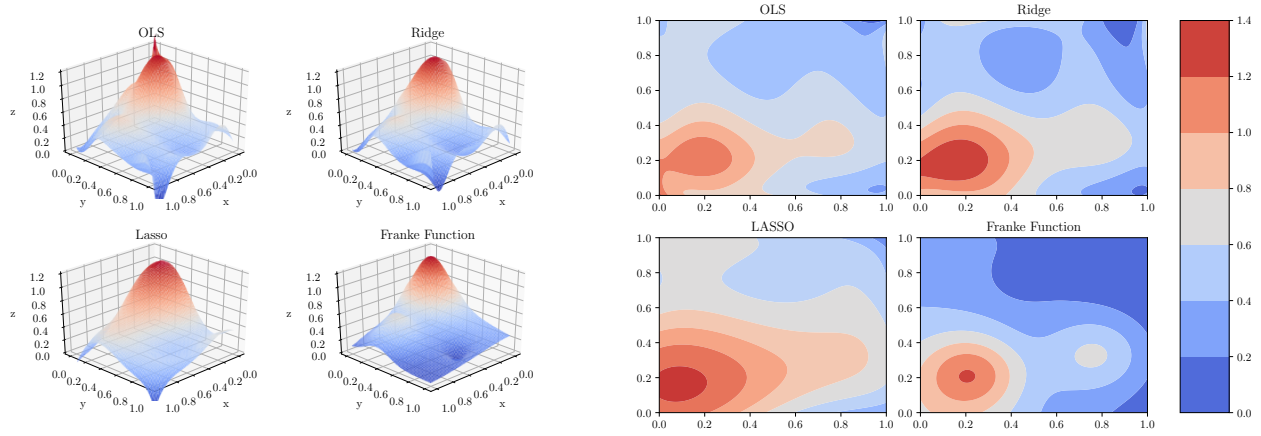
(a) OLS, N=500 (b) Ridge (c) LASSO

FIG. 10: $M = 100$ bootstrapped MSE for OLS, Ridge and LASSO regression on the Terrain data for the λ parameters yielding the best results for $k = 5$ fold cross-validation.



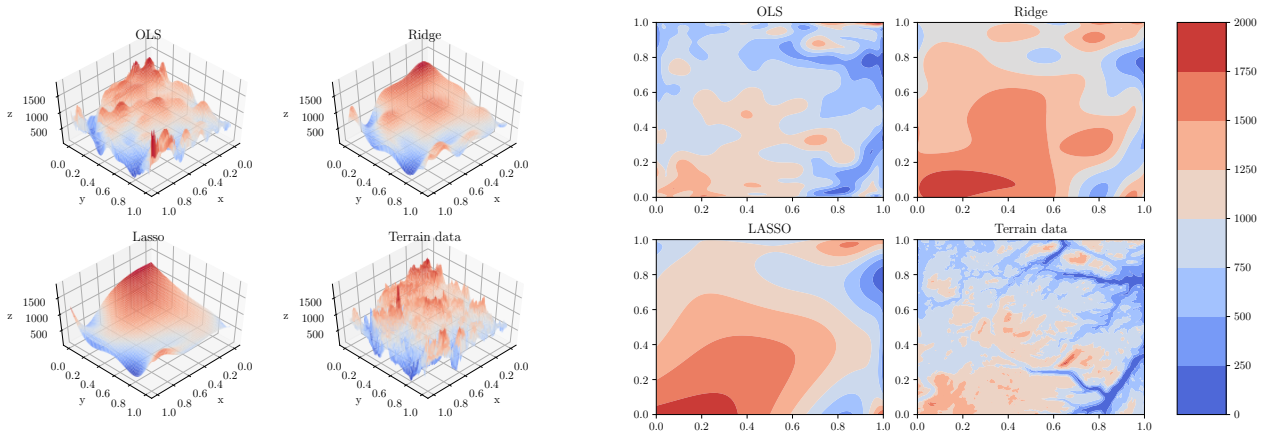
(a) OLS, Best Ridge & LASSO (b) Ridge regression (c) LASSO regression

FIG. 11: MSE for $k = 5$ cross-validated OLS, Ridge and LASSO regression performed on the terrain data



(a) (b)

FIG. 12: Predictions of the Franke function for a 7th order polynomial & optimal penalty parameters λ performed with OLS, Ridge and LASSO regression compared with the true Franke function



(a) (b)

FIG. 13: Predictions of the terrain data for a 25th order polynomial & optimal penalty parameters λ performed with OLS, Ridge and LASSO regression compared with the true terrain data