Regression analysis and resampling methods

by
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Abstract

We apply Ordinary Least Squares (OLS), Ridge and Lasso Regression to a set of simulated data to find the best algorithm that can fit the data well and then use the results to find a fit to my own data. We find that OLS performs reasonably well for simple models but breaks for models of higher complexity when applied to the simulated data. Ridge and Lasso regression perform better and are more robust at higher complexity albeit at the cost of more time spent finding the correct hyperparameters. For my own data Lasso Regression failed to find a good solution under certain conditions. Ridge Regression performed better than OLS at the cost of higher complexity.

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1 Introduction

Finding solutions to linear problems is as old as modern science itself.[1] For simple linear models it is a good and simple way to find solutions to easier problems without the necessity of modern computers. With the origin of computers however previously unsolvable problems could be solved employing machines to perform tedious calculations. More complex problems however bring computational problems with them and the more complex the problems become, the more difficult they become to solve with the easy algorithm of OLS.
Ridge and Lasso regression employ different methods of restricting the problems arising from OLS by restricting the possible space of the solution. This comes at the cost of higher computation time and the necessity to find a fitting hyperparameter.
Another problem is the availability of computation time. Testing on the whole set of available data might take a long time or the data is too sparse to give a proper estimate. Bootstrap resampling and cross validation offer problems to this solution.
In this report in 2 I will first give an introduction into the theory behind the regression algorithms. I will show their differences and evaluate potential systematic errors. I explain how the error is calculated from the data and how different resampling techniques work and when they might be used. In 3 I evaluate the different tasks given for the project based on the previously explained algorithms. The tasks from the project sheet are shown one at a time in the order they were give with the results each discussed in their corresponding part. Lastly I give an overview of the results in 4.

2 Basics

2.1 Regression Techniques

2.1.1 Ordinary Least squares

Ordinary Least squares (OLS) is probably the most basic regression function. With OLS it is possible to solve linear expressions it is however not able to solve problems that cannot be written in the form of a linear expression. A linear expression is of the form

$$\vec{y} = \underline{X} * \vec{\beta} \tag{1}$$

where $\underline{X}$ is the feature matrix, $\vec{\beta}$ the parameters and $\vec{y}$ the result vector of the equation. $\underline{X}$ is a generalised matrix and does not correspond to the coordinate x in a cartesian coordinate system. For our case, $\underline{X}$ contains information about

both coordinates x and y for every n-th pair of coordinates x_n and y_n. In the case for a system of order P and N dimensions, $\vec{X}_n$ = the n-th row of $\underline{X}$ takes the form

$$\vec{X}_n = \sum_{i=0}^{P} \sum_{j=0}^{i} x_n^{(i-j)} y_n^j \tag{2}$$

Where each part of the above sum is sorted into the columns of the matrix. E.g. for P = 2 and N = 6, $\underline{X}$ takes the form

$$\underline{X} = \begin{pmatrix} 1 & x_1 & y_1 & x_1^2 & x_1 y_1 & y_1^2 \\ 1 & x_2 & y_2 & x_2^2 & x_2 y_2 & y_2^2 \\ 1 & x_3 & y_3 & x_3^2 & x_3 y_3 & y_3^2 \\ 1 & x_4 & y_4 & x_4^2 & x_4 y_4 & y_4^2 \\ 1 & x_5 & y_5 & x_5^2 & x_5 y_5 & y_5^2 \\ 1 & x_6 & y_6 & x_6^2 & x_6 y_6 & y_6^2 \end{pmatrix}$$

$\vec{\beta}$ will be a vector of length

$$len(\vec{\beta}) = \sum_{i=1}^{P} i = \frac{(P+1) * (P+2)}{2} = 6 \tag{3}$$

Equation 1 can be rewritten to find an analytical solution to $\vec{\beta}$ [2]

$$\vec{\beta} = (\underline{X}^T \underline{X})^{-1} \underline{X}^T \vec{y} \tag{4}$$

For this $\vec{\beta}$ the sum of squared residuals is minimised:

$$r = \sum_i (\tilde{y}_i - y_i)^2 \tag{5}$$

Where $\tilde{y}_i = \vec{X}_i \vec{\beta}$ is the i-th result for the i-th row of the feature matrix based on the results obtained for the parameter matrix.

2.1.2 Ridge Regression

Ridge Regression works similar to OLS but has an additional term in the matrix to be inverted. This parameter shrinks the contribution from the original feature matrix such that large values of λ force the parameters towards 0 and low values of λ cause no shrinkage. The parameter vector can then be calculated as[3]

$$\vec{\beta} = (\underline{X}^T \underline{X} + \lambda * \mathbf{I})^{-1} \underline{X}^T \vec{y} \tag{6}$$

where λ is an additional parameter and $\mathbf{I}$ is the identity matrix. The dimensions of $\mathbf{I}$ are chosen that way that they match $\underline{X}^T \underline{X}$.

2.1.3 Lasso Regression

Lasso regression minimises the following equation:[3]

$$\min_{\beta} \frac{1}{N} \left\| \vec{y} - \underline{X}\vec{\beta} \right\|_2^2 + \lambda \left\| \beta \right\|_1 \tag{7}$$

This can be rewritten to [4]

$$\min_{\beta} \left\| \vec{y} - \underline{X}\vec{\beta} \right\|_2^2 \tag{8}$$

but applies additional constraints to the parameter variable β. $\beta \in B(\lambda)$ where

$$B(\lambda) = \{x \in \mathbb{R}^n : \left\| x \right\|_1 < \lambda\} \tag{9}$$

$B(\lambda)$ is a ball of radius $0 < \lambda < \infty$ dependent on the chosen norm $\left\| \cdot \right\|_1$. This norm with λ restricts the size of the regression parameter β.
Whereas ridge regression only was able to shrink the size of the coefficients, applying the norm to the coefficients, Lasso not only applies an upper bound to the coefficients but also forces "budgeting" onto the parameters or may even set some parameters to zero. If one parameter becomes large, other parameters have to be small to stay within the boundaries given by the norm and λ.
Scikit-learn uses the 1-norm[5], here the sum of the absolute values of the coefficients has to be smaller than λ.
Contrary to OLS and Ridge, Lasso Regression can not be solved analytically but only computationally. In this case the search for an optimal solution is stopped if either of two conditions is true:[5]

1. The calculated solution converges. Convergence in the case of scikit learn's implementation is defined as the change between two iterations being smaller than a predefined tolerance.

2. A maximum number of iterations was reached. To avoid searching for an ideal solution where none exists, after a predetermined amount of iterations the search is stopped.

2.2 Computational restraints

When solving $(\underline{X}^T\underline{X})^{-1}$ in equ. 4 or $(\underline{X}^T\underline{X} + \lambda * \mathbf{I})^{-1}$ in equ. 6 it is important to remember the condition number of a matrix defined as the relation between the absolute values of the largest and smallest singular value of the matrix. The condition number describes how accurate the computed result is in terms of machine accuracy.
Calculating the feature matrix for a high order polynomial will lead to entries that

are several orders of magnitude apart from the largest values. In such a case the condition number may be large. Even if the problem has in theory an analytical solution, the result will be heavily influenced by machine inaccuracy.
Calculating the condition number for a feature matrix with $x, y \in [0, 1]$ with a resolution of 0.01, the condition number is of the order 10^4 for a degree p = 3, 10^7 for p = 5 and 10^{15} for p = 10. Considering the machine epsilon of $\epsilon = 2^{53} \approx 1.1 * 10^{-16}$ for double precision values, a degree of p=10 is already too imprecise to yield proper results using default matrix inversion techniques.
A similar problem arises when centering and scaling the data yielding high condition numbers.
A solution to this computational problem is for example numpys pinv function, which calculates the pseudoinverse of the feature matrix based on singular value decomposition.[6] This makes it possible to use matrix inversion even at higher degrees, but the results should still be treated carefully.

2.3 Confidence Interval

To find the confidence interval of our results we need to find the variance in our parameter variable β. This is given in the diagonal of the following matrix: $\sigma^2 = (\underline{X}^T \underline{X})^{-1}$. We can then calculate the error as:

$$\Delta\beta_i = 1.96 \frac{\sigma_i}{\sqrt{N}} \tag{10}$$

Where $\Delta\beta_i$ is the difference in β_i to stay within a 95% confidence interval, N is the sample size (= the amount of coordinates in our training set) and σ_i is the positive square root of the i-th diagonal element of the aforementioned matrix. The factor 1.96 is a result of our choice of a 95% interval and the assumption that the noise is normal distributed.
To make computation easier and my code reusable, I use numpys pinv-function to calculate the final result, but still invert the matrix normally to get an estimate of the variance and subsequently the error.

2.4 Franke Function

$$\begin{aligned} f(x,y) = \frac{3}{4}\left(-\frac{(9x-2)^2}{4} - \frac{(9y-2)^2}{4}\right) + \frac{3}{4}\left(-\frac{(9x+1)^2}{49} - \frac{(9y+1)^2}{10}\right) \\ + \frac{1}{2}\left(-\frac{(9x-7)^2}{4} - \frac{(9y-3)^2}{4}\right) - \frac{1}{5}\left(-(9x-4)^2 - (9y-7)^2\right) \end{aligned} \tag{11}$$

Equation 11 shows the Franke function which is used in the interval $x, y \in [0, 1]$ to generate testing data. Figure 1 also shows a plot of the franke function. In

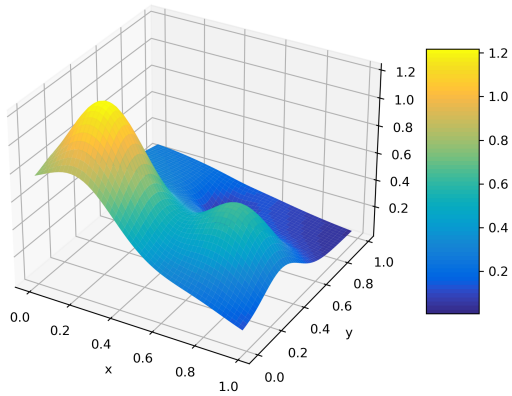


Figure 1: Franke function

the chosen interval the values of the franke function are positive and $\lesssim 1.2$. The function has one global maximum, one global minimum and a local maximum.

2.5 Sampling

2.5.1 Bootstrap Resampling

In Bootstrap resampling instead of using the whole set of data (which may be several thousands or hundreds of thousands samples large), only a smaller portion of the data is used to calculate their respective error. The samples are randomly drawn from the whole set of data and may be drawn several times. The error is then estimated as the average error of the sample errors.[7]

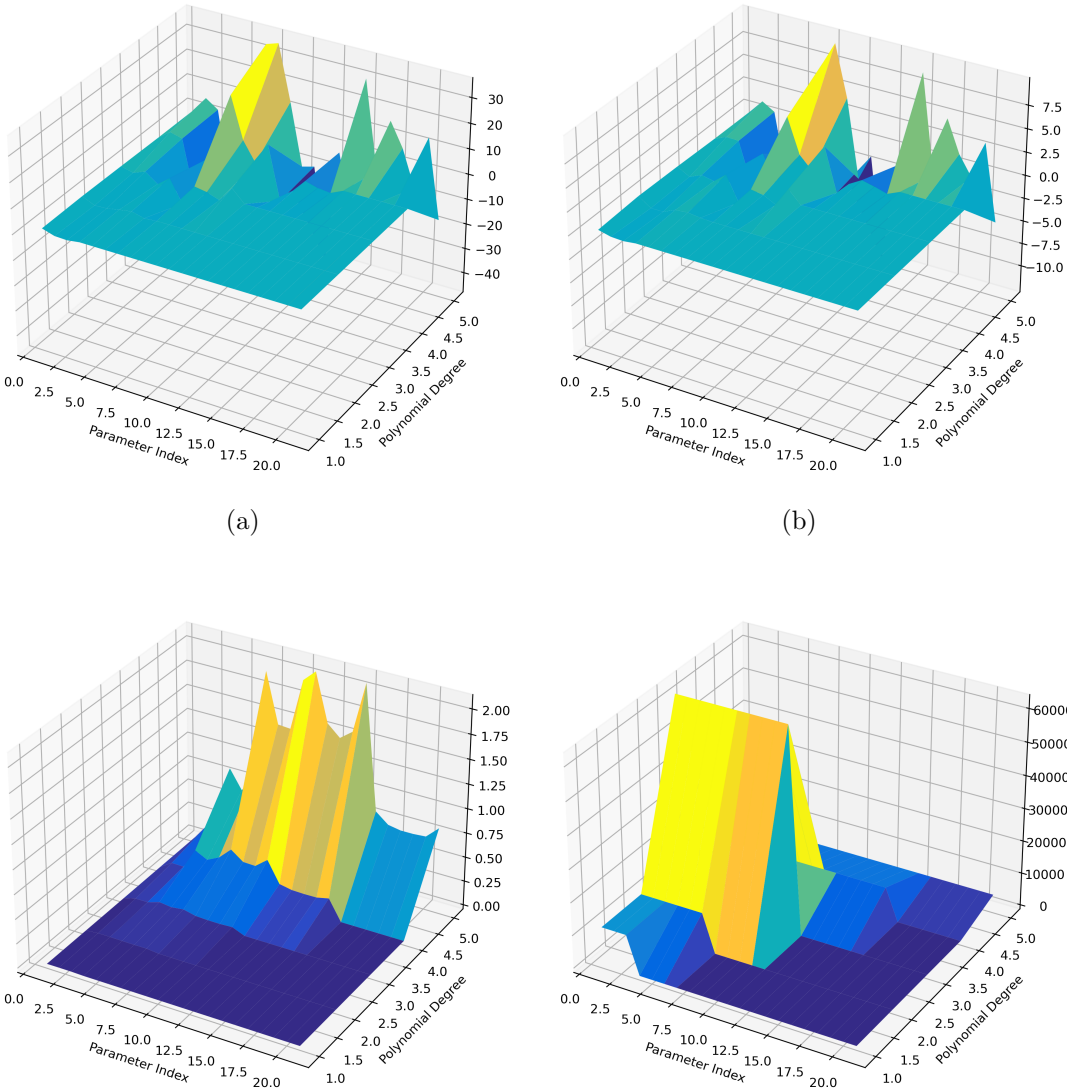
2.5.2 Cross Validation

k-fold Cross Validation is a technique that can for example be used when the amount of available data is small. Here the data is split into k equal sized parts ("folds"). Then it is iterated over the folds such that each fold will be the testing data once and the rest of the folds will be used for training. This gives an amount of k different estimates for the parameters and error, for which the mean can be used as a global estimate.[7]

3 Tasks

3.1 OLS on Franke Function

The data for the following graphs was created by creating a grid of x- and y- coordinates with a fixed resolution of 0.02 between 0 and 1. This gives a total sample size of $N = 2500$. The grid was applied to the Franke function and randomly distributed noise centered around 0 with a standard deviation of 1 and an amplitude of 0.1 was added to the values. The data was then randomly split into 80% training $N_{train} = 2000$ and 20% test data $N_{test} = 500$. The x- and y- coordinate grid was conglomerated into a single feature matrix corresponding to a polynomial of increasing degree between 1 and 5. The data from the Franke function was then fitted onto the polynomial using OLS.
Figure 2 shows how the parameter values and errors behave under scaling for different complexities. The right axis in each plot shows the polynomial degree, the left axis the parameter index within beta. Because a model with lower degree can be interpreted as a model with higher complexity where the parameters with higher index are all zero, we can plot the parameter values as a surface plot, where the z-axis corresponds to the value of the parameter.
In the top row (figs. 2a and 2b) the parameter values are plotted, in the bottom row (figs. 2c and 2d) their respective errors are shown. The left column corresponds to the original data in the feature matrix being processed, in the right column, the data has been centered with mean 0 and scaled to variance 1. The parameters are affected in that regard, that they are scaled by the same transformation as the feature data. Their behaviour relative to each other is unchanged.
The error however has to be calculated by inverting the product of the feature matrix with its transpose. As shown above this produces large errors when applied to the scaled data. Otherwise the error is within a few percent of the produced parameters.
In fig. 3 we see how the different models fit the data. The top row shows how the mean squared error for training and test data behaves and the bottom row shows the R^2 value of the fit for training and test data. The left column shows again the unchanged feature data, the right column shows scaled data.
In both cases we can see a decrease in error and increase in goodness of the fit towards higher complexity in both training and testing data. We can already see how the R^2 value starts to level out at around 0.9 for the scaled version, whereas the unscaled data is still rising but below the level of the scaled data. In general, the scaled data performs slightly better in terms of the goodness of the fit but has slightly higher error values.
Train and test data both show a good correllation and the difference between their values is not significant.



(a) (b)

(c) (d)

Figure 2: Parameter values (top row) and their corresponding estimate errors (bottom row) for unscaled data (left column) and scaled data (right column) using OLS

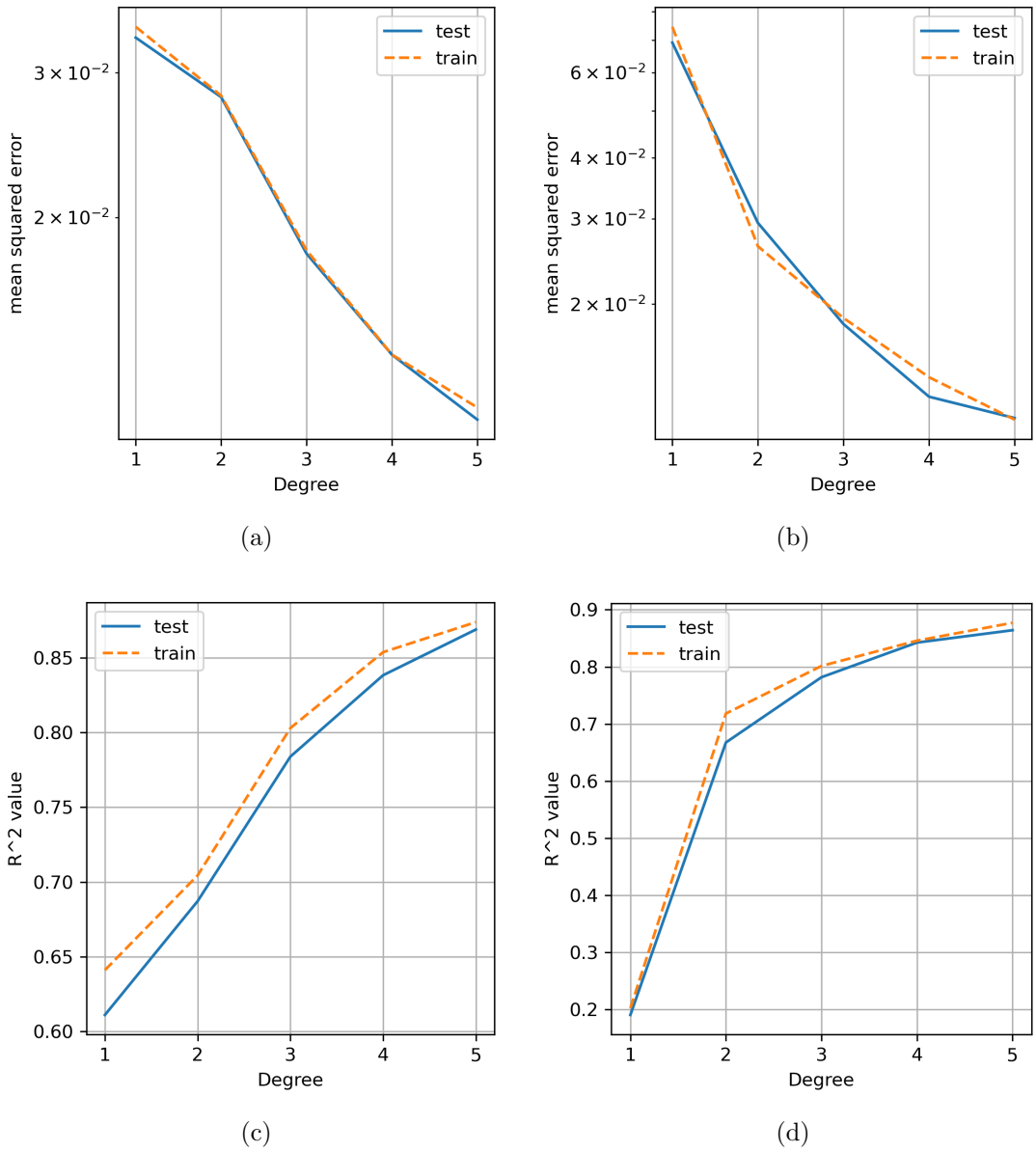
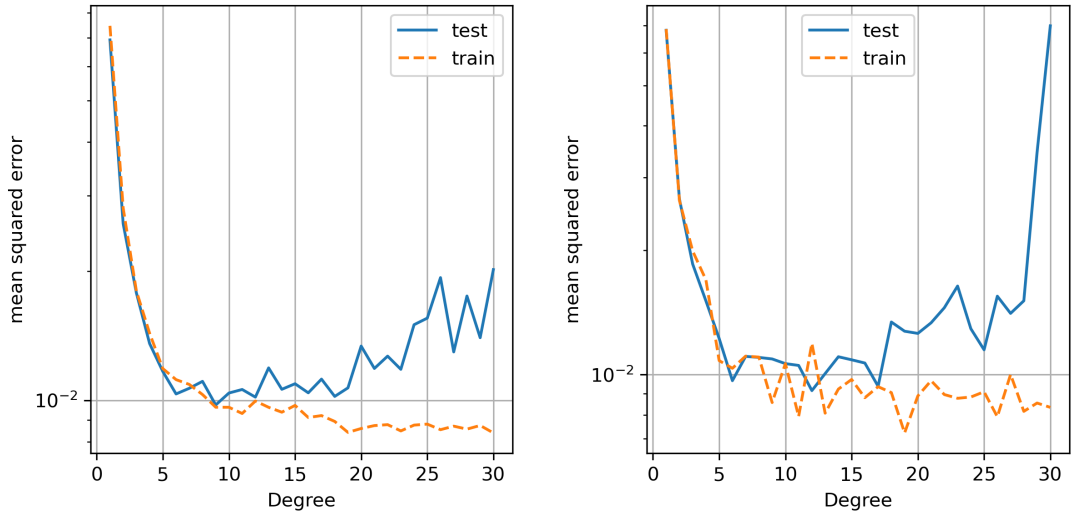


Figure 3: Mean squared error (top row) and R^2 value (bottom row) for unscaled data (left column) and scaled data (right column) using OLS plotted against the complexity degree of the model



(a) (b)

Figure 4: Mean squared error for higher order degrees using standard evalution (left) and bootstrap with 200 samples (right)

3.2 Bias- Variance Tradeoff and Resampling

In the previous section we saw training and test data error values in good agreement with each other. Here we want to show the Bias- Variance tradeoff. This is the effect, that the more complicated our model is and the better our model fits the training data the worse it will fit the testing data. The data for this part is the same as for the previous part and again OLS is used to perform the fit.
To perform analysis of the data, we resample using the bootstrap algorithm. Figure 4 shows the Bias-Variance tradeoff. The figure shows the same evaluation once done as in the previous task (left) but with a higher degree of the polynomial and once using the bootstrap resampling technique using $n = 200$ samples. We can see that while the accuracy of the training data increases towards higher complexity of the model, the accuracy of the testing data decreases. Comparing the standard technique to bootstrap, we see that although the original graph is more smooth, there is only a small difference between the two graphs, showing that a sample size of 10% of the training data set still gives a good approximation. For complex models this could be used to reduce computing time.

Next I rephrase the expectation value of the cost function:

$$\begin{aligned}
\left\langle (y-\tilde{y})^2 \right\rangle &= \left\langle (f(x)+\epsilon-\tilde{y})^2 \right\rangle \\
&= \left\langle f^2(x)+\epsilon^2+\tilde{y}^2+2f(x)\epsilon-2f(x)\tilde{y}-2\tilde{y}\epsilon \right\rangle \\
&= \left\langle (f(x)-\tilde{y})^2 \right\rangle + 2\left\langle f(x)-\tilde{y} \right\rangle \left\langle \epsilon \right\rangle + \left\langle \epsilon^2 \right\rangle \\
&= \left\langle (f(x)-\tilde{y})^2 \right\rangle + 0 + \sigma^2 \\
&= \left\langle (f(x)-\tilde{y}-\langle\tilde{y}\rangle+\langle\tilde{y}\rangle)^2 \right\rangle + \sigma^2 \\
&= \left\langle ((f(x)-\langle\tilde{y}\rangle)-(\tilde{y}-\langle\tilde{y}\rangle))^2 \right\rangle + \sigma^2 \\
&= \left\langle (f(x)-\langle\tilde{y}\rangle)^2 \right\rangle + \left\langle (\tilde{y}-\langle\tilde{y}\rangle)^2 \right\rangle - 2\left\langle (f(x)-\langle\tilde{y}\rangle)(\tilde{y}-\langle\tilde{y}\rangle) \right\rangle + \sigma^2 \\
&= \left\langle (f(x)-\langle\tilde{y}\rangle)^2 \right\rangle + \left\langle (\tilde{y}-\langle\tilde{y}\rangle)^2 \right\rangle - 2(f(x)-\langle\tilde{y}\rangle)\left\langle \tilde{y}-\langle\tilde{y}\rangle \right\rangle + \sigma^2 \\
&= \left\langle (f(x)-\langle\tilde{y}\rangle)^2 \right\rangle + \left\langle (\tilde{y}-\langle\tilde{y}\rangle)^2 \right\rangle - 2(f(x)-\langle\tilde{y}\rangle)(\langle\tilde{y}\rangle-\langle\tilde{y}\rangle) + \sigma^2 \\
&= \left\langle (f(x)-\langle\tilde{y}\rangle)^2 \right\rangle + \left\langle (\tilde{y}-\langle\tilde{y}\rangle)^2 \right\rangle + \sigma^2 \\
&= \text{BIAS} + \text{VARIANCE} + \text{BACKGROUND-NOISE}
\end{aligned} \tag{12}$$

From the first to the second line I expanded the quadratic equation. Then I reorganised depending on the order of ϵ. Here I used that the expectation value of two sums is the sum of two expectation values. If two variables are independent, then the expectation value of the product is equal to the product of the expectation values of the two variables. I used this to arrive on the third line. Because our error ϵ is randomly distributed around 0, its expectation value vanishes and the expectation value of its square is equal to the variance σ^2. This was shown and used in the first homework sheet this semester.[1] I then added and subtracted $\langle\tilde{y}\rangle$ in the remaining term and again expanded the quadratic expression. After reshaping and using the same rules as above I arrive on the seventh line. Here I use the same rule for two products and the for a sum, giving me the difference between two times the same term.

$$\left\langle (f(x)-\langle\tilde{y}\rangle)^2 \right\rangle \tag{13}$$

Equation 13 is the expectation value of the difference between the original data and the expectation value of the predicted data. This term is called the Bias and describes how well the model fits the training data. The more complex the model is, the better the training data can be fitted and the lower the bias becomes.

$$\left\langle (\tilde{y}-\langle\tilde{y}\rangle)^2 \right\rangle \tag{14}$$

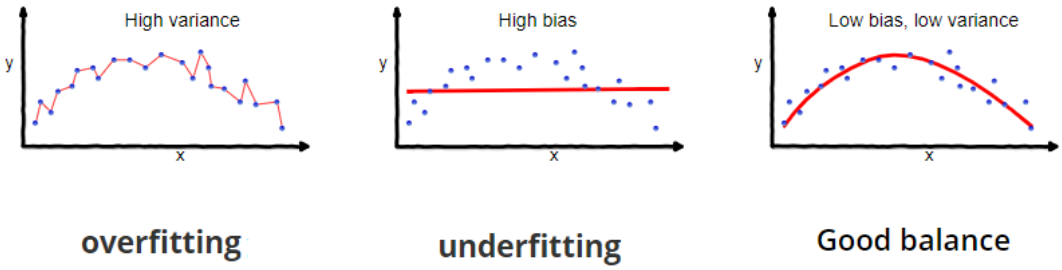
The term in equ. 14 describes the difference between the predicted data and their expected outcome. This describes how much the model will move around its mean

[1] https://compphysics.github.io/MachineLearning/doc/Projects/2020/hw1/html/hw1.html

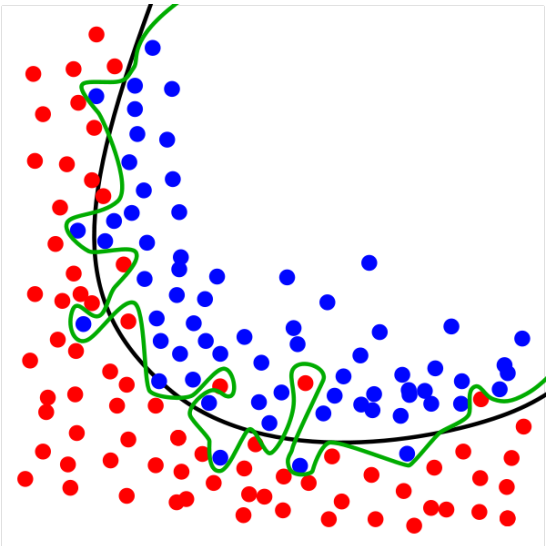
value. The more complex the model is, the more this value will increase.
σ^2 describes the remaining background noise. The sum of the three terms will give the total testing error. When training models and by this creating a predictor, we can reduce the bias by increasing the complexity of our model. Then our model will fit the training data better and better the more complex the model becomes. When complexity rises the model will move more and therefore the variance will increase.
None of these are dependent on the sample size (which is equivalent to resolution in our case) which means that the trend in bias and variance will not change for different resolutions. This of course assumes that the model complexity is independent of the sample size.
When training a model and creating a predictor it is important to find a good spot in between, where the model is complex enough to extract enough information from the training data but is not too complex. The phenomenon of increasing variance at the cost of bias is called overfitting and occurs for example when the model becomes so complex that it fits not only the underlying distribution of the data but also the added random noise. In this case predictions will become worse the more complex the model becomes.
This is shown exemplary in fig. 5a.[8] The blue dots show data of some distribution which could come from a second order polynomial with randomly added noise. The first graph shows a fit that perfectly matches all of the data. If new data (e.g. from testing or validation) is added, the difference between prediction and the true result will vary much and lead to high variance.
For the second graph a very simple model is chosen. The variance in the prediction will be low but the model also does not fit the training data well, leading to high bias.
At last a model in between is shown. The model fits the underlying distribution but ignores the noise. This is the ideal case, where bias and variance are at their lowest.
Figure 5b shows another example of this. There are two distributions in red and blue dots with two predictors in black and green. The green predictor follows the underlying distribution including the randomly added noise, giving high variance and clearly overfitting. The black predictor ignores the noise and gives a good fit.

3.3 Cross Validation

We perform the same data analysis as in the previous part, this time splitting the data into 5 and 10 folds. The results of this analysis can be seen in fig. 6. Figure 6a shows the result for 5 folds, 6b for 10 folds. The two curves follow the same shape and are very similar to the results produced using bootstrap resampling.
The increase in variance is less distinct than before but still notable.

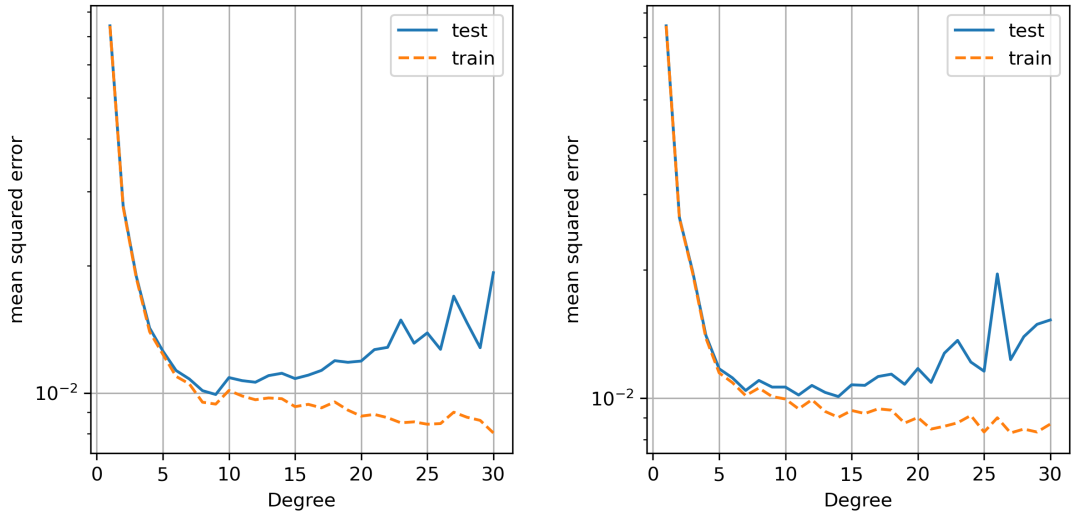


(a)



(b)

Figure 5: Example of the Bias Variance Tradeoff (a) [8] and overfitting (b) [9].



(a) (b)

Figure 6: Mean squared error for higher order degrees using cross validation with 5 folds (left) and 10 folds (right)

3.4 Ridge Regression with Resampling

In this task we are to test several choices for λ using both bootstrap resampling and cross validation. We are also to evaluate the bias variance tradeoff from our results obtained using bootstrap resampling on ridge regression. Figure 7 shows the results of this analysis. The top row shows the mean squared error of this computation and the bottom row the R^2 value. The left column shows the computation for cross validation using $k = 5$ and the right column uses bootstrap with $n = 200$. For the sake of reducing computation time and forcing a more sparse set of data, I have reduced the resolution to 0.05, resulting in $N = 400$.
The effect of shrinkage is clearly visible in the R^2 value. High values of the parameter λ force the parameters to vanish. This is a bad fit to the data and the goodness of the fit decreases rapidly for λ approaching 10^2.
On the lower side we can see the opposite effect and observe already the Bias Variance tradeoff. Train and Test results for the mean squared errors are each plotted in the same colour for the same degree of the polynomial but the test data uses a normal line and the training data a dashed line. Observing especially the polynomial degrees 9 and 10, we can see a split between test and training data at around $\lambda \approx 10^0$.
I will therefore use a value of $\lambda = 1$ to study the bias variance tradeoff using bootstrap resampling further. Figure 8 shows the result of this analysis. In fig.

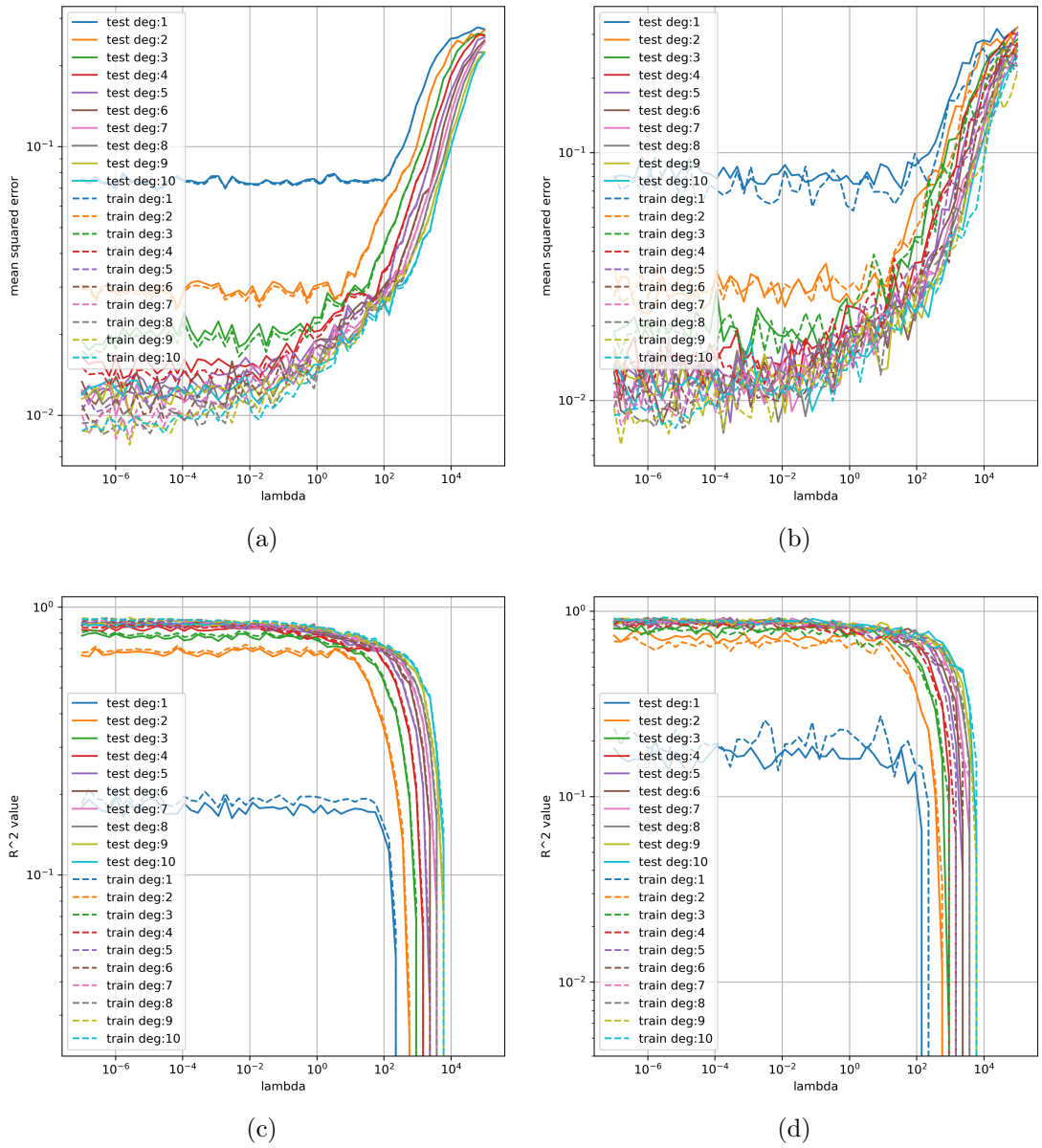
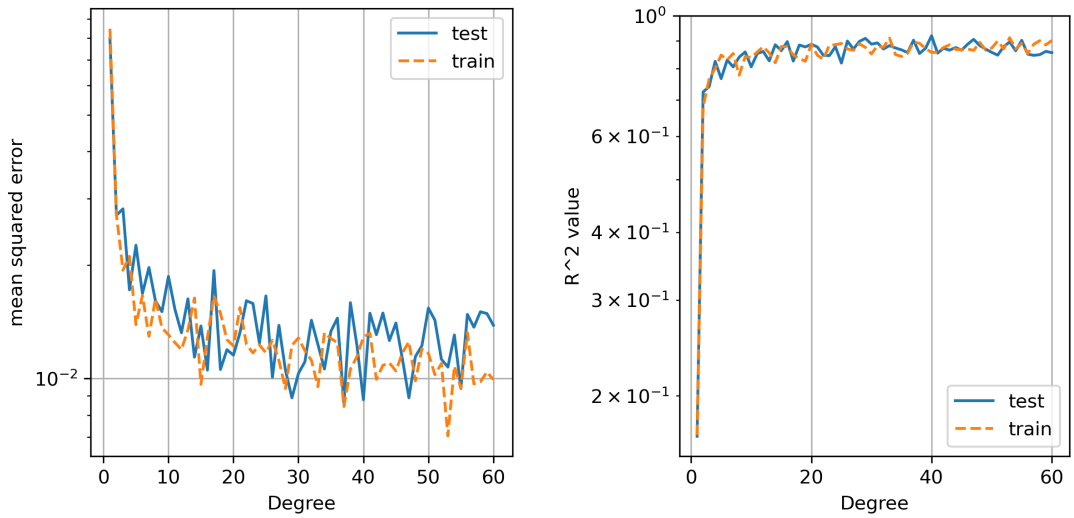


Figure 7: Mean squared error (top row) and R^2 value (bottom row) for higher order degrees using cross validation with 5 folds (left) and bootstraps with $n = 200$ (right)



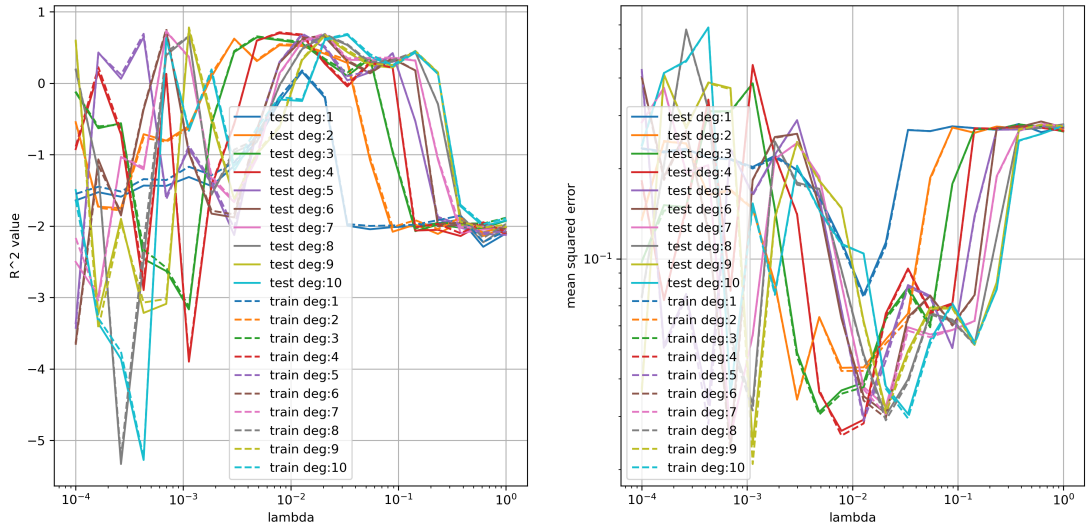
(a) (b)

Figure 8: Mean squared error (left) and R^2 value for a higher order polynomial fit using ridge regression with $\lambda = 1$

8b we see the R^2 value and in fig. 8a the mean squared value each plotted for test and training data using ridge regression with $\lambda = 1$ and bootstrap resampling with $n = 200$. This time we cannot see a divergence at higher order polynomials even when going as high as $p = 60$. The obtained mean squared error is not as good as with OLS, but it is more robust to even very high degrees.

3.5 Lasso Regression with resampling

Applying Lasso regression to the data, I choose the same approach as for the previous task using a Resolution of 0.05. Using the R^2 value as an indicator for the goodness of the fit we see that Lasso regression in general performs poorly for values of λ below 10^-3. As we have seen in the first task, our parameter values operate in the range of 10^1 for low-order polynomials. Restricting the possible values to such a value several orders of magnitude below this, a bad fit is not unexpected. For increasing values of λ we can see better fits to the data. The first order polynomial peaks at $\approx 10^{-2}$, second and third order perform better in a whole range of values around this peak. With increasing complexity, the best values of λ increase towards the order of 10^{-1}. The maximum R^2 value achieved by models of different complexity is not much different, only the parameter value λ where the best fit is achieved, changes. The only exception is the first order polynomial which performed worse.



(a) (b)

Figure 9: R^2 value (left) and mean squared error (right) for different values of λ using lasso regression with 5-fold cross validation

We can see a similar development when analysing the mean squared error. The MSE for the first order polynomial has its lowest point for the same value of λ as the R^2 value had its peak. The higher orders perform again better but only to about the same level, where each degree achieves its peak at a slightly higher value than the degree before.
In both figures we can also see that there is no significant difference between the test data (full lines) and the training data (dashed lines).
Choosing a best λ to perform Bias Variance tradeoff in this context is difficult for two reasons. First, there is no best lambda that can be chosen for all degrees. The best value increases with complexity of the model. Secondly, we see no increase in performance for higher complexity. The second order polynomial already performs as well as the tenth order polynomial. I therefore perform this analysis twice, once choosing $\lambda_1 = 2 * 10^{-2}$ to match the best value achieved for the tenth order polynomial and then once for $\lambda_2 = 2*10^{-1}$, one order magnitude higher to possibly match higher order polynomials.
Figure 10 shows the analysis of the bias variance tradeoff for lasso regression. The analysis was performed using bootstrap resampling with $n = 200$. The top row shows the mean squared error, the bottom row the R^2 value of the fit. On the left the parameter $\lambda_1 = 2 * 10^{-2}$ is used and $\lambda_2 = 2 * 10^{-1}$ on the right.
Comparing to the results for the first analysis to find a suitable parameter, λ_1

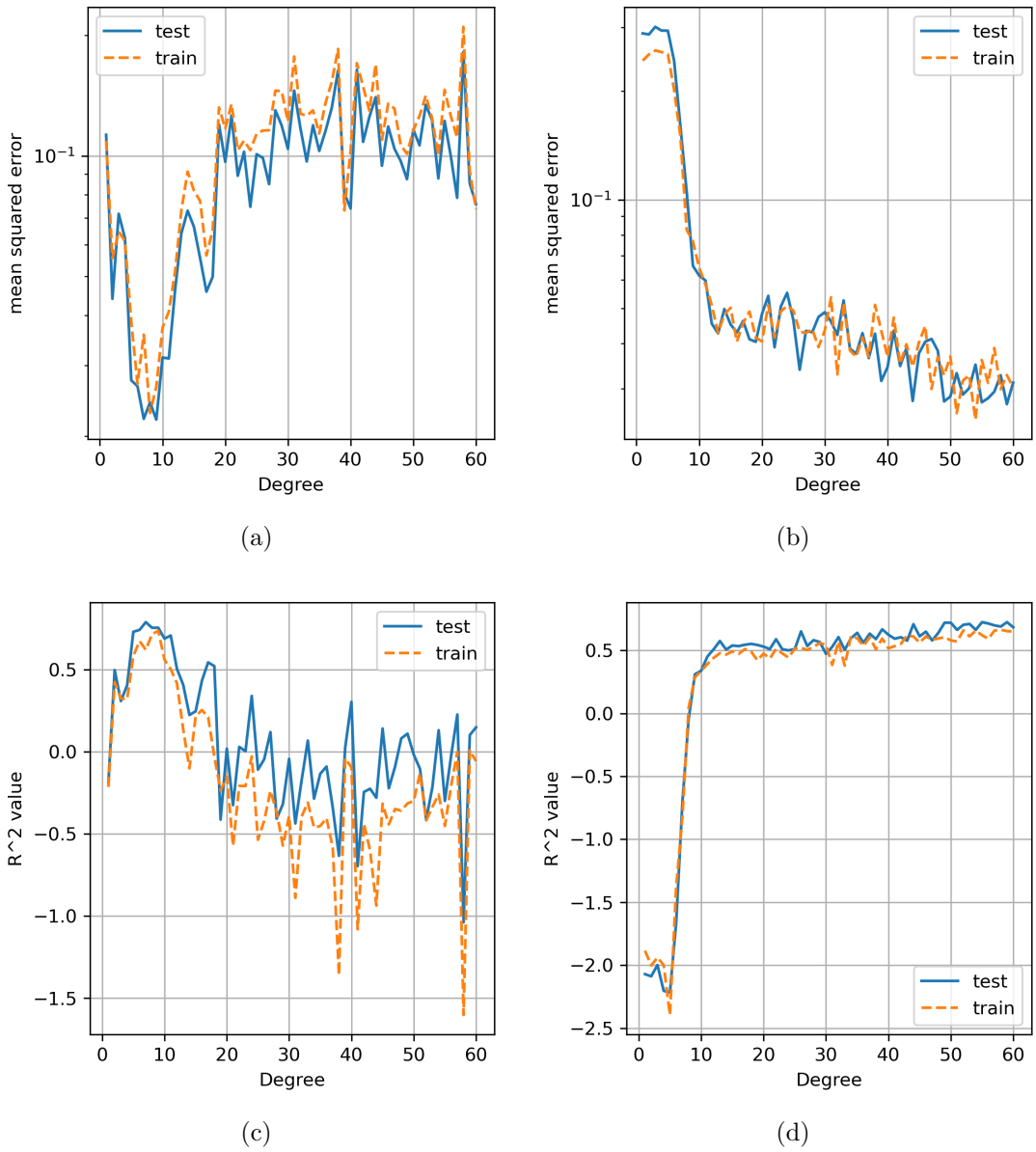
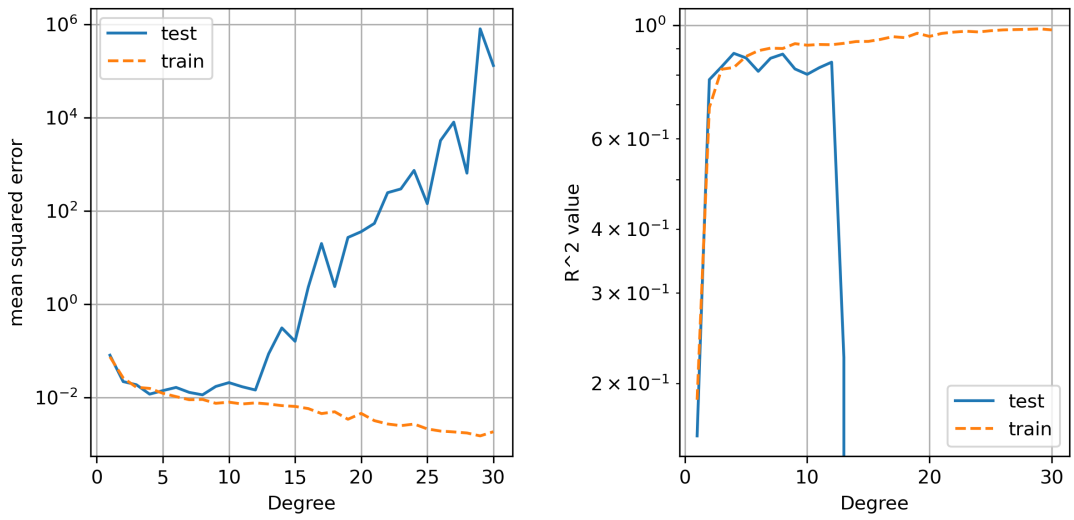


Figure 10: Mean squared error (top row) and R^2 value (bottom row) for higher order degrees using bootstrap resampling with $n = 200$ applied to lasso regression with $\lambda_1 = 2 * 10^{-2}$ (left) and $\lambda_2 = 2 * 10^{-1}$ (right)



(a) (b)

Figure 11: Mean squared error (left) and R^2 value (right) for ordinary least squares performed on my own data.

fits the data well in the range of low order polynomials. It reaches its best fit at $p \approx 10$, the value for which it was chosen. The goodness of the fit decreases afterwards and the error values increase for both test and training data.
For λ_2 we can see that the fit only becomes valid for $p > 10$. For lower orders, the fit is not usable and shows a low R^2 value as well as high errors. Afterwards, the error decreases rapidly and we see that the fit performs quite well in the regions where λ_1 failed.
The mean squared error is also slightly lower and the R^2 value is slightly higher than for λ_1. Both values are still improving when the highest displayed degree was reached.
For neither of the fits we can see a significant difference between test and training data, meaning that the fit is again quite robust and reduces overfitting.

3.6 Fitting own data

Instead of using terrain data I use data that I had available from previous experiments. I never performed regression analysis this way on the data but rather used a pre-trained model to compute the data. The data does not strictly follow an integer polynomial within its boundaries, but should still be describable by one nonetheless.
Figure 11 shows how my own data performs against ordinary least squares. The

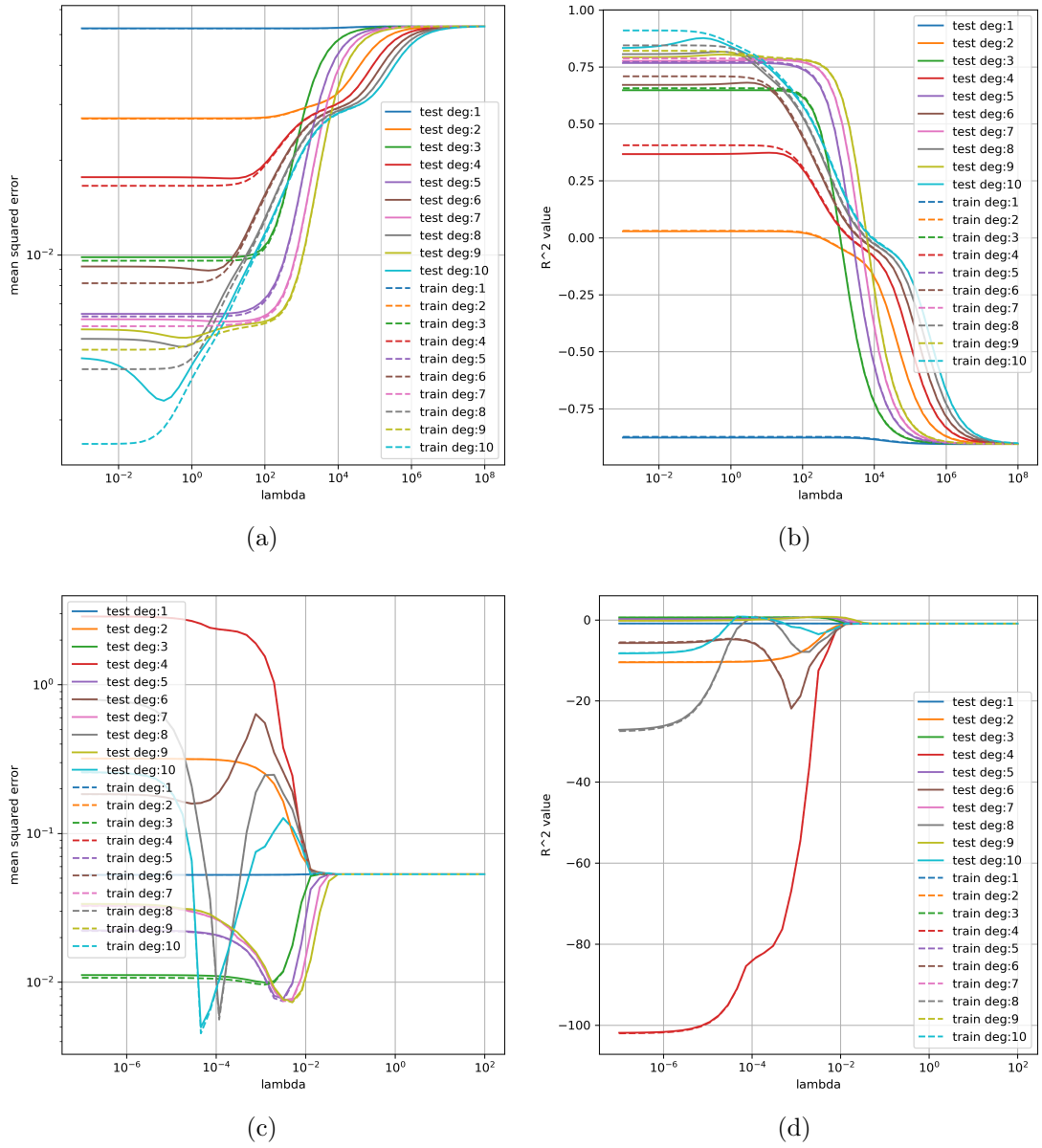
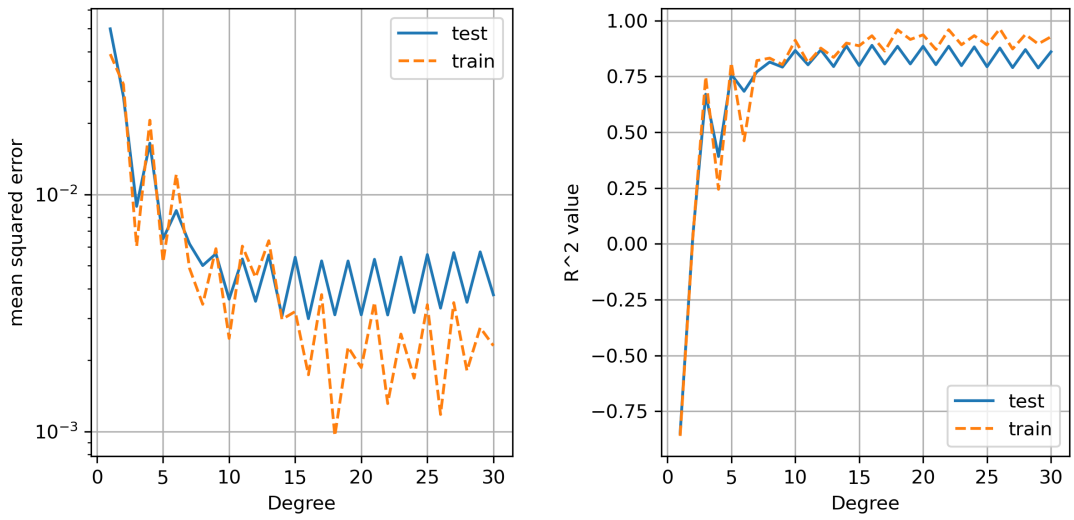


Figure 12: Mean squared error (left) and R^2 value (right) for ridge (top row) and lasso regression (bottom row). A degree up to 10 has been chosen and different parameters for λ are shown each. The data was evaluated using 5-fold cross validation.

analysis was performed using cross validation with 5 folds.
We can clearly see the that for a degree of up to 6 the performance of the model improves. Afterwards the goodness of the fit decreases for testing data while the performance of training data improves. This is a clear indicator of overfitting.
For ridge and lasso regression I performed evaluation of a polynomial degree up to 10. The graphs shown in fig. 12 shown this analysis for different values of λ chosen. The mean squared error is shown in the left column R^2 value on the right, Ridge regression in the top row and Lasso regression in the bottom. I again performed the analysis using cross validation with 5 folds.
For ridge regression we can see that the performance of the model still improves for higher degrees. A separation between training and testing data can be observed beginning at degree 6. Both the mean squared error and R^2 value show good and constant performance for $\lambda \leq 10^2$ for a polynomial of degree 3 or higher. There are also values for λ where ridge regression performs best but these values highly depend on the degree of the polynomial. For $p = 6$ this is at $\lambda_6 \approx 10^1$, for $p = 8$ at $\lambda \approx 10^0$ and for $p = 10$ at $\lambda \approx 2 * 10^{-1}$. First and second order show bad performance. This is not due to the method chosen, they are not complex enough to fit the data well.
For lasso regression only degrees of uneven order perform well. Even order polynomials are fitted poorly for all chosen values of λ. The regression algorithm probably overestimates the influence of even order polynomials and its less inclined to do so when fitting uneven order polynomials.
For the uneven order polynomials best performance was achieved for $\lambda_3 \approx 2 * 10^{-3}$ for p=3, $\lambda_5 \approx 3 * 10^{-3}$ for p=5 and $\lambda_{7+} \approx 5 * 10^{-3}$ for $p > 7$.
Comparing the three fits with each other, while Ridge and Lasso are more robust than OLS, Lasso breaks down for half of the possible feature matrixes and is therefore not usable.
Figure 13 shows the behaviour of ridge regression when choosing an optimal parameter $\lambda = 2 * 10^{-1}$ according to the best parameter for a polynomial for degree 10 as found above. Although the fit is quite robust and there is no increase in error for the testing data towards higher degrees of the fit and no decrease in R^2 value over the same range of degrees, the mean squared error achieved this way is only marginally better than for OLS.
We can see here as well that the fit performs differently for uneven degrees than for even degrees. The mean squared error depending on the complexity follows a zig-zag pattern where the highs and lows are alternating between even and uneven degrees.
The fit also does not get better at a degree $p = 8$ and the complexity is therefore only slightly higher than for OLS.
Overall for Ridge regression some effort had to be put into finding the optimal



(a) (b)

Figure 13: Mean squared error (left) and R^2 value (right) for ordinary ridge regression with $\lambda = 10$ performed on my own data

parameter. This then led only to a very small increase in goodness of the fit while making the fit slightly more complex.
Depending on where and how the achieved results need to be applied, one has to make an evaluation whether the additionally spent time to find this model and the added complexity to the model are worth it. If the desired result was to find a good and simple fit, then OLS would have been sufficient. If the desired outcome was the best fit, then ridge regression would be better. One could even argue that in this case a further evaluation of Lasso regression with more time spent on evaluating the parameters and increasing the allowed time to find a converging solution would have yielded a better result and may have been the way to go. Because the goal of this project was to purely evaluate the different regression methods I did not spend any more time finding the best possible fit.

4 Conclusion

In the search for a fit for a given set of data one might be tempted to apply OLS because it is simple to implement based on the highest order available model because it fits the data best. We have however shown the problems arising from using a simple OLS model extended to higher degrees. This problem can be resolved by using more robust models in the form of ridge or lasso regression

that suppress overfitting. This comes at the cost of increased time finding the best hyperparameter and might depending on the problem not even be the best solution.

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Python Code

The python code used to create the data this report is based on can be found in the following github repository: https://github.uio.no/Pascalsa/FYS4155 or at the end of this report. Each task has its own function that creates figures put into subfolders labeled according to the task they belong to.

```python
from typing import Tuple

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from matplotlib.figure import Figure
from sklearn import linear_model
from sklearn.preprocessing import scale
from sklearn.utils import shuffle

import colormaps as cmaps


def franke(x: np.array, y: np.array, noise_level: float) -> np.array:
    """
    Calculates the value of the franke function for x and y coordinates and adds random noise based
    on the noise level
    :param x: x-coordinate
    :param y: y-coordinate
    :param noise_level: noise level
    :return: Values of the franke function for the x-y pairs
    """
    if x.any() < 0 or x.any() > 1 or y.any() < 0 or y.any() > 1:
        # Breaks if the interval of x and y is outside [0,1]
        print("Franke function is only valid for x and y between 0 and 1.")
        return None
    term1 = 0.75 * np.exp(-(0.25 * (9 * x - 2) ** 2) - 0.25 * ((9 * y - 2) ** 2))
```

```
    term2 = 0.75 * np.exp(-((9 * x + 1) ** 2) / 49.0 - 0.1 * (9 * y + 1))
    term3 = 0.5 * np.exp(-(9 * x - 7) ** 2 / 4.0 - 0.25 * ((9 * y - 3) ** 2))
    term4 = -0.2 * np.exp(-(9 * x - 4) ** 2 - (9 * y - 7) ** 2)
    noise = np.random.normal(0, 1, term4.shape)
    return term1 + term2 + term3 + term4 + noise_level * noise


def plot_franke():
    """
    plots the franke function for x,y between 0 and 1
    """
    x, y = create_grid(RESOLUTION)
    z = franke(x, y, 0)
    fig = plt.figure(figsize=(6, 6), dpi=300)
    ax = fig.gca(projection='3d')
    surf = ax.plot_surface(x, y, z, cmap=cmaps.parula, linewidth=0)
    fig.colorbar(surf, shrink=0.5, aspect=5)
    ax.set_xlabel("x")
    ax.set_ylabel("y")
    fig.tight_layout()
    fig.savefig("images/franke.png")


def r2_error(y_data: np.array, y_model: np.array) -> float:
    """
    Calculates R squared based on predicted and true data.
    """
    return 1 - np.sum((y_data - y_model) ** 2) / np.sum((y_data - np.mean(y_data)) ** 2)


def mse_error(y_data: np.array, y_model: np.array) -> float:
    """
```

```
    Calculates mean squared error based in predicted and true data
    """
    return np.sum((y_data - y_model) ** 2) / np.size(y_model)


def coords_to_polynomial(x: np.array, y: np.array, p: int) -> np.array:
    """
    Calculates the feature matrix based on input coordinates x and y and the given degree of the
    polynomial
    :param x: x vector
    :param y: y vector
    :param p: degree of polynomial
    :return: feature matrix
    """
    if x.shape != y.shape:
        # Breaks if x and y are of different shapes
        print("mismatch between size of x and y vector")
        return None
    # Preparing x and y and pre-allocating the feature matrix X
    x = x.flatten()
    y = y.flatten()
    feat_matrix = np.zeros(shape=(len(x), max_mat_len(p)))
    k = 0
    for i in range(p + 1):
        for j in range(i + 1):
            feat_matrix[:, k] = x ** (i - j) * y ** j
            k += 1
    return feat_matrix


def solve_lin_equ(y: np.array, x: np.array, solver: str = "ols", la: float = 1) -> Tuple[
        np.array, np.array]:
    """
```

```
    Solves linear equation of type y = x*beta. This can be done using ordinary least squares (OLS),
    ridge or lasso regression. For ridge and lasso, an additional parameter l for shrinkage /
    normlization needs to be provided.
    :param y: solution vector of linear problem
    :param x: feature vector or matrix of problem
    :param solver: solver. Can be ols, ridge or lasso
    :param la: shrinkage / normalization parameter for ridge or lasso
    :return: parameter vector that solves the problem & variance of parameter vector
    """
    beta = np.zeros(x.shape[0])
    var = np.zeros(beta.shape)
    if solver == "ols":
        var = np.linalg.inv(x.transpose() @ x)
        beta = np.linalg.pinv(x) @ y
    elif solver == "ridge":
        var = np.linalg.inv(x.transpose() @ x + la * np.identity(x.shape[1]))
        beta = var @ x.transpose() @ y
    elif solver == "lasso":
        clf = linear_model.Lasso(alpha=la, max_iter=MAX_ITER)
        clf.fit(x, y)
        beta = clf.coef_
        var = np.zeros(shape=(1, 1))
    return beta, np.abs(var.diagonal())


def create_grid(res: float) -> Tuple[np.array, np.array]:
    """
    Creates a parameter grid for x and y in [0,1] with a given resolution
    :param res: resolution of the grid
    :return: Parameter grid
    """
    x = np.arange(0, 1, res)
    y = np.arange(0, 1, res)
```

```
    x, y = np.meshgrid(x, y)
    return x, y


def create_data(deg: int, cross_validation: int = 1, x: np.array = None, y: np.array = None,
                z: np.array = None) \
        -> Tuple[np.array, np.array, np.array, np.array]:
    """
    Creates the data that is used for the regression. Depending on the given degree of the
    polynomial a feature matrix will be created. Also data for the franke function for this feature
    matrix is calculated. If cross validation is to be performed, the parameter with a value larger
    than one has to be set. For a value equal 1, the data is split into 80:20 training and test
    data. For cross validation, the data will be split into equal folds depending on the number
    given.
    If values for x,y and z are provided, no feature matrix is created but instead the given values
    are passed on. The function also performs scaling of the data, if necessary.
    :param deg: Degree of the polynomial
    :param cross_validation: Number of folds for cross validation. Default: 1. This means a split
        in 80:20 training:test without cross validation
    :param x: x-vector
    :param y: y-vector
    :param z: z-vector
    :return: arrays containing feature and result vectors split into training and test
    """
    # creating coordinate vectors if none were provided
    if x is None or y is None:
        x, y = create_grid(RESOLUTION)
        z = franke(x, y, NOISE_LEVEL).flatten()
    # calculating feature matrix
    feature_mat = coords_to_polynomial(x, y, deg)
```

```
    # scaling
    if SCALE_DATA:
        feature_mat = scale(feature_mat, axis=1)
    # calculation z-vector if none was provided
    if z is None:
        z = franke(x, y, NOISE_LEVEL).flatten()
    # dimensions of the feature matrix
    n = int(feature_mat.shape[0])
    m = int(feature_mat.shape[1])
    # k will be the amount of folds
    # test_l is the length of the test split
    # train_l is the length of the training split
    if cross_validation == 1:
        # 80:20 split in train and test data
        k = 1
        test_l = int(np.floor(n * 0.2))
        train_l = n - test_l
    else:
        # split into k folds, length depends on amount of folds
        k = cross_validation
        test_l = int(np.floor(n / k))
        train_l = n - test_l
    # randomizing order of feature matrix and result vector and allocating split variables
    feature_mat, z = shuffle(feature_mat, z, random_state=RANDOM_SEED)
    feature_mat_train = np.zeros(shape=(k, train_l, m))
    feature_mat_test = np.zeros(shape=(k, test_l, m))
    z_train = np.zeros(shape=(k, train_l))
    z_test = np.zeros(shape=(k, test_l))
    for i in range(k):
        # For each split the first test_l amount of data is removed from the training set. The same
        # array of data is then the test set for this fold.
        feature_mat_train[i, :, :] = np.delete(feature_mat,
                                               np.arange(i
                                                   * test_l,
                                                   (i + 1)
                                                   * test_l,
```

```
                                                    1, int),
                                                axis=0)
        feature_mat_test[i, :, :] = feature_mat[i * test_l
            :(i + 1) * test_l, :]
        z_train[i, :] = np.delete(z, np.arange(i * test_l,
            (i + 1) * test_l, 1, int), axis=0)
        z_test[i, :] = z[i * test_l:(i + 1) * test_l]
    # reshaping to make it easier in the coming functions.
        The first two indeces are left in their
    # previous relative and are the length and height of
        the feautres. The now last index represents
    # the fold.
    feature_mat_train = np.transpose(feature_mat_train, (1,
        2, 0))
    feature_mat_test = np.transpose(feature_mat_test, (1,
        2, 0))
    z_train = np.transpose(z_train, (1, 0))
    z_test = np.transpose(z_test, (1, 0))
    return feature_mat_train, feature_mat_test, z_train,
        z_test


def predict(beta: np.array, feature_mat: np.array) -> np.
    array:
    """
    Predicts result of linear equation: y = x*beta
    :param beta: parameter matrix
    :param feature_mat: feature matrix
    :return:
    """
    return feature_mat @ beta


def err_from_var(var: np.array, sample_size: int) -> np.
    array:
    """
    Calculates the error from its variance
    :param var: variance
    :param sample_size: Sample size
    :return: error based on variance and sample size
```

```
    """
    return 1.97 * np.sqrt(var) / np.sqrt(sample_size)


def train(deg: int, cross_validation: int = 1, bootstraps: int = 0, solver: str = "ols",
          la: float = 1,
          x: np.array = None, y: np.array = None, z: np.array = None) -> \
        Tuple[np.array, np.array, np.array, np.array, np.array, np.array, np.array]:
    """
    Calculates fit based on given degree. If cross validation of bootstraps are given, the
    corresponding algorithms will be applied. If noe data for x,y and z are given, data will be
    created from / for the franke function, otherwise the provided data will be used
    :param deg: Degree of the polynomial to be fitted onto
    :param cross_validation: amount of folds for cross validation. Default:1 means 80:20 split
    :param bootstraps: amount of bootstraps for bootstrap evaluation
    :param solver: Algorithm for solving. Can be ols, ridge or lasso
    :param la: parameter for ridge and lasso regression
    :param x: x-vector
    :param y: y-vector
    :param z: z-vector
    :return: Regression parameter vector, error and variance of parameter vector, test & training data R squqared value and mean squared error
    """
    # creates feature matrix and result vector
    feature_mat_train, feature_mat_test, z_train, z_test = create_data(deg, cross_validation, x=x,
                                                                       y
```

```
    # declares variables for results
    test_rs = np.zeros(shape=cross_validation)
    test_ms = np.zeros(shape=cross_validation)
    train_rs = np.zeros(shape=cross_validation)
    train_ms = np.zeros(shape=cross_validation)
    beta = np.zeros(feature_mat_test.shape[1])
    var = np.zeros(beta.shape)
    err = np.zeros(beta.shape)
    # looping over folds for cross validation
    for i in range(cross_validation):
        # solving the linear equation, calculating error for parameter vector
        beta, var = solve_lin_equ(z_train[:, i].flatten(), feature_mat_train[:, :, i],
                                  solver=solver, la=la)
        err = err_from_var(var, len(z_train[:, i]))
        if bootstraps > 0:
            # If bootstrap resampling is to be evaluated, randomly select samples from the training
            # data. The index variable may contain the same values several times
            train_l = feature_mat_train.shape[0]
            train_inds = np.random.randint(0, high=train_l, size=bootstraps)
            train_x = feature_mat_train[train_inds, :, i]
            train_z = z_train[train_inds, i]
            test_x = feature_mat_test[:, :, i]
            test_z = z_test[:, i]
        else:
            # No bootstrap: Every result is part of the sample
            test_x = feature_mat_test[:, :, i]
            train_x = feature_mat_train[:, :, i]
            test_z = z_test[:, i]
```

```
            train_z = z_train[:, i]
        # Calculate errors based on the chosen samples
        test_rs[i] = r2_error(test_z, predict(beta, test_x))
        test_ms[i] = mse_error(test_z, predict(beta, test_x))
        train_rs[i] = r2_error(train_z, predict(beta, train_x))
        train_ms[i] = mse_error(train_z, predict(beta, train_x))
    # average over the folds
    test_r = np.average(test_rs)
    train_r = np.average(train_rs)
    test_m = np.average(test_ms)
    train_m = np.average(train_ms)
    return test_r, train_r, test_m, train_m, beta, var, err


def max_mat_len(maxdeg: int) -> int:
    """
    Calculates the size of the polyonmial based on its degree
    :param maxdeg: degree of polynomial
    :return: size of the polynomial
    """
    return int((maxdeg + 2) * (maxdeg + 1) / 2)


def train_degs(maxdeg: int, cross_validation: int = 1, bootstraps: int = 0, solver: str = "ols",
               la: float = 1,
               x: np.array = None, y: np.array = None, z: np.array = None) \
        -> Tuple[np.array, np.array, np.array, np.array, np.array, np.array, np.array]:
    """
    This is a wrapper for the function "train", that loops over all the degrees given in maxdeg
    :param maxdeg: highest order degree to be trained
```

```
    :param cross_validation: amount of folds for cross validation. Default:1 means 80:20 split
    :param bootstraps: amount of bootstraps for bootstrap evaluation
    :param solver: Algorithm for solving. Can be ols, ridge or lasso
    :param la: parameter for ridge and lasso regression
    :param x: x-vector
    :param y: y-vector
    :param z: z-vector
    :return: Regression parameter vector, error and variance of parameter vector, test & training data R squqared value and mean squared error
    """
    # declare variables so that the values can be assigned in the loop
    beta = np.zeros(shape=(maxdeg, max_mat_len(maxdeg)))
    var = np.zeros(shape=(maxdeg, max_mat_len(maxdeg)))
    err = np.zeros(shape=(maxdeg, max_mat_len(maxdeg)))
    test_r = np.zeros(shape=(maxdeg, 1))
    train_r = np.zeros(shape=(maxdeg, 1))
    test_m = np.zeros(shape=(maxdeg, 1))
    train_m = np.zeros(shape=(maxdeg, 1))
    # looping over every degree to be trained
    for i in range(maxdeg):
        print("training degree: " + str(i + 1))
        t = train(i + 1, cross_validation=cross_validation, bootstraps=bootstraps, solver=solver,
                  la=la, x=x, y=y, z=z)
        b = t[4]
        beta[i, 0:len(b)] = b
        v = t[5]
        var[i, 0:len(v)] = v
        e = t[6]
        err[i, 0:len(e)] = e
        test_r[i] = t[0]
        train_r[i] = t[1]
        test_m[i] = t[2]
        train_m[i] = t[3]
```

```
    return test_r.ravel(), train_r.ravel(), test_m.ravel(), train_m.ravel(), beta, var, err


def print_errors(x_values: np.array, errors: np.array, labels: list, name: str, logy: bool = False,
                 logx: bool = False,
                 xlabel: str = "Degree", ylabel: str = "error value", d: int = 6) -> Figure:
    """
    Helper function to create similar looking graphs. All the graphs where mean squared errors or
    the r_squared value are plotted and shown in the report are plotted using this function
    :param x_values: values for x axis
    :param errors: values for y axis
    :param labels: plot labels
    :param name: filename
    :param logy: plot y logarithmically?
    :param logx: plot x logarithmically?
    :param xlabel: label for x
    :param ylabel: label for y
    :param d: size of plot
    :return: the created figure
    """
    # creating new figure
    fig = plt.figure(figsize=(d, d), dpi=300)
    # plotting every given value
    for i in range(len(errors)):
        label = labels[i]
        # linestyle depends on test or train data
        if label.__contains__("train"):
            linestyle = "--"
        else:
            linestyle = "-"
        plt.plot(x_values, errors[i], label=labels[i], linestyle=linestyle)
    plt.legend()
    plt.grid()
    ax = fig.gca()
```

```
    ax.set_xlabel(xlabel)
    ax.set_ylabel(ylabel)
    if logy:
        plt.yscale('log')
    if logx:
        plt.xscale('log')
    fig.tight_layout()
    fig.savefig("images/" + name + ".png", dpi=300)
    return fig


def print_cont(deg: int, data: np.array, name: str, zlabel:
    str) -> Figure:
    """
    Similar as above but for contour data where the axes
       depend on the degree of the polynome
    :param deg: degree of the polynomial
    :param data: z-values
    :param name: filename
    :param zlabel: label for z axis
    :return: the create figure
    """
    # x axis is the parameter index
    x = np.linspace(1, max_mat_len(deg), max_mat_len(deg))
    # axis is the polynomial index
    y = np.linspace(1, deg, deg)
    x, y = np.meshgrid(x, y)
    fig = plt.figure(figsize=(6, 6), dpi=300)
    ax = fig.gca(projection='3d')
    ax.plot_surface(x, y, data, cmap=cmaps.parula)
    ax.set_xlabel("Parameter Index")
    ax.set_ylabel("Polynomial Degree")
    ax.set_zlabel(zlabel)
    fig.tight_layout()
    fig.savefig("images/" + name + ".png", dpi=300)
    return fig


def read_data_file() -> pd.DataFrame:
    """
```

```
    Reads file with own data into pandas data frame
    :return: File content as dataframe
    """
    data_file = DATA_FILE
    return pd.read_csv(data_file, delimiter=",")


def get_data() -> Tuple[np.array, np.array, np.array]:
    """
    I used some data that I had left over from my previous position. This is calculated magnetic
    field data from some permanent magnet configuration. The data does not follow a strictly
    integer-polynomial trend but can be described not too badly by a polynom within the boundaries.
    I made the data more sparse by randomly removing 90% of the original data.
    :return: prepared data
    """
    data = read_data_file()
    x = np.array(data["x"])
    y = np.array(data["y"])
    z = np.array(data["z"])
    cutoff = int(np.floor(len(z) * .1))
    x, y, z = shuffle(x, y, z, random_state=RANDOM_SEED)
    x = x[:cutoff]
    y = y[:cutoff]
    z = z[:cutoff]
    z = z / np.max(z)
    return x, y, z


def print_data() -> Figure:
    """
    Prints my data to image file
    :return: The created figure
    """
    x, y, z = get_data()
    fig = plt.figure(figsize=(8, 8), dpi=300)
    ax = fig.gca(projection='3d')
```

```
    ax.scatter(x, y, z, c='y', marker='o')
    ax.set_xlabel("x")
    ax.set_ylabel("y")
    ax.set_zlabel("B")
    fig.savefig("images/data.png", dpi=300)
    return fig


def train_print_diff_lambdas(deg: int, minorder: int, maxorder: int, cross_validation: int = 1,
                             bootstraps: int = 0,
                             solver: str = "ridge", x: np.array = None, y: np.array = None,
                             z: np.array = None,
                             task: str = "a", d: int = 6) -> None:
    """
    Wrapper functino around "train_degs", that is able to handle different parameters for ridge and
    lasso and automatically prints the resulting diagramms.
    :param deg: maximum degree for which to train
    :param minorder: minimum order of magnitude for parameter
    :param maxorder: maximum order of magnitude for parameter
    :param cross_validation: folds for cross validation
    :param bootstraps: amount of bootstraps
    :param solver: ridge or lasso
    :param x: x vector
    :param y: y vector
    :param z: z vector
    :param task: task this belongs to, to sort the figures into the correct folder
    :param d: size of the figure
    :return: None
    """
    if task == "f" or task == "e":
        logy = False
    else:
```

```
        logy = True
    order = np.array([minorder, maxorder])
    n = int(np.linalg.norm(order, 1) * 5)
    test_r = np.zeros(shape=(deg, n))
    train_r = np.zeros(shape=(deg, n))
    test_m = np.zeros(shape=(deg, n))
    train_m = np.zeros(shape=(deg, n))
    # different parameters created based on the orders given before, equally spaced on a logarithmic
    # scale
    lambdas = np.logspace(order[0], order[1], num=n)
    i = 0
    # iterating over lambdas
    for la in lambdas:
        test_r[:, i], train_r[:, i], test_m[:, i], train_m[:, i], beta, var, err = train_degs(
            maxdeg=deg,
            cross_validation=cross_validation,
            bootstraps=bootstraps,
            solver=solver, la=la, x=x,
            y=y, z=z)
        i = i + 1
    # refactoring shape of error and label vectors
    errors = np.append(test_m, train_m, axis=0)
    labels = [[], []]
    for i in range(deg):
        labels[0].extend(["test deg:" + str(i + 1)])
        labels[1].extend(["train deg:" + str(i + 1)])
    # https://stackoverflow.com/a/952952
    labels = [item for sublist in labels for item in sublist]
    # plotting mean squared error
    print_errors(lambdas, errors, labels,
                 task + "/" + solver + "_mse_cross_" + str(cross_validation) + "_boot_" + str(bootstraps), logx=True, logy=True,
                 xlabel="lambda", d=d, ylabel="mean squared error")
    errors = np.append(test_r, train_r, axis=0)
    print_errors(lambdas, errors, labels,
```

```
                    task + "/" + solver + "_R_squared_cross_" + str(cross_validation) + "_boot_" + str(
                        bootstraps), logx=True, logy=logy,
                    xlabel="lambda", d=d, ylabel="R^2 value")


def train_print_single_lambda(deg: int, la: float = 0, cross_validation: int = 1,
                              bootstraps: int = 0,
                              solver: str = "ridge", x: np.array = None, y: np.array = None,
                              z: np.array = None,
                              task: str = "a", d: int = 6):
    """
    Same as "train_print_diff_lambdas" but only for a single lambda
    :param deg: maximum degree for which to train
    :param la: lambda for which to plot
    :param cross_validation: folds for cross validation
    :param bootstraps: amount of bootstraps
    :param solver: ridge or lasso
    :param x: x vector
    :param y: y vector
    :param z: z vector
    :param task: task this belongs to, to sort the figures into the correct folder
    :param d: size of the figure
    :return: None
    """
    if task == "f" or task == "e":
        logy = False
    else:
        logy = True
    test_r, train_r, test_m, train_m, beta, var, err = train_degs(maxdeg=deg,
                                                                 cross_
                                                                 =
                                                                 cro
```

```
                                                
```

```
                    logy=True, ylabel="mean squared error", d=d)
    errors = [test_r, train_r]
    print_errors(np.linspace(1, deg, deg), errors, labels,
                    task + "/" + solver + "_R_squared_deg" + str(deg) + "_cross_" +
                    str(cross_validation) + "_Boot_" + str(bootstraps) + "_lambda_" + str(la),
                    logy=logy, ylabel="R^2 value", d=d)


def task_a():
    deg = 5
    test_r, train_r, test_m, train_m, beta, var, err = train_degs(deg)
    print_cont(deg, err, "a/ols_error_scaling_" + SCALE_DATA.__str__(), "Parameter error")
    print_cont(deg, beta, "a/ols_betas_scaling_" + SCALE_DATA.__str__(), "Parameter values")
    errors = [test_m, train_m]
    labels = ["test", "train"]
    print_errors(np.linspace(1, deg, deg), errors, labels,
                    "a/ols_mse_scaling_" + SCALE_DATA.__str__(),
                    logy=True, ylabel="mean squared error", d=4)
    errors = [test_r, train_r]
    print_errors(np.linspace(1, deg, deg), errors, labels,
                    "a/ols_R_squared_scaling_" + SCALE_DATA.__str__(),
                    ylabel="R^2 value", d=4)


def task_b():
    deg = MAX_DEG
    bootstraps = np.array([0, BOOTSTRAPS])
    for bs in bootstraps:
        train_print_single_lambda(deg=deg, bootstraps=bs, solver="ols", task="b", d=4)

```

```python

def task_c():
    deg = MAX_DEG
    cross_validation = np.array([5, 10])
    for cr in cross_validation:
        train_print_single_lambda(deg=deg, cross_validation=cr, task="c", solver="ols", d=4)


def task_d():
    deg = 10
    bootstraps = BOOTSTRAPS
    cross_validation = CROSS_VALIDATION
    minorder = -7
    maxorder = 5
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder,
                             cross_validation=cross_validation,
                             solver="ridge", task="d", d=6)
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder, bootstraps=bootstraps,
                             solver="ridge", task="d", d=6)
    best_l = 1
    train_print_single_lambda(deg=MAX_DEG * 2, la=best_l, bootstraps=bootstraps, solver="ridge",
                              task="d", d=4)


def task_e():
    deg = 10
    cross_validation = CROSS_VALIDATION
    bootstraps = BOOTSTRAPS
    minorder = -4
    maxorder = 0
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder,
                             cross_validation=cross_validation,
                             solver="lasso", task="e", d=6)
```

```
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder, bootstraps=bootstraps,
                             solver="lasso", task="e", d=6)
    best_l = 2e-2
    train_print_single_lambda(deg=MAX_DEG * 2, la=best_l, bootstraps=bootstraps, solver="lasso",
                              task="e", d=4)
    best_l = 2e-1
    train_print_single_lambda(deg=MAX_DEG * 2, la=best_l, bootstraps=bootstraps, solver="lasso",
                              task="e", d=4)


def task_f():
    x, y, z = get_data()
    deg = MAX_DEG
    cross_validation = CROSS_VALIDATION
    bootstraps = BOOTSTRAPS
    test_r, train_r, test_m, train_m, _, _, _ = train_degs(deg)
    errors = [test_m, train_m]
    labels = ["test", "train"]
    print_errors(np.linspace(1, deg, deg), errors, labels,
                 "f/ols_mse",
                 logy=True, ylabel="mean squared error", d=4)
    errors = [test_r, train_r]
    print_errors(np.linspace(1, deg, deg), errors, labels,
                 "f/ols_R_squared",
                 ylabel="R^2 value", logy=True, d=4)

    deg = 10
    minorder = -3
    maxorder = 8
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder,
                             cross_validation=cross_validation,
                             solver="ridge", task="f", x=x, y=y, z=z, d=6)
```

```
    minorder = -7
    maxorder = 2
    train_print_diff_lambdas(deg=deg, minorder=minorder, maxorder=maxorder,
                                cross_validation=cross_validation,
                                solver="lasso", task="f", x=x, y=y, z=z, d=6)
    best_l = 2*10**-1
    deg = MAX_DEG
    train_print_single_lambda(deg=deg, la=best_l, bootstraps=bootstraps, solver="ridge", task="f",
                                x=x, y=y, z=z, d=4)


def show_cond_numbers():
    """
    Calculates and prints condition numbers for different feature matrices
    :return: None
    """
    x, y = create_grid(0.1)
    x3 = coords_to_polynomial(x, y, 3)
    x5 = coords_to_polynomial(x, y, 5)
    x10 = coords_to_polynomial(x, y, 10)
    c3 = np.linalg.cond(x3.transpose() @ x3)
    c5 = np.linalg.cond(x5.transpose() @ x5)
    c10 = np.linalg.cond(x10.transpose() @ x10)
    x3 = scale(x3, axis=1)
    x5 = scale(x5, axis=1)
    x10 = scale(x10, axis=1)
    c3s = np.linalg.cond(x3.transpose() @ x3)
    c5s = np.linalg.cond(x5.transpose() @ x5)
    c10s = np.linalg.cond(x10.transpose() @ x10)
    print("condition numbers for different degress of the polynomial:\n"
          "deg3: %f\ndeg5: %f\ndeg10:%f\nSame for centered data:\ndeg3: %f\ndeg5: %f\ndeg10:%f" % (
              c3, c5, c10, c3s, c5s, c10s))

```

```

NOISE_LEVEL = 0.1
MAX_DEG = 30
RESOLUTION = .02
RANDOM_SEED = 1337
BOOTSTRAPS = 200
BEST_L = 1e-2
DATA_FILE = "files/data.csv"
np.random.seed(RANDOM_SEED)
CROSS_VALIDATION = 5
MAX_ITER = 100000

show_cond_numbers()
SCALE_DATA = False
plot_franke()

task_a()
SCALE_DATA = True
task_a()
task_b()
task_c()
RESOLUTION = .05
task_d()
task_e()
MAX_ITER = 1000
task_f()
```

```
# New matplotlib colormaps by Nathaniel J. Smith, Stefan van der Walt,
# and (in the case of viridis) Eric Firing.
#
# This file and the colormaps in it are released under the CC0 license /
# public domain dedication. We would appreciate credit if you use or
# redistribute these colormaps, but do not impose any legal restrictions.
#
# To the extent possible under law, the persons who associated CC0 with
# mpl-colormaps have waived all copyright and related or
```

```
    neighboring rights
# to mpl-colormaps.
#
# You should have received a copy of the CC0 legalcode
    along with this
# work.  If not, see <http://creativecommons.org/
    publicdomain/zero/1.0/>.

# import colormaps as cmaps
# plt.imshow(my_image, cmap=cmaps.viridis)

__all__ = ['magma', 'inferno', 'plasma', 'viridis', 'parula
    ']

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from matplotlib.colors import ListedColormap

cmaps = {}
for (name, data) in (('magma', _magma_data),
                     ('inferno', _inferno_data),
                     ('plasma', _plasma_data),
                     ('viridis', _viridis_data),
                     ('parula', _parula_data)):
    cmaps[name] = ListedColormap(data, name=name)

magma = cmaps['magma']
inferno = cmaps['inferno']
plasma = cmaps['plasma']
```

```
viridis = cmaps['viridis']
parula = cmaps['parula']
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