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FYS-STK3155

Project 1

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[HTTPS://GITHUB.COM/BRAGEWISETH/MACHINELEARNINGPROJECTS](https://github.com/bragewiseth/machinelearningprojects)

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Abstract

In this paper, we delve into the realm of machine learning model optimization and evaluation. Our study encompasses various regression techniques, including Ordinary Least Squares (OLS), Ridge, and Lasso regression, to analyze their effectiveness in handling simple and more complex datasets. Additionally, we employ bootstrap resampling and cross-validation methodologies to rigorously assess model performance and enhance generalization. A significant portion of our investigation is dedicated to understanding the delicate balance between bias and variance. We explore how regularization methods like Ridge and Lasso impact bias-variance trade-offs, offering insights into the stability and predictive power of these models. Furthermore, we provide empirical evidence of the benefits of cross-validation and bootstrap techniques in mitigating overfitting and improving model robustness. We found that { ..results.. }. Additionally we verify and compare our findings with well established theory and libraris such as SKLearn.

Keywords: Linear Regression, Scaling, Bias & Variance

1. Introduction

Machine learning has emerged as a powerful tool in data analysis, providing the ability to uncover complex patterns and relationships in diverse datasets. But, at its core, machine learning is all about finding functions that capture the underlying structure of the data. The use of machine learning algorithms to approximate functions is the essence of this paper.

Our motivation for this research lies in the exploration of machine learning techniques to approximate the terrain on our planet, which can perhaps be described by such a function. Earth's terrain exhibits peaks and troughs, hills and valleys, much like some polynomial functions. Fortunately, we can employ standard linear regression techniques to approximate polynomials, but the terrain presents its own set of challenges. Firstly, the terrain's true underlying function may not be a polynomial at all, and its complexity may vary significantly from one location to another. Secondly, our landscape is teeming with small, intricate details. Some regions are characterized by flat and smooth surfaces, while others are marked by rough and uneven terrain. Focusing too much on these minute details can lead to model overfitting, making it crucial to strike a careful balance between model complexity and generalization. In this context, regularization and resampling techniques, including Ridge and Lasso regression with bootstrap and cross validation, have proven indispensable. By introducing regularization and resampling, we aim to find the sweet spot between bias and Variance. And getting the best predictions we can with our assumptions.

To embark on this exploration, we will begin with a simpler case: "Franke's function." which mimics our real terrain data. This function serves as a foundational starting point, allowing us to assess our model's performance in a controlled environment before venturing into the complexity of real-world terrain data. Through this gradual progression, we provide ourselves with a framework that can be applied to more complex and varied real-world terrain datasets.

Data: We begin by introducing the dataset used for our analysis, highlighting data collection and preprocessing procedures. Understanding the characteristics of the terrain data is fundamental to our modeling endeavor.

Methods and Scaling: Next, we delve into the methodology, encompassing the implementation of polynomial regression models and the application of regularization techniques such as Ridge and Lasso. Additionally, we will discuss the importance of proper scaling for model stability and convergence.

Bias-Variance Trade-off: A significant portion of our study will revolve around the critical concept of bias and variance. We'll explore how regularization methods influence this trade-off and delve into the fine balance between model complexity and generalization.

Results: In this section, we will present the outcomes of our experiments, showcasing the performance of different models and regularization techniques. Through empirical evidence, we aim to provide insights into the effectiveness of our approach.

Conclusion: Finally, we will summarize the key findings and their implications for terrain modeling with machine learning. Our conclusion will underscore the importance of regularization in achieving accurate representations of complex terrains and provide a perspective on future research directions.

2. Data

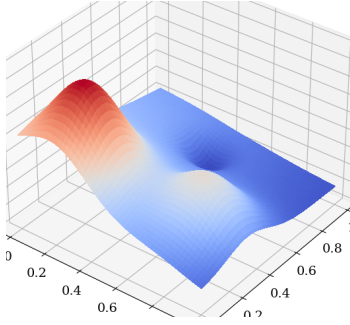
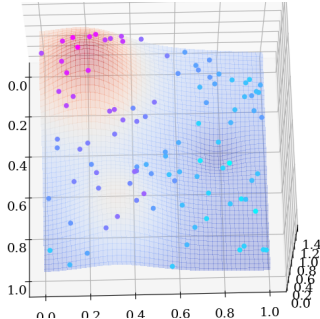


Figure 1: franke's function with noise

3. linear regression models

Figure 2: franke's function

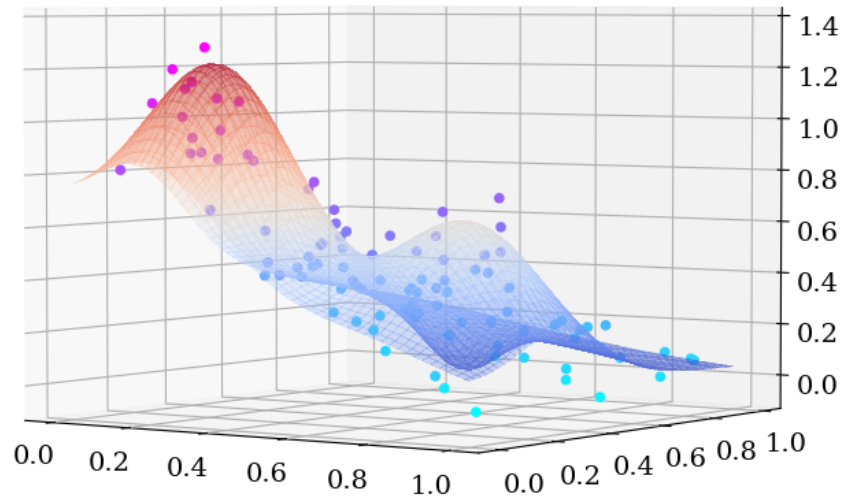


$$mse(\mathbf{y}, \tilde{\mathbf{y}}) = \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2,$$

$$r^2(\mathbf{y}, \tilde{\mathbf{y}}) = 1 - \frac{\sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2}{\sum_{i=0}^{n-1} (y_i - \bar{y})^2},$$

$$\bar{y} = \frac{1}{n} \sum_{i=0}^{n-1} y_i.$$

Data



3.1 Ordinary Least Squares (OLS)

3.2 Ridge Regression

3.3 lasso Regression

3.4 Scaling

Table 1: unscaled sample design matrix fitting one-dimensional polynomial of degree 5

1.	0.	0.	0.	0.	0.
1.	0.25	0.0625	0.01562	0.00391	0.00098
1.	0.5	0.25	0.125	0.0625	0.03125
1.	0.75	0.5625	0.42188	0.31641	0.2373
1.	1.	1.	1.	1.	1.

Table 2: scaled sample design matrix fitting one-dimensional polynomial of degree 5

0.	-1.41421	-1.0171	-0.83189	-0.728	-0.66226
0.	-0.70711	-0.84758	-0.7903	-0.71772	-0.65971
0.	0.	-0.33903	-0.49913	-0.56348	-0.58075
0.	0.70711	0.50855	0.29116	0.10488	-0.0433
0.	1.41421	1.69516	1.83016	1.90431	1.94603

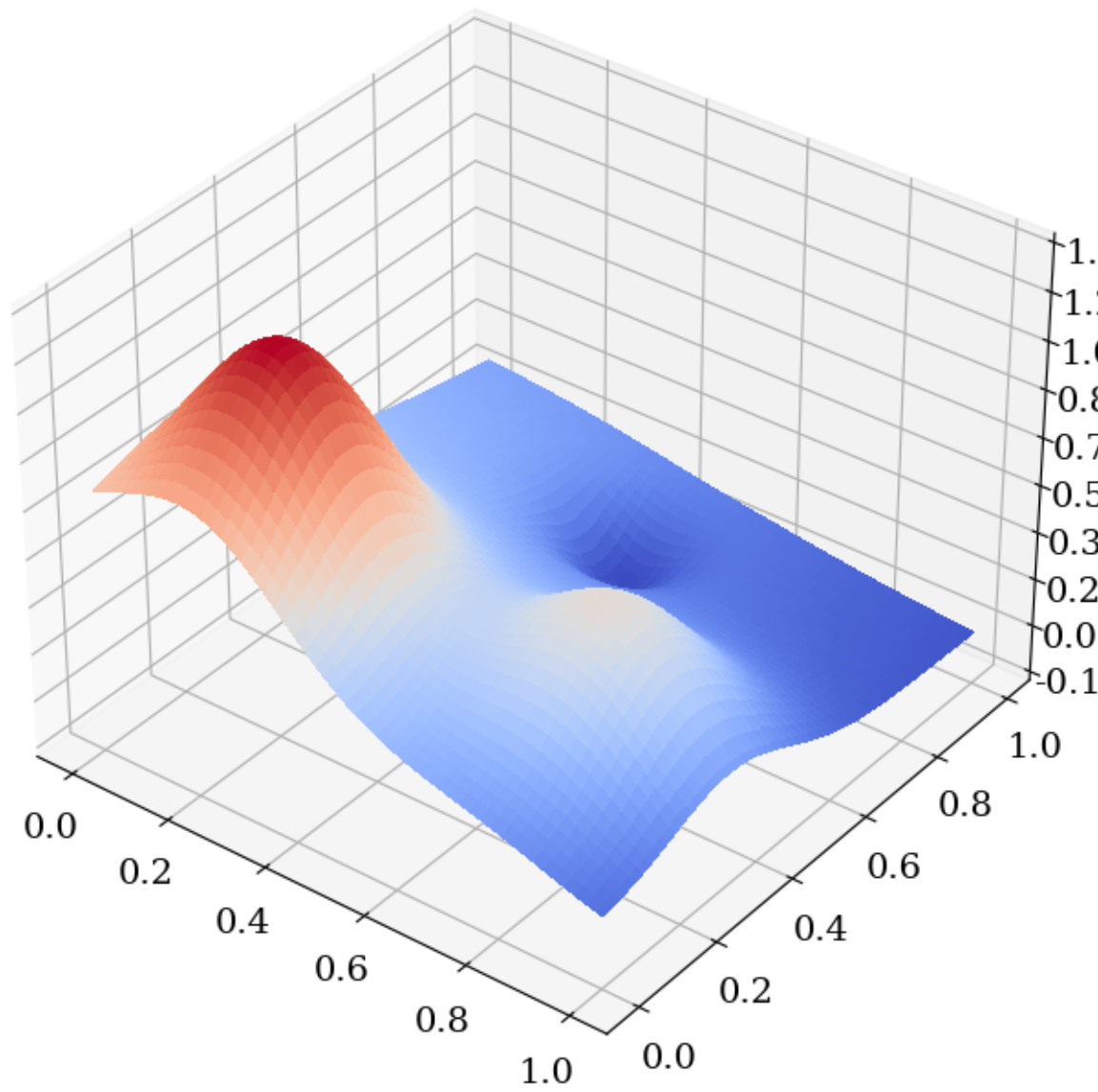
mse for ols on unscaled data:	0.010349396022903145
mse for ols on scaled data:	0.010349396024145656
mse for ridge on unscaled data:	0.02106077418650843
mse for ridge on scaled data:	0.01782525371566323

first x_{unscaled} and x_{scaled} is not that different, the original data was close to zero-centered and not that spread out, which means that initially by just looking at the data scaling is not that necessary. when we add the polynomial terms we can now see that some of the entries of x_{unscaled} get really small as an example $0.1^5 = 0.00001$ this makes the columns of x_{unscaled} live in their own order of magnitude and scaling should be considered to bring them back to the same order of magnitude. the act of not scaling results in β spanning from -50 to 48 while scaling gives a smaller span from -10 to 13 . now this alone may not justify why we should scale this data set, as scaled and unscaled ols yields the same mse. however when doing ridge regression the cost function is directly dependent on the magnitude of β_i . now with each β_i varying alot, some are getting more penalized than others. as we can see the mse for unscaled data is much higher than for scaled data in the ridge case. this leads us to conclude that we should scale the data, making it easier to tweak λ and giving us nicer numbers to work wi

4. Results and Discussion

as we increase the order of the polynomial fit we see a corresponding decrease in mse and increase in r^2 .

True function



we see that ols remains constant since it is not a function of λ . for the mse from the training set we see that the mse will increase for larger values of λ for ridge regression. this is expected since the ols will give the best approximation for the data it has been trained on (compared to ridge), while ridge punishes the weights from becoming too large and therefore gives a not so tight fit. this can explain why ridge does better than ols for some values of λ . as stated before the ols will try to fit the model to the best of its ability to the training data, this includes the noise which might not generalize to the test set, hence giving ridge a greater score. the term for this is called *****overfitting*****. and balancing between overfitting and underfitting is called the *****bias variance tradeoff*****.

4.1 confidence interval

the assumption we have made is that there exists a continuous function $f(x)$ and a normal distributed error $\epsilon \sim N(0, \sigma^2)$ which describes our data $y = f(x) + \epsilon$ we then approximate this function $f(x)$ with our model \tilde{y} from the solution of the linear regression equations (ordinary least squares ols), that is our function f is approximated by \tilde{y} where we minimized $(y - \tilde{y})^2$, with $\tilde{y} = x^T \beta$. the matrix x is the so-called design or feature matrix. $y_i \sim N(x_i^T \beta, \sigma^2)$, that is y follows a normal distribution with mean value $x^T \beta$ and variance σ^2 . we can use this when we define a so-called confidence interval for the parameters β . a given parameter β_j is given by the diagonal matrix element of the above matrix. ??

5. bias & variance

$$\begin{aligned} \text{var}(\tilde{y}) &= E[(\tilde{y} - E[\tilde{y}])^2] = E[\tilde{y}^2] - E[\tilde{y}]^2 \\ E[\tilde{y}^2] &= E[\tilde{y}]^2 + \text{var}(\tilde{y}) \end{aligned}$$

$$\begin{aligned} E[y^2] &= E[(f + \epsilon)^2] = E[f^2 + 2f\epsilon + \epsilon^2] \\ &= E[f^2] + 2E[f\epsilon] + E[\epsilon^2] \\ &= E[f^2] + 2E[f]E[\epsilon] + E[\epsilon^2] \\ &= E[f^2] + \sigma^2 \end{aligned}$$

$$\begin{aligned} E[y\tilde{y}] &= E[f\tilde{y} + \epsilon\tilde{y}] \\ &= E[f\tilde{y}] + E[\epsilon\tilde{y}] \\ &= E[f\tilde{y}] + E[\epsilon]E[\tilde{y}] \\ &= E[f\tilde{y}] \end{aligned}$$

$$\begin{aligned}
 [(\mathbf{y} - \tilde{\mathbf{y}})^2] &= [\mathbf{y}^2] - 2[\mathbf{y}\tilde{\mathbf{y}}] + [\tilde{\mathbf{y}}^2] \\
 &= \mathbf{f}^2 + \sigma^2 - 2\mathbf{f}[\tilde{\mathbf{y}}] + [\tilde{\mathbf{y}}^2] \\
 &= \mathbf{f}^2 + \sigma^2 - 2\mathbf{f}[\tilde{\mathbf{y}}] + [\tilde{\mathbf{y}}]^2 + \text{var}(\tilde{\mathbf{y}}) \\
 &= (\mathbf{f} - [\tilde{\mathbf{y}}])^2 + \text{var}(\tilde{\mathbf{y}}) + \sigma^2
 \end{aligned}$$

$$\begin{aligned}
 \text{bias}[\tilde{y}] &= [(\mathbf{y} - [\tilde{\mathbf{y}}])^2] = [\mathbf{y}^2] - 2[\mathbf{y}][\tilde{\mathbf{y}}] + [\tilde{\mathbf{y}}^2] \\
 &= \mathbf{f}^2 + \sigma^2 - 2\mathbf{f}[\tilde{\mathbf{y}}] + [\tilde{\mathbf{y}}]^2 \\
 &= (\mathbf{f} - [\tilde{\mathbf{y}}])^2 + \sigma^2
 \end{aligned}$$

to find $[\tilde{\mathbf{y}}]$ we can use bootstrap to get different samples for $\tilde{\mathbf{y}}$ and then take the mean of that distribution. the term *variance* refers to how spread out our observations are. we can for our case think of the observations \tilde{y}_i as either individual predictions, or the mean of predictions from one test set.

in a sense the bias resembles the mathematical definition for variance, we can see that the bias term is a distance measure of \mathbf{y} from the expected value of $\tilde{\mathbf{y}}$. if we take the individual observations approach this can be thought of as a high bias will then result in a large band around $\tilde{\mathbf{y}}$ in which y_i will exist. the variance term is a measure of how much the $\tilde{\mathbf{y}}$ varies around its own mean. in other terms a high variance model will experience large variance in the predicted values $\tilde{\mathbf{y}}$ from one test set to another. or as a result of this a large variance in score if you will. now these two terms are in a sense opposites, it is likely that a model with high bias will have low variance and vice versa. this is something we as designers of the model get to tune, if we value a lower bias more than we value a low variance or vice versa, we can choose a model accordingly

Appendix

appendix

Derivation of The Optimal Parameters β

OLS

The expression for the standard Mean Squared Error (MSE) which we used to define our cost function and the equations for the ordinary least squares (OLS) method, was given by the optimization problem

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \left\{ (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \right\}.$$

can also be written as

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2 = \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2,$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2$$

$$\hat{\beta}_{\text{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y},$$

Ridge

We know that

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 = \frac{2}{n} \mathbf{X}^T \mathbf{X} \beta - \frac{2}{n} \mathbf{X}^T \mathbf{y}$$

The minimization of ridge addition alone is

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \lambda \|\beta\|_2^2 = \frac{2}{n} \lambda \beta$$

adding these two we get

$$\frac{\partial \left[\frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_2^2 \right]}{\partial \beta} = 0 = \frac{2}{n} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}) \beta - \frac{2}{n} \mathbf{X}^T \mathbf{y} \implies \beta = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_2^2$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2 = \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2,$$

$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_2^2$$

$$\hat{\beta}_{\text{Ridge}} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y},$$

SVD

Use the singular value decomposition of an $n \times p$ matrix \mathbf{X} (our design matrix)

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

where \mathbf{U} and \mathbf{V} are orthogonal matrices of dimensions $n \times n$ and $p \times p$, respectively, and $\mathbf{\Sigma}$ is an $n \times p$ matrix which contains the singular values only. This material was discussed during the lectures of week 35.

Show that you can write the OLS solutions in terms of the eigenvectors (the columns) of the orthogonal matrix \mathbf{U} as

$$\tilde{\mathbf{y}}_{\text{OLS}} = \mathbf{X}\beta = \sum_{j=0}^{p-1} \mathbf{u}_j \mathbf{u}_j^T \mathbf{y}.$$

$$\mathbf{X}^T \mathbf{X} = \mathbf{V} \mathbf{\Sigma}^T \mathbf{U}^T \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T = \mathbf{V} \mathbf{\Sigma}^T \mathbf{\Sigma} \mathbf{V}^T = \mathbf{V} \mathbf{\Sigma}^2 \mathbf{V}^T$$

$$\tilde{\mathbf{y}}_{\text{OLS}} = \mathbf{X}\beta = \mathbf{X} \left(\mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T \left(\mathbf{V} \mathbf{\Sigma}^2 \mathbf{V}^T \right)^{-1} \mathbf{V} \mathbf{\Sigma}^T \mathbf{U}^T \mathbf{y} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T \mathbf{V}^{T-1} \mathbf{\Sigma}^{2-1} \mathbf{V}^{-1} \mathbf{V} \mathbf{\Sigma}^T \mathbf{U}^T \mathbf{y}$$

using the orthogonality of \mathbf{V} and \mathbf{U} we get. Multiplying with $\mathbf{\Sigma}$ removes columns from \mathbf{U} with eigenvalues equal to zero.

$$\tilde{\mathbf{y}}_{\text{OLS}} = \mathbf{U} \mathbf{U}^T \mathbf{y} = \sum_{j=0}^{p-1} \mathbf{u}_j \mathbf{u}_j^T \mathbf{y}$$

Math Behind the Confidence Interval section

We can assume that y follows some function f with some noise ϵ

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

$$\tilde{\mathbf{y}} = \mathbf{X}\beta.$$

$$\mathbb{E}(y_i) = \sum_j x_{ij} \beta_j = \mathbf{X}_{i,*} \beta$$

$$\text{Var}(y_i) = \sigma^2$$

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

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

$$\mathbb{E}[\mathbf{y}] = \mathbb{E}[f(\mathbf{x}) + \epsilon] = \mathbb{E}[f(\mathbf{x})] + \mathbb{E}[\epsilon_i]$$

The expected value of ϵ_i is 0, $f(x)$ is a non-stochastic variable and is approximated by $\mathbf{X}\beta$

$$\mathbb{E}[y_i] = \mathbf{X}_{i,*}\beta$$

The variance is defined as

$$Var(y_i) = \mathbb{E}[(y_i - \mathbb{E}[y_i])^2] = \mathbb{E}[y_i^2 - 2y_i\mathbb{E}[y_i] + \mathbb{E}[y_i]^2] = \mathbb{E}[y_i^2] - \mathbb{E}[y_i]^2$$

$$Var(y_i) = \mathbb{E}[(\mathbf{X}_{i,*}\beta)^2 + 2\epsilon\mathbf{X}_{i,*}\beta + \epsilon^2] - (\mathbf{X}_{i,*}\beta)^2$$

$$Var(y_i) = (\mathbf{X}_{i,*}\beta)^2 + 2\mathbb{E}[\epsilon]\mathbf{X}_{i,*}\beta + \mathbb{E}[\epsilon^2] - (\mathbf{X}_{i,*}\beta)^2$$

$$Var(y_i) = \mathbb{E}[\epsilon^2] = \sigma^2$$

for the expected value of β we can insert the definition of β from earlier

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

$$\begin{aligned} Var(\hat{\beta}) &= \mathbb{E}\{[\beta - \mathbb{E}(\beta)][\beta - \mathbb{E}(\beta)]^T\} \\ &= \mathbb{E}\{[(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - \beta][(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - \beta]^T\} \\ &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbb{E}\{\mathbf{y} \mathbf{y}^T\} \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} - \beta \beta^T \\ &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \{\mathbf{X} \beta \beta^T \mathbf{X}^T + \sigma^2 \mathbf{I}\} \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} - \beta \beta^T \\ &= \beta \beta^T + \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1} - \beta \beta^T = \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}, \end{aligned}$$

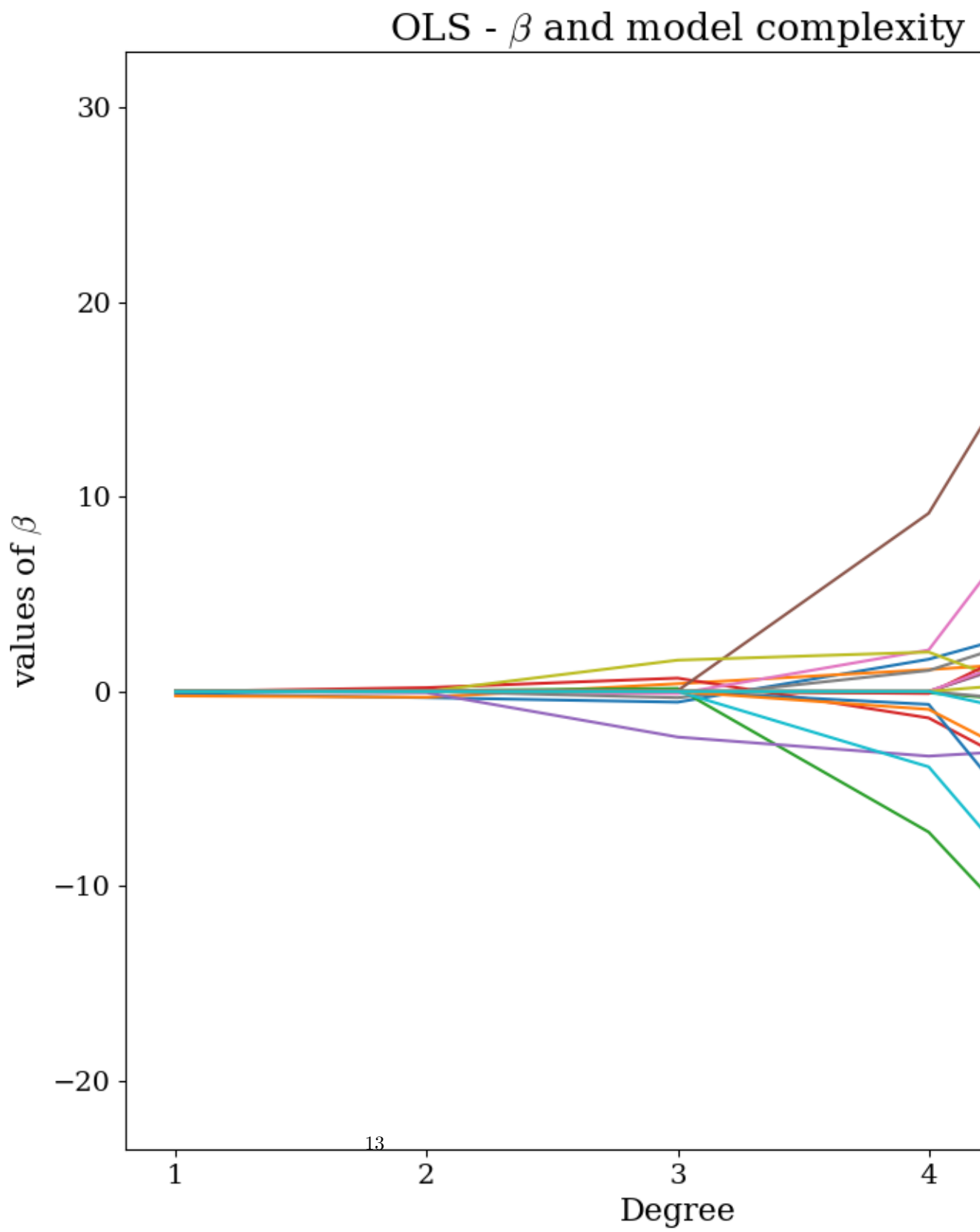
ridge

$$\mathbb{E}[\hat{\beta}^{\text{Ridge}}] = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta.$$

$$Var[\hat{\beta}^{\text{Ridge}}] = \sigma^2 [\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}]^{-1} \mathbf{X}^T \mathbf{X} \{[\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}]^{-1}\}^T,$$

$$\mathbb{E}[\hat{\beta}^{\text{Ridge}}] = \mathbb{E}\left[(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbf{y}\right] = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbb{E}[\mathbf{Y}] = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta$$

$$\begin{aligned} Var(\hat{\beta}^{\text{Ridge}}) &= \mathbb{E}\{[\beta - \mathbb{E}(\beta)][\beta - \mathbb{E}(\beta)]^T\} \\ &= \mathbb{E}\left\{\left[(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbf{y} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta\right] \left[(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbf{y} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta\right]^T\right\} \\ &= \mathbb{E}\left\{(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbf{y} \mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta \beta^T (\mathbf{X}^T \mathbf{X}) (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1}\right\} \\ &= (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T \mathbb{E}\{\mathbf{y} \mathbf{y}^T\} \mathbf{X} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta \beta^T (\mathbf{X}^T \mathbf{X}) (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \\ &= (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \mathbf{X}^T (\mathbf{X} \beta \beta^T \mathbf{X}^T + \sigma^2 \mathbf{I}) \mathbf{X} (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} - (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} (\mathbf{X}^T \mathbf{X}) \beta \beta^T (\mathbf{X}^T \mathbf{X}) (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_{pp})^{-1} \end{aligned}$$



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