

Machine Learning for Physicists - First Assignment

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1 Theory Part

1) You are training a ridge regression model with zero regularization. How does the training loss behave for $n < d$? Explain your answer.

If we are training ridge regression model with $\lambda = 0$, we are in the domain of linear regression, where $\hat{w} = (X^T X)^{-1} X^T y$. In this case there is only a general solution for \hat{w} if $X^T X$ exists, ie, if $n \geq d$. Thinking in terms of rank (or non trivial eigenvalues), they are a increasing function for $n < d$. For this reasons, if we plot the train error (loss) we would see that it would decrease until $\alpha = \frac{n}{d} = 1$

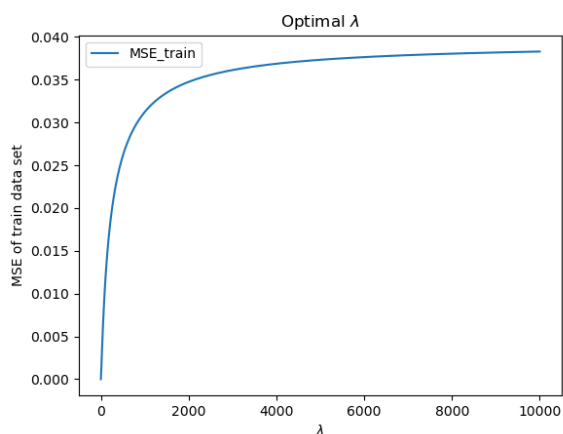
2) Let $X \in \mathbb{R}^{n \times d}$ be the training data matrix and $y \in \mathbb{R}^n$ be the labels. Under what condition on X and y is ridge regression with zero regularization able to exactly fit the training points?

As it was explained on 1), there is only a general solution for \hat{w} , in the zero regularization regime, if there are at least as many parameters as equations (ie $n \geq d$) provided they are linearly independent, this means that the matrix $X^T X$ is full rank, hence invertible. Furthermore, the augmented matrix $[X|y]$ has to be the same rank as X , in order to avoid fits that the same X has two different y 's.

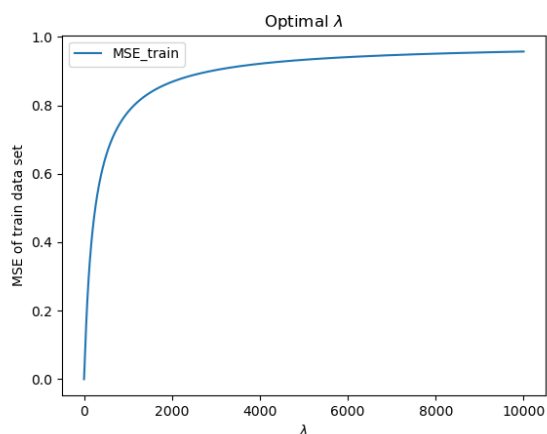
3) You train ridge regression several times with fixed n and increasing regularization λ . How do you expect the training error to depend on λ ? Express the training error at $\lambda = \infty$ in terms of the labels of the training set $y = (y_1, y_2, \dots, y_n)$. Explain your reasoning.

Regarding the **training** error, as $\lambda \rightarrow \infty$, tending to a horizontal asymptote to the variance ($= \sigma^2 = \frac{\sum (y - \bar{y})^2}{n}$) of the training set y . As the regularization strength approaches high values, the training does not depend on the input, hence the the output tends to a mean value, this means that the mean squared error is actually the variance!

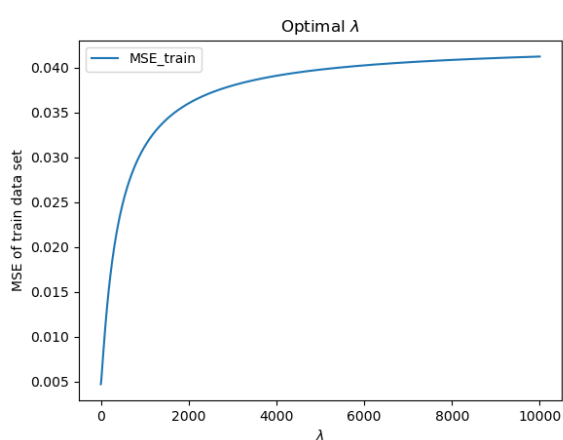
Bonus for 3: I slightly modified the code done in main.py and created main2.py (committed in Github) in order to produced this plots who illustrate the aforementioned behaviour.



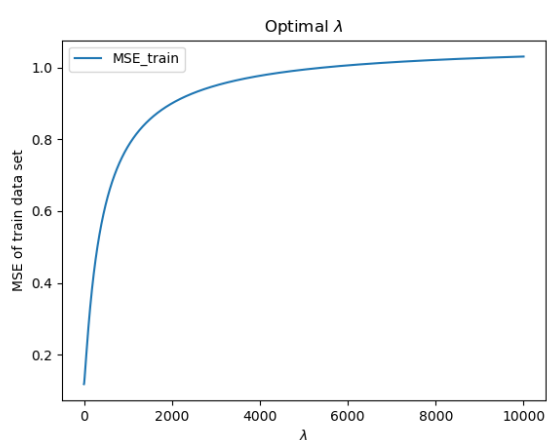
(a) $\sigma^2 = (0.2)^2 = 0.04$, $n=80$.



(b) $\sigma^2 = (1.0)^2 = 1.0$, $n=80$.



(c) $\sigma^2 = (0.2)^2 = 0.04$, $n=150$.



(d) $\sigma^2 = (1.0)^2 = 1.0$, $n=150$.

Figure 1: Optimal λ for Ridge Regression, considering training data set.

2 Acknowledgments

I would like to thank Francisco Simões and Arianna Alonso Bizzi for having very useful debates with me regarding this assignment and the course, in general.