# Machine Learning 1 Prof. Schmidt-Thieme, Randolf Scholz

**Deadline: Th. November 28<sup>th</sup> , 13:00** Drop your printed or legible handwritten submissions into the boxes at Samelsonplatz. Alternatively upload a .pdf file via LearnWeb. (e.g. exported Jupyter notebook)

## **1.** $L^1$ regularization

**A.** [7p] Fit a linear regression model (including bias) with  $L^1$  regularization to the dataset from Table 1 by performing 2 iterations of coordinate descent (update each parameter twice). Use  $\beta^{(0)} = 0$  and  $\lambda = 1$ .

$x_1$	$x_2$	y
1	1	1.4
1	-1	1.6
-1	0	0.5
-1	-1	0.6

#### Table 1

**B.** [3p] The elastic-net model is a linear model with a mix of  $L^1$  and  $L^2$  regularization.

$$L^{\text{enet}}(\beta) = \frac{1}{2N} \|y - X\beta\|_2^2 + \lambda \left(\alpha \|\beta\|_1 + (1-\alpha)\frac{1}{2}\|\beta\|_2^2\right)$$

Note that if  $\alpha = 1$ , elastic net is the same as LASSO and for  $\alpha = 0$  it is the same as RIDGE regression. For  $\alpha \in (0, 1)$  it is something in between. We trained an Elastic Net model 4 times on a regression task, each time choosing a different trade-off  $\alpha \in \{0, 0.25, 0.5, 1\}$ . The resulting regularization paths, as well as the number of non-zero coefficients at different total regularization strength  $\lambda$  is shown in Figure 1. Explain which figure corresponds to which choice of  $\alpha$ .

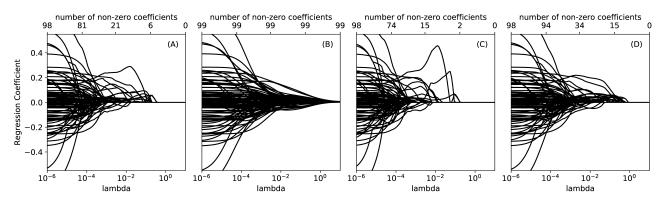


Figure 1: Regularization paths of the 4 models

#### 2. Variable Selection – Programming

#### (10 points)

Use the following code to load the famous "Boston Housing" dataset (alternatively data-files will be uploaded to the LearnWeb as well)

```
import numpy as np
from sklearn.datasets import load_boston
np.random.seed(2019)
dataset = load_boston()
Xdata = dataset['data']
Ydata = dataset['target']
N, M = Xdata.shape
ridx = np.random.permutation(N)
split = int(0.8*N)
Xtrain = Xdata[ridx[:split]]
Ytrain = Ydata[ridx[:split]]
Xvalid = Xdata[ridx[split:]]
Yvalid = Ydata[ridx[split:]]
```

#### 1/2

## (10 points)

**A.** [7p] Implement both forward search and backward search and apply them to the provided data using a linear regression model. At the start of each outer loop, report the currently selected variables V as well as the loss on the training and validation set.

**B.** [3p] Repeat the experiment 100 times using random train/valid splits (you'll need to remove np.random. seed(2019)). Whats the average improvement of forward/backward search compared to fitting with the whole dataset? How often does each of the 13 variables end up in the final selection?

## **3**<sup>\*</sup> Parameter Variance – OLS vs Ridge Regression (5 points)

For the following problem, we assume that the ground truth is is a linear function  $y(x) = x^{\mathsf{T}}\hat{\beta} + \epsilon$  with  $\epsilon \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ and we are given a **finite** data sample (X, Y). From the lecture we know that the ordinary least squares (OLS) estimator  $\hat{\beta}^{\text{OLS}} = (X^{\mathsf{T}}X)^{-1}X^{\mathsf{T}}Y$  satisfies:

- $\mathbb{E}[\hat{\beta}^{\text{OLS}}] = \hat{\beta}$
- $\mathbb{V}[\hat{\beta}^{\text{OLS}}] = (X^{\mathsf{T}}X)^{-1}\sigma^2$

In particular, we note that the OLS estimator is unbiased!

**A.** [2p] Show that the RIDGE estimator  $\hat{\beta}^{\text{RIDGE}} = (X^{\mathsf{T}}X + \lambda \mathbb{I})^{-1}X^{\mathsf{T}}y$  satisfies

- $\mathbb{E}[\hat{\beta}^{\text{RIDGE}}] = (X^{\mathsf{T}}X + \lambda \mathbb{I})^{-1}X^{\mathsf{T}}X\hat{\beta}$
- $\mathbb{V}[\hat{\beta}^{\mathrm{RIDGE}}] = (X^{\mathsf{T}}X + \lambda \mathbb{I})^{-1}X^{\mathsf{T}}X(X^{\mathsf{T}}X + \lambda \mathbb{I})^{-1}\sigma^{2}$

In particular, we note that the RIDGE estimator is biased!

**B.** [3p] Given two covariance matrices  $\Sigma_A$  and  $\Sigma_B$ , we say that  $\Sigma_A$  is strictly greater than  $\Sigma_B$  (in symbols  $\Sigma_A > \Sigma_B$ ) iff  $\Sigma_A - \Sigma_B$  is positive definite. (This is the so called Löwner order). Show that  $\hat{\beta}^{\text{OLS}}$  has strictly greater variance than  $\hat{\beta}^{\text{RIDGE}}$ 

**Hint:** Note that  $(X^{\mathsf{T}}X)^{-1}$  and  $X^{\mathsf{T}}X + \lambda \mathbb{I}$  commute. More generally, if p and q are polynomial functions, then p(A)q(A) = q(A)p(A) and likewise  $q(A)^{-1}p(a) = p(A)q(A)^{-1}$  for any square matrix A.