# Regularization in Linear Regression

## Applied Machine Learning for Educational Data Science

true

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# Regularization

Regularization is a general strategy to incorporate additional penalty terms into the model fitting process and used not just for regression but a variety of other types of models. The idea behind the regularization is to constrain the size of regression coefficients with the purpose of reducing their sampling variation and, hence, reducing the variance of model predictions. These constrains are typically incorporated into the loss function to be optimized. There are two commonly used regularization strategy: **ridge penalty** and **lasso penalty**. In addition, there is also **elastic net**, a mixture of these two strategies.

### Ridge Regression

## Ridge Penalty

Remember that we formulated the loss function for the linear regression as the sum of squared residuals across all observations. For ridge regression, we add a penalty term to this loss function and this penalty term is a function of all the regression coefficients in the model. Assuming that there are P regression coefficients in the model, the penalty term for the ridge regression would be

$$\lambda \sum_{i=1}^{P} \beta_p^2,$$

where  $\lambda$  is a parameter that penalizes the regression coefficients when they get larger. Therefore, when we fit a regression model with ridge penalty, the loss function to minimize becomes

$$Loss = \sum_{i=1}^{N} \epsilon_{(i)}^2 + \lambda \sum_{i=1}^{P} \beta_p^2,$$

$$Loss = SSR + \lambda \sum_{i=1}^{P} \beta_p^2.$$

Let's consider the same example from the previous class. Suppose we fit a simple linear regression model such that the readability score is the outcome (Y) and average word length is the predictor (X). Our regression model is

$$Y = \beta_0 + \beta_1 X + \epsilon,$$

and let's assume the set of coefficients are  $\{\beta_0, \beta_1\} = \{7.5, -2\}$ , so my model is

$$Y = 7.5 - 2X + \epsilon.$$

Then, the value of the loss function when  $\lambda = 0.2$  would be equal to 27.433.

```
readability_sub <- read.csv('https://raw.githubusercontent.com/uo-datasci-specialization/c4-ml-fall-202
d <- readability_sub[,c('mean.wl','target')]
b0 = 7.5
b1 = -2
d$predicted <- b0 + b1*d$mean.wl
d$error <- d$target - d$predicted
d</pre>
```

```
mean.wl
                 target predicted
                                         error
  4.603659 -2.58590836 -1.7073171 -0.87859129
  3.830688 0.45993224 -0.1613757
                                    0.62130790
 4.180851 -1.07470758 -0.8617021 -0.21300545
 4.015544 -1.81700402 -0.5310881 -1.28591594
  4.686047 -1.81491744 -1.8720930
                                   0.05717559
6
 4.211340 -0.94968236 -0.9226804 -0.02700194
 4.025000 -0.12103065 -0.5500000 0.42896935
8 4.443182 -2.82200582 -1.3863636 -1.43564218
9 4.089385 -0.74845172 -0.6787709 -0.06968077
10 4.156757 0.73948755 -0.8135135
                                    1.55300107
11 4.463277 -0.96218937 -1.4265537
                                    0.46436430
12 5.478261 -2.21514888 -3.4565217
                                    1.24137286
13 4.770492 -1.21845136 -2.0409836
                                    0.82253224
14 4.568966 -1.89544351 -1.6379310 -0.25751247
15 4.735751 -0.04101056 -1.9715026
16 4.372340 -1.83716516 -1.2446809 -0.59248431
17 4.103448 -0.18818586 -0.7068966 0.51871069
18 4.042857 -0.81739314 -0.5857143 -0.23167886
19 4.202703 -1.86307557 -0.9054054 -0.95767016
20 3.853535 -0.41630158 -0.2070707 -0.20923088
```

```
lambda = 0.2
loss <- sum((d\( \frac{b0^2}{2} + \frac{b1^2}{2} \)
loss</pre>
```

#### [1] 27.43364

Notice that when  $\lambda$  is equal to 0, the loss function is identical to SSR; therefore, it becomes a linear regression with no regularization. As the value of  $\lambda$  increases, the degree of penalty linearly increases. Technically, the  $\lambda$  can take any positive value between 0 and  $\infty$ .

As we did in the previous lecture, imagine that we computed the loss function with the ridge penalty term for every possible combination of the intercept ( $\beta_0$ ) and the slope ( $\beta_1$ ). Let's say the plausible range for the intercept is from -10 to 10 and the plausible range for the slope is from -2 to 2. Now, we also have to think different values of  $\lambda$  because the surface we try to minimize is dependent on the value  $\lambda$  and different values of  $\lambda$  yield different estimates of  $\beta_0$  and and  $\beta_1$ .

You can try a number of different values for  $\lambda$  using the shiny app at this link and explore how the loss function value and coefficient estimates change for different values of  $\lambda$ . Note that when  $\lambda$  is equal to zero, it should be equivalent of what we have seen in the earlier lecture. Try values of 1, 5, 10, 50, and 100.

Below is also a demonstration of what happens to loss function and the regression coefficients for increasing levels of ridge penalty  $(\lambda)$ .

#### **Model Estimation**

Matrix Solution The matrix solution we learned before for regression without regularization can also be applied to estimate the coefficients from ridge regression given the  $\lambda$  value. Given that

- Y is an N x 1 column vector of observed values for the outcome variable,
- X is an N x (P+1) \*\*design matrix\* for the set of predictor variables including an intercept term,
- $\beta$  is an (P+1) x 1 column vector of regression coefficients,
- I is a (P+1) x (P+1) identity matrix,
- and  $\lambda$  is positive real-valued number,

the set of ridge regression coefficients can be estimated using the following matrix operation.

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathbf{T}}\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{Y}$$

Now, suppose we want to predict the readability score by using the two predictors, the average word length  $(X_1)$  and number of sentences  $(X_2)$ . Our model will be

$$Y_{(i)} = \beta_0 + \beta_1 X_{1(i)} + \beta_2 X_{2(i)} + \epsilon_{(i)}.$$

If we estimate the ridge regression coefficients by using  $\lambda = .5$ , the estimates would be  $\{\beta_0, \beta_1, \beta_2\} = \{0.277, -.593, 0.097\}$ .

```
Y <- as.matrix(readability_sub$target)
X <- as.matrix(cbind(1,readability_sub$mean.wl,readability_sub$sents))
lambda <- 0.5</pre>
```

```
beta <- solve(t(X)%*%X + lambda*diag(ncol(X)))%*%t(X)%*%Y
beta</pre>
```

```
[,1]
[1,] 0.27693153
[2,] -0.59327091
[3,] 0.09692781
```

If we change the value of  $\lambda$  to 2, then we will get a different set of estimates for the regression coefficients.

```
Y <- as.matrix(readability_sub$target)
X <- as.matrix(cbind(1,readability_sub$mean.wl,readability_sub$sents))

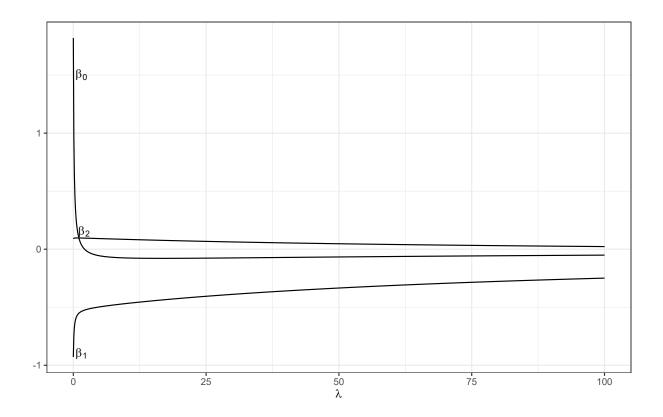
lambda <- 2
beta <- solve(t(X)%*%X + lambda*diag(ncol(X)))%*%t(X)%*%Y

beta
```

```
[,1]
[1,] 0.006012867
[2,] -0.526374942
[3,] 0.095845692
```

We can manipulate the value of  $\lambda$  from 0 to 100 with increments of .1 and calculate the regression coefficients for every possible value of  $\lambda$ . Note the regression coefficients will shrink towards zero, but will never be exactly equal to zero in ridge regression.

```
Y <- as.matrix(readability_sub$target)</pre>
X <- as.matrix(cbind(1,readability_sub$mean.wl,readability_sub$sents))</pre>
lambda \leftarrow seq(0,100,.1)
         <- data.frame(matrix(nrow=length(lambda),ncol=4))</pre>
beta[,1] <- lambda
for(i in 1:length(lambda)){
  beta[i,2:4] \leftarrow t(solve(t(X))%*X + lambda[i]*diag(ncol(X)))%*Xt(X)%*XY)
}
ggplot(data = beta) +
  geom line(aes(x=X1,y=X2))+
  geom_line(aes(x=X1,y=X3))+
  geom_line(aes(x=X1,y=X4))+
  xlab(expression(lambda))+
  ylab('')+
  theme bw()+
  annotate(geom='text',x=1.5,y=1.5,label=expression(beta[0]))+
  annotate(geom='text',x=2,y=.15,label=expression(beta[2]))+
  annotate(geom='text',x=1.5,y=-.9,label=expression(beta[1]))
```



Standardized Variables We haven't considered a very important issue for the model estimation. This issue is not necessarily important if you have only one predictor. However, it is critical whenever you have more than one predictor. Different variables have different scales and therefore the magnitude of the regression coefficients for different variables will be dependent on the scales of the variables. A regression coefficient for a predictor with a range from 0 to 100 will be very different than a regression coefficient for a predictor with a range from 0 to 1. Therefore, if we work with the unstandardized variables, ridge penalty will be amplified for the coefficients of those variables with a larger range of values.

Therefore, it is critical that we standardize variables before we use ridge regression. Let's do the example in the previous section, but we now first standardize the variables in our model.

```
Y <- as.matrix(readability_sub$target)

X <- as.matrix(cbind(readability_sub$mean.wl,readability_sub$sents))

# Standardize Y

Y <- scale(Y)

Y</pre>
```

[,1]
[1,] -1.49010043
[2,] 1.58384679
[3,] 0.03504552
[4,] -0.71410074
[5,] -0.71199490
[6,] 0.16122446

```
[7,] 0.99752285
 [8,] -1.72837656
 [9,] 0.36431202
[10,] 1.86598181
[11,] 0.14860203
[12,] -1.11591963
[13,] -0.11002472
[14,] -0.79326406
[15,] 1.07828135
[16,] -0.73444792
[17,] 0.92974794
[18,] 0.29473442
[19,] -0.76059743
[20,] 0.69952720
attr(,"scaled:center")
[1] -1.109433
attr(, "scaled:scale")
[1] 0.9908565
# Standardized X
  X <- scale(X)</pre>
 X
            [,1]
                        [,2]
 [1,] 0.6695829 -0.7833675
 [2,] -1.3062112 1.6269940
```

```
[3,] -0.4111573 0.7231084
 [4,] -0.8336993 -0.7833675
 [5,] 0.8801752 -0.9340151
 [6,] -0.3332238  0.8737560
 [7,] -0.8095289 -0.3314247
 [8,] 0.2593876 -1.2353102
 [9,] -0.6449529 -0.4820723
[10,] -0.4727448 2.3802319
[11,] 0.3107526 0.4218133
[12,] 2.9051581 -0.3314247
[13,] 1.0960262 -0.3314247
[14,] 0.5809039 -0.6327199
[15,]
      1.0072258 1.0244036
[16,] 0.0783096
                  0.4218133
[17,] -0.6090069 -0.9340151
[18,] -0.7638842 -0.9340151
[19,] -0.3553022 -0.7833675
[20,] -1.2478105 1.0244036
attr(, "scaled:center")
[1] 4.341704 12.200000
attr(, "scaled: scale")
[1] 0.3912203 6.6380086
```

When we standardize the variables, the mean all variables become zero. So, the intercept estimate for any regression model with standardized variables is guaranteed to be zero. Note that our design matrix doesn't have a column of ones anymore because it is unnecessary (it would be a column of zeros if we had).

First, let's check the coefficients of the regression model with standardized variables when there is no ridge penalty.

```
lambda <- 0
beta.s <- solve(t(X)%*%X + lambda*diag(ncol(X)))%*%t(X)%*%Y
beta.s</pre>
```

```
[,1]
[1,] -0.3666326
[2,] 0.6049359
```

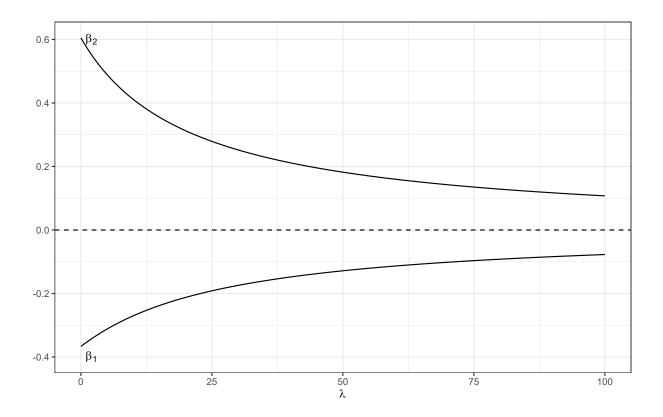
Now, let's increase the ridge penalty to 0.5.

```
lambda <- 0.5
beta.s <- solve(t(X)%*%X + lambda*diag(ncol(X)))%*%t(X)%*%Y
beta.s</pre>
```

```
[,1]
[1,] -0.3604763
[2,] 0.5908420
```

Below, we can manipulate the value of  $\lambda$  from 0 to 100 with increments of .1 as we did before and calculate the standardized regression coefficients for every possible value of  $\lambda$ .

```
Y <- as.matrix(readability_sub$target)</pre>
X <- as.matrix(cbind(readability_sub$mean.wl,readability_sub$sents))</pre>
Y <- scale(Y)
X <- scale(X)</pre>
lambda <- seq(0,100,.1)
                                       <- data.frame(matrix(nrow=length(lambda),ncol=3))</pre>
beta
beta[,1] <- lambda
for(i in 1:length(lambda)){
         beta[i,2:3] \leftarrow t(solve(t(X)) * X + lambda[i] * diag(ncol(X))) * X + (X) * X + lambda[i] * diag(ncol(X))) * X + (X) 
ggplot(data = beta) +
         geom_line(aes(x=X1,y=X2))+
         geom_line(aes(x=X1,y=X3))+
         xlab(expression(lambda))+
         ylab('')+
         theme bw()+
         geom_hline(yintercept=0,lty=2) +
         annotate(geom='text',x=2,y=.60,label=expression(beta[2]))+
         annotate(geom='text',x=2,y=-.4,label=expression(beta[1]))
```



glmnet() function Similar to lm function, we can use glmnet() function from the glmnet package to run a regression model with ridge penalty. There are many arguments of the glmnet() function. For now, the arguments we need to know are

- x: an N x P input matrix, where N is the number of observations and P is the number of predictor
- y: an N x 1 input matrix for the outcome variable
- alpha: a mixing constant for lasso and ridge penalty. When it is zero, the ridge regression is conducted
- lambda: penalty term
- intercept: set FALSE to avoid intercept for standardized variables

If you want to fit the linear regression without any regularization, you can specify alpha = 0 and lambda = 0.

```
intercept=FALSE)
coef(mod)
```

```
3 x 1 sparse Matrix of class "dgCMatrix" s0
(Intercept) .
V1 -0.3666327
V2 0.6049359
```

We can also increase the penalty term  $(\lambda)$ .

```
3 x 1 sparse Matrix of class "dgCMatrix"
s0
(Intercept) .
V1 -0.2720458
V2 0.4145987
```

#### NOTE

A careful eye should catch the fact that the coefficient estimates we obtained from glmnet() function for the two standardized variables (average word length and number of sentences) are different when the penalty term ( $\lambda$ ) is 0.5. When we apply the matrix solution above for the ridge regression, we obtained the estimates of -0.360 and 0.591 for the two predictors, respectively, at  $\lambda = 0.5$ . When we enter the same value in glmnet(), we obtained the estimates of -0.27 and 0.414. So, what is wrong? Where does this discrepancy come from?

In fact, there is nothing wrong. It appears that what lambda argument in glmnet indicates is  $\frac{\lambda}{N}$ . In most statistics textbook, the penalty term for the ridge regression is specified as

$$\lambda \sum_{i=1}^{P} \beta_p^2.$$

On the other hand, if we examine Equation 1-3 in this paper written by the developers of the glmnet package, we can see that the penalty term applied is equivalent of

$$\lambda N \sum_{i=1}^{P} \beta_p^2.$$

Therefore, if we want to get the identical results, then we should use  $\lambda = 0.5/20$ .

```
3 x 1 sparse Matrix of class "dgCMatrix" s0
(Intercept) .
V1 -0.3606303
V2 0.5911903
```

Note that these numbers are still slightly different. We can attribute this difference to numerical approximation glmnet is using when optimizing the loss function. glmnet doesn't use the closed form matrix solution for ridge regression. This is a good thing because there is not always a closed form solution for different types of regularization approaches (e.g., lasso). Therefore, the computational approximation in glmnet is very needed moving forward.

Tuning the Hyperparameter  $\lambda$  The  $\lambda$  parameter in ridge regression is called a hyperparameter. In the context of machine learning, the parameters in a model can be classified into two types: parameters and hyperparameters. The parameters of the model are typically estimated from data and not set by users. In the context of ridge regression, regression coefficients,  $\{\beta_0, \beta_1, ..., \beta_P\}$ , are parameters to be estimated from data. On the other hand, the hyperparameters are not estimable, most of the time due to the fact that there is no first order or second order derivatives for these hyperparameters. Therefore, they must be set by the users. In the context of ridge regression, penalty term,  $\{\lambda\}$ , is a hyperparameter.

The process of deciding what value to use for a hyperparameter is called **tuning**, and it is most of the time a trial-error process. The idea is simple. We try many different values of a hyperparameter and check how well the model performs based on a certain criteria (e.g., MAE, MSE, RMSE) using a k-fold cross validation. Then, we pick the value of a hyperparameter that provides the best performance.

#### Using Ridge Regression to Predict Readability Scores

In this section, we will apply ridge regression to predict the readability scores from all predictors in the dataset. We will use the caret package and use 10-fold cross validation to evaluate the model performance for different levels of penalty term  $(\lambda)$ .

```
# Load the packages
  require(caret)
  require(recipes)
 require(finalfit)
  require(glmnet)
# Import the dataset
  readability <- read.csv('https://raw.githubusercontent.com/uo-datasci-specialization/c4-ml-fall-2021/s
# Initial preparation (remove variables with large amount of missingness)
  require(finalfit)
 missing_ <- ff_glimpse(readability)$Continuous</pre>
 flag_na <- which(as.numeric(missing_$missing_percent) > 80)
 readability <- readability[,-flag_na]</pre>
# Set the random seed for reproducibility
  set.seed(10152021)
# Train/Test Split
           <- sample(1:nrow(readability), round(nrow(readability) * 0.9))</pre>
  read_tr <- readability[loc, ]</pre>
 read_te <- readability[-loc, ]</pre>
# Blueprint
  blueprint \leftarrow recipe(x = readability,
                      vars = colnames(readability),
                      roles = c(rep('predictor',990),'outcome')) %>%
    step_zv(all_numeric()) %>%
    step_nzv(all_numeric()) %>%
    step_impute_mean(all_numeric()) %>%
    step_normalize(all_numeric_predictors()) %>%
    step_corr(all_numeric(),threshold=0.9)
# Cross validation settings
  cv <- trainControl(method = "cv",</pre>
                     p = 10)
# Tune Grid
  # Here, we have to specify different values of lambda we want to try
  # This should be a dataframe with columns named are the same as
  # the tuning parameters available for the engine we are using
  # In order to get which parameters are available to tune for glmnet
  # run the following code
```

```
caret::getModelInfo()$glmnet$parameters
 # This indicates there are two hyperparameters available to tune for the glmnet
 # For ridge regression, we know that we will fix the value of alpha to 0
 # Let's assume that the lambda values we want to try are 1, 5, 10, and 100.
   # Remember how almnet multiplies the lambda by sample size (N)
   # In this case, the sample size is 2834
    # So, for instance a lambda value of 1 would be 2834
    \# You can try larger values and explore, but in this case a max value of 3
    \# for lambda would be more than enough. I don't think it will improve performance
   # beyond this value
   # Also, note that there are 100 values, and for every lambda value we will do
    # 10-fold cross validation, so it can take a very long time to search this
    # grid
 grid \leftarrow data.frame(alpha = 0, lambda = seq(0.01,3,.01))
 grid
# Train the model
 ridge <- caret::train(blueprint,</pre>
                                 = read_tr,
                        data
                                = "glmnet",
                        method
                        trControl = cv,
                        tuneGrid = grid)
    # This training took about 3 minutes in my computer
 ridge$results
 ridge$bestTune
 plot(ridge)
```

```
alpha lambda
                     RMSE Rsquared
                                          MAE
                                                  RMSESD RsquaredSD
                                                                         MAESD
1
           0.01 0.5750266 0.6963298 0.4593452 0.02221126 0.02504427 0.01591786
2
           0.02 0.5750266 0.6963298 0.4593452 0.02221126 0.02504427 0.01591786
3
           0.03 0.5750266 0.6963298 0.4593452 0.02221126 0.02504427 0.01591786
4
           0.04 0.5750266 0.6963298 0.4593452 0.02221126 0.02504427 0.01591786
5
           0.05 0.5750266 0.6963298 0.4593452 0.02221126 0.02504427 0.01591786
6
           0.06 0.5745666 0.6967386 0.4590050 0.02225662 0.02504704 0.01598661
7
           0.07 0.5712485 0.6996988 0.4565815 0.02230691 0.02459360 0.01604447
8
           0.08 0.5685228 0.7021324 0.4546089 0.02237512 0.02421407 0.01606915
9
           0.09 0.5662201 0.7041939 0.4529484 0.02244372 0.02389469 0.01613219
10
           0.10 0.5642541 0.7059545 0.4515073 0.02251416 0.02361760 0.01621680
11
          0.11 0.5625415 0.7074888 0.4502566 0.02260880 0.02338194 0.01633059
12
       0 0.12 0.5610403 0.7088395 0.4491550 0.02266965 0.02315986 0.01642020
13
       0 0.13 0.5597290 0.7100172 0.4481867 0.02276865 0.02298978 0.01656136
       0 0.14 0.5585670 0.7110617 0.4473259 0.02285591 0.02283001 0.01671961
14
```

```
0.15 0.5575110 0.7120154 0.4465375 0.02289951 0.02265871 0.01685539
15
16
            0.16 0.5565852 0.7128485 0.4458319 0.02300219 0.02255260 0.01703982
            0.17 0.5557408 0.7136111 0.4451867 0.02307682 0.02243425 0.01718752
17
            0.18 \ 0.5549560 \ 0.7143224 \ 0.4445800 \ 0.02314049 \ 0.02231704 \ 0.01731194
18
19
            0.19 0.5542713 0.7149406 0.4440584 0.02322135 0.02223021 0.01743259
20
            0.20\ 0.5536309\ 0.7155207\ 0.4435804\ 0.02329190\ 0.02213983\ 0.01755151
            0.21 0.5530515 0.7160482 0.4431387 0.02334379 0.02204746 0.01765745
21
            0.22\ 0.5525135\ 0.7165381\ 0.4427113\ 0.02340350\ 0.02196900\ 0.01776944
22
23
            0.23 0.5520265 0.7169810 0.4423191 0.02347386 0.02191345 0.01788628
24
            0.24 0.5515700 0.7173971 0.4419665 0.02353869 0.02185562 0.01798902
25
            0.25 0.5511610 0.7177708 0.4416443 0.02359267 0.02179608 0.01808423
            0.26 0.5507690 0.7181299 0.4413370 0.02364697 0.02173856 0.01818548
26
            0.27 0.5504161 0.7184534 0.4410616 0.02370846 0.02169912 0.01828827
27
            0.28 0.5500793 0.7187632 0.4408025 0.02377001 0.02166221 0.01838929
28
29
            0.29 0.5497709 0.7190474 0.4405627 0.02382146 0.02162040 0.01847420
30
            0.30 0.5494945 0.7193030 0.4403503 0.02386048 0.02157649 0.01854237
31
            0.31 0.5492296 0.7195488 0.4401459 0.02389958 0.02153393 0.01861073
            0.32 0.5489850 0.7197761 0.4399596 0.02394483 0.02150092 0.01868874
32
33
            0.33 0.5487566 0.7199890 0.4397816 0.02399354 0.02147442 0.01877180
34
            0.34 0.5485379 0.7201937 0.4396066 0.02404177 0.02144866 0.01885293
35
            0.35 0.5483402 0.7203793 0.4394449 0.02408424 0.02142247 0.01892259
            0.36 0.5481604 0.7205489 0.4392937 0.02412281 0.02139804 0.01898807
36
            0.37 0.5479885 0.7207118 0.4391463 0.02416112 0.02137427 0.01905715
37
            0.38 0.5478269 0.7208656 0.4390013 0.02419849 0.02135132 0.01912452
38
            0.39 0.5476842 0.7210021 0.4388713 0.02423388 0.02133245 0.01918348
39
40
            0.40 0.5475483 0.7211330 0.4387460 0.02426895 0.02131414 0.01923465
41
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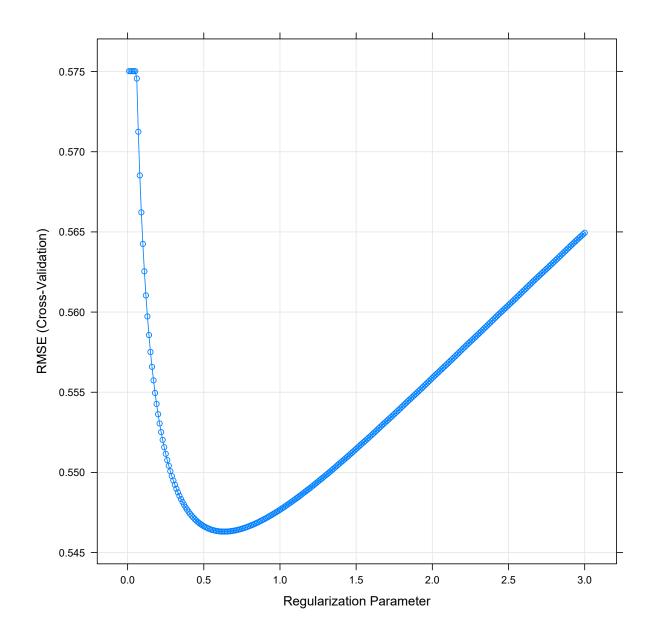
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alpha lambda 63 0 0.63



Lasso Regression

Lasso Penalty

Elastic Net