Homework_1

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```
set.seed(123123)
sl_tr =
  read_csv(here::here("solubility_train.csv")) %>%
  janitor::clean_names()

sl_ts =
  read_csv(here::here("solubility_test.csv")) %>%
  janitor::clean_names()

x_ts = model.matrix(solubility ~ ., sl_ts)[, -1]

y_ts = sl_ts$solubility
```

Q1

```
sl_lm =
  train(solubility~.,
        data = sl_tr,
        method = "lm",
        trControl =
          trainControl(
            method = "repeatedcv",
            number = 10,
            repeats = 5
          ))

print("the RMSE of the model is")
```

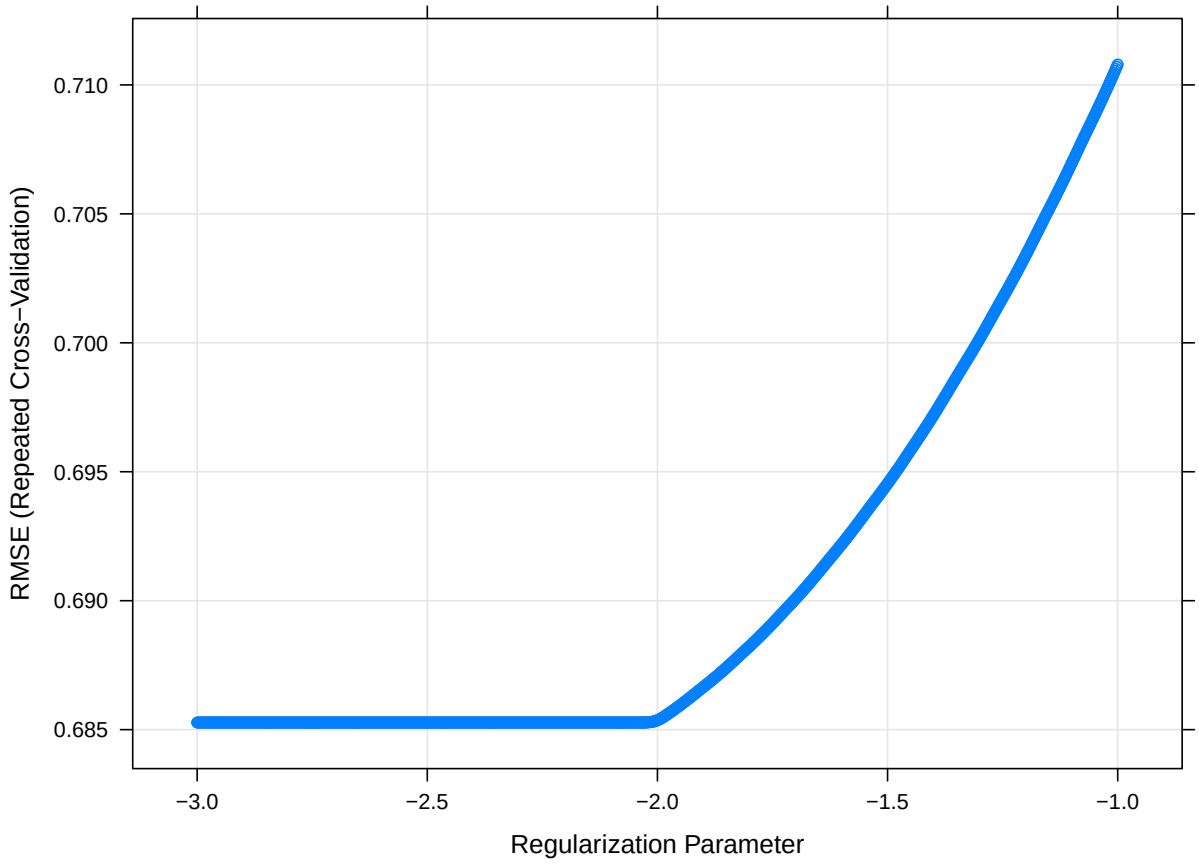
```
## [1] "the RMSE of the model is"
```

```
RMSE(predict(sl_lm,newdata = sl_ts),sl_ts$solubility)
```

```
## [1] 0.746
```

Q2

```
sl_ridge =
  train(
    solubility ~ .,
    data = sl_tr,
    method = "glmnet",
    tuneGrid =
      expand.grid(alpha = 0,
            lambda = exp(seq(from = -1,to =-3, length = 1000))),
    trControl =
      trainControl(method = "repeatedcv",
                   number = 10,
                   repeats = 5),
    preProcess = c("center","scale")
  )

plot(sl_ridge, xTrans = log)
```




```
sl_ridge$bestTune
```

```
##     alpha lambda
```

```
## 485     0  0.131
```

```
print("the RMSE of the model is")
```

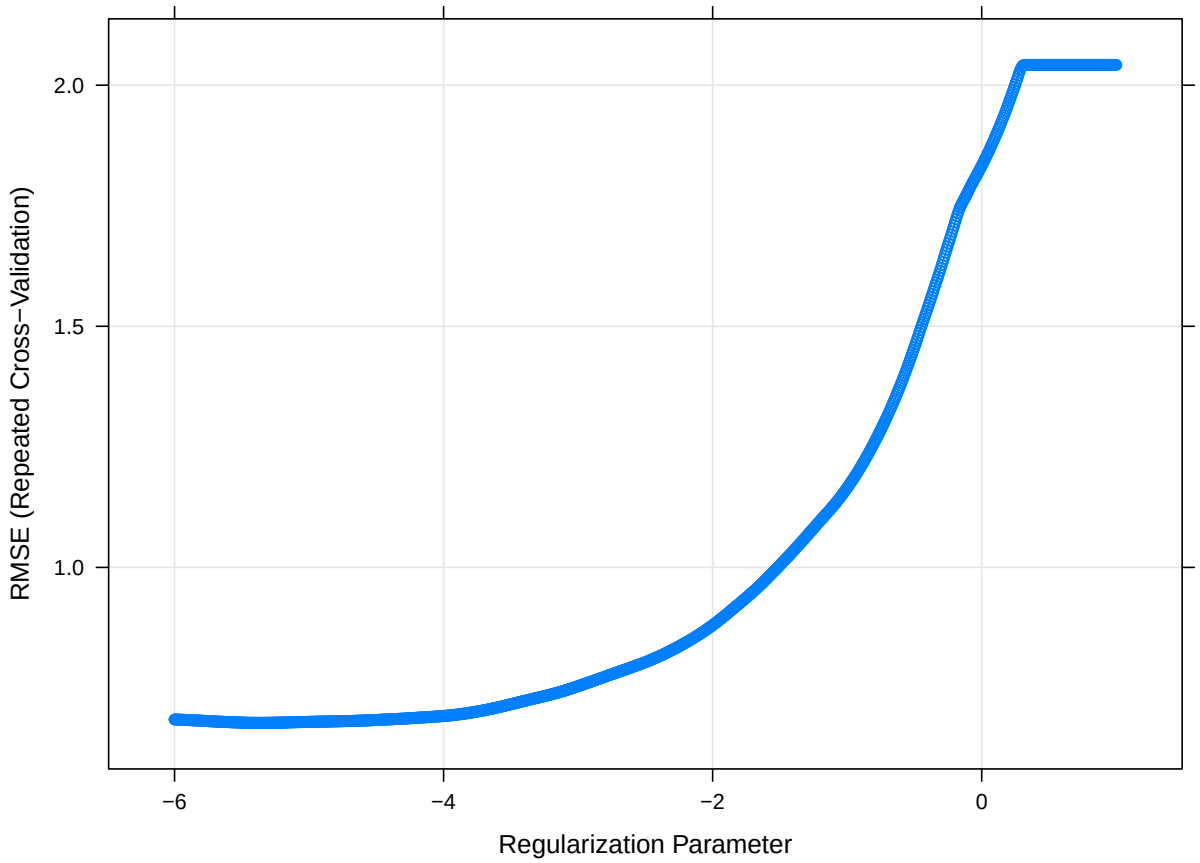
```
## [1] "the RMSE of the model is"
```

```
RMSE(predict(sl_ridge,newdata = sl_ts),sl_ts$solubility)
```

```
## [1] 0.717
```

Q3

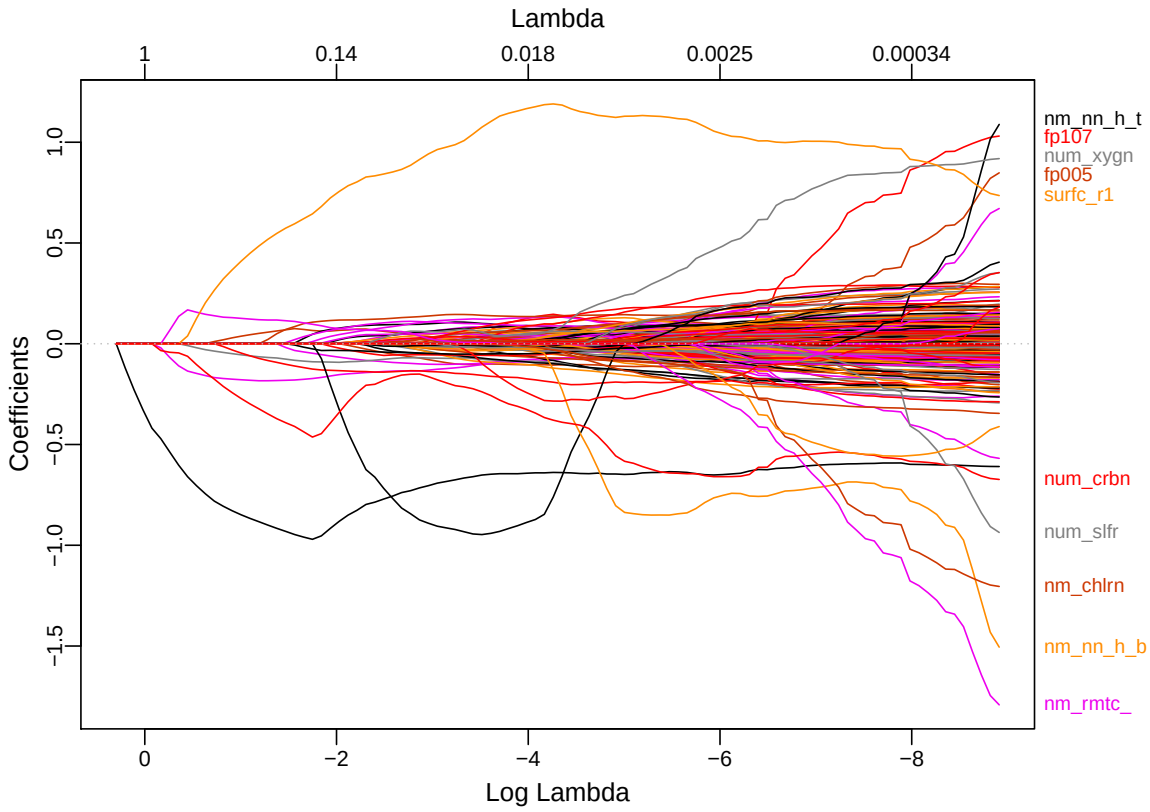
```
sl_lasso =
  train(
    solubility~.,
    data = sl_tr,
    method = "glmnet",
    tuneGrid =
      expand.grid(alpha = 1,
             lambda = exp(seq(-6,to=1,length = 1000))),
    trControl =
      trainControl(
        method = "repeatedcv",
        number = 10,
        repeats = 5
      ),
    preProcess =
      c("center","scale")
  )

sl_lasso_1se =
  cv.glmnet(model.matrix(solubility~.,sl_tr)[,-1],
          sl_tr$solubility,
          alpha = 1,
          lambda = exp(seq(-6,1,length =1000))
          )

plot(sl_lasso,xTrans = log)
```




```
sl_lasso$bestTune
```

```
##    alpha  lambda
## 89     1 0.00459
```

```
plotmo::plot_glmnet(
  sl_lasso$finalModel
)
```




```
print("we have following parameters left")
```

```
## [1] "we have following parameters left"
```

```
sum(coef(sl_lasso$finalModel, s = sl_lasso$bestTune$lambda)!=0)
```

```
## [1] 148
```

```
print("the RMSE of the model is")
```

```
## [1] "the RMSE of the model is"
```

```
RMSE(predict.train(sl_lasso,newdata = sl_ts),sl_ts$solubility)
```

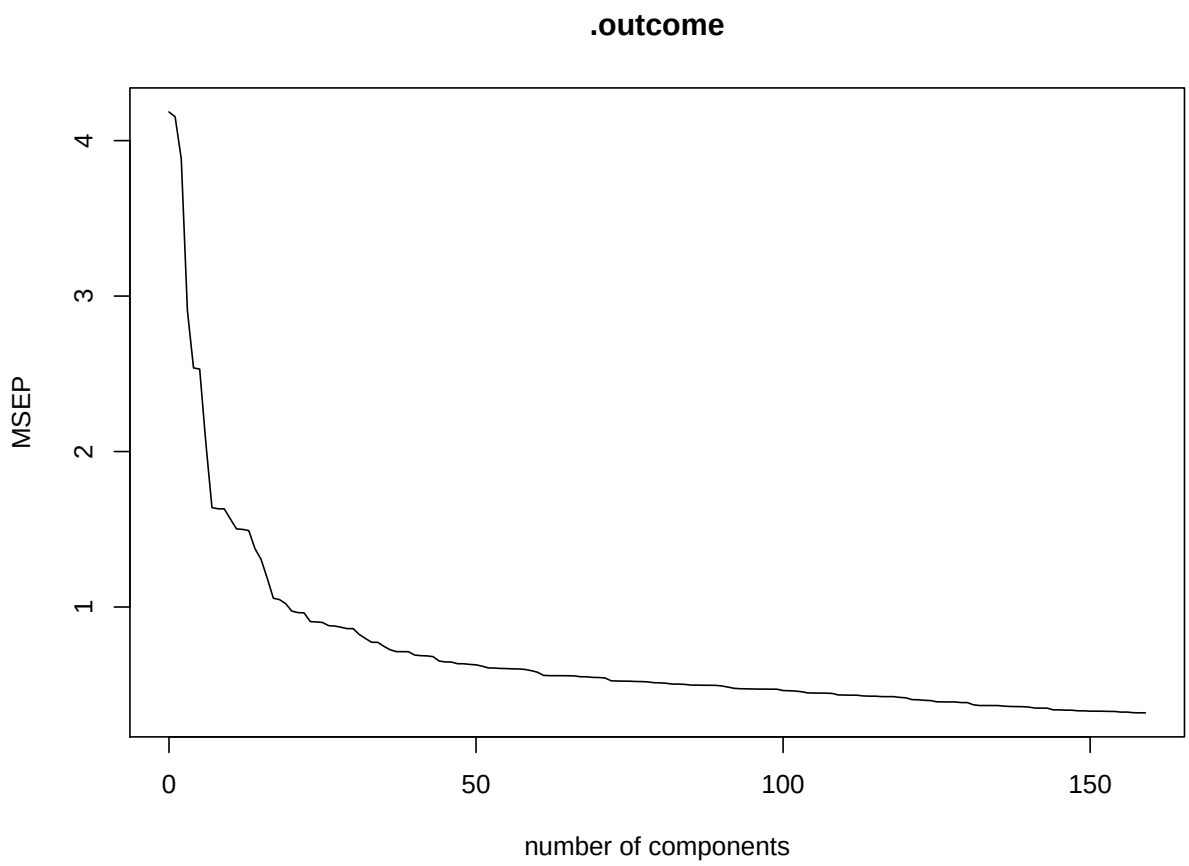
```
## [1] 0.706
```

Q4

```
sl_pcr =
  train(
    solubility~.,
    data = sl_tr,
    method = "pcr",
    tuneGrid =
      expand.grid(ncomp = seq(1,ncol(sl_tr))),
    preProcess = c("center","scale"),
    trControl =
      trainControl(
        method = "repeatedcv",
        number = 10,
        repeats = 5
      )
  )

sl_pcr$bestTune
```

```
##     ncomp
## 159   159
```

```
validationplot(sl_pcr$finalModel,val.type = "MSEP")
```



```r
print("the RMSE of the model is")
```

```
## [1] "the RMSE of the model is"
```

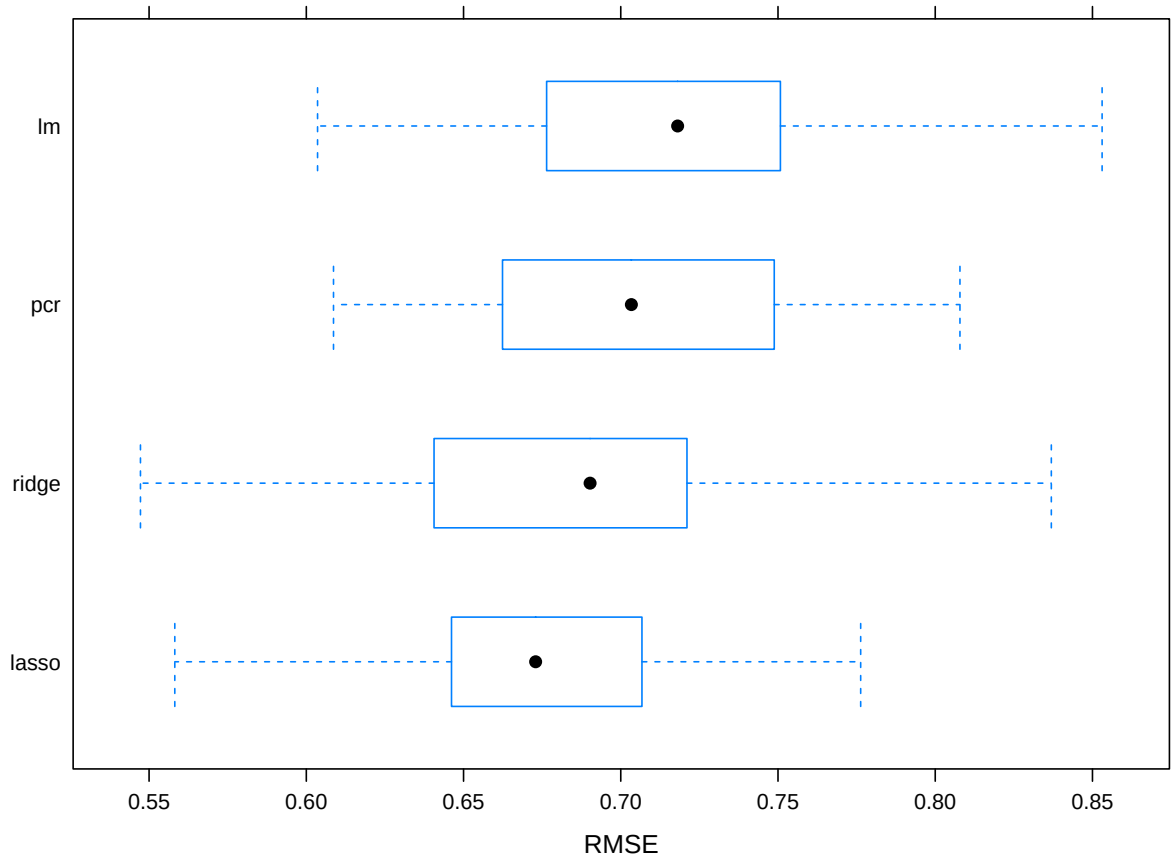
```r
RMSE(predict(sl_pcr,x_ts),y_ts)
```

```
## [1] 0.739
```

```r
resam =
  resamples(list(
    lm = sl_lm,
    ridge = sl_ridge,
    lasso = sl_lasso,
    pcr = sl_pcr
  ))

summary(resam)
```

```
##
## Call:
## summary.resamples(object = resam)
##
## Models: lm, ridge, lasso, pcr
## Number of resamples: 50
##
## MAE
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.446   0.508  0.538 0.533   0.556 0.635    0
## ridge 0.426   0.491  0.522 0.522   0.557 0.640    0
## lasso 0.444   0.498  0.512 0.519   0.543 0.606    0
## pcr   0.445   0.514  0.541 0.544   0.574 0.643    0
##
## RMSE
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.604   0.678  0.718 0.716   0.750 0.853    0
## ridge 0.547   0.641  0.690 0.685   0.721 0.837    0
## lasso 0.558   0.647  0.673 0.678   0.706 0.776    0
## pcr   0.609   0.663  0.703 0.707   0.748 0.808    0
##
## Rsquared
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.798   0.859  0.880 0.878   0.898 0.924    0
## ridge 0.822   0.869  0.886 0.887   0.912 0.932    0
## lasso 0.850   0.876  0.893 0.891   0.903 0.929    0
## pcr   0.816   0.863  0.886 0.881   0.900 0.921    0
```

```r
bwplot(resam, metric = "RMSE")
```



By the resampling result, we can see that Lasso method has the best/lowest mean RMSE and MAE, as well as the highest R^2. Lasso will be chosen to use out of the four for its predictivity and goodness of fit.