P8106 Homework 1

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```
# Import data

sol_train =
  read_csv("./data/solubility_train.csv") %>%
  janitor::clean_names()

sol_test =
  read_csv("./data/solubility_test.csv") %>%
  janitor::clean_names()

x_train = model.matrix(solubility ~., sol_train)[, -1]
y_train = sol_train$solubility

x_test = model.matrix(solubility ~., sol_test)[,-1]
y_test = sol_test$solubility

ctr <- trainControl(method = "repeatedcv", number = 10, repeats = 5)
```

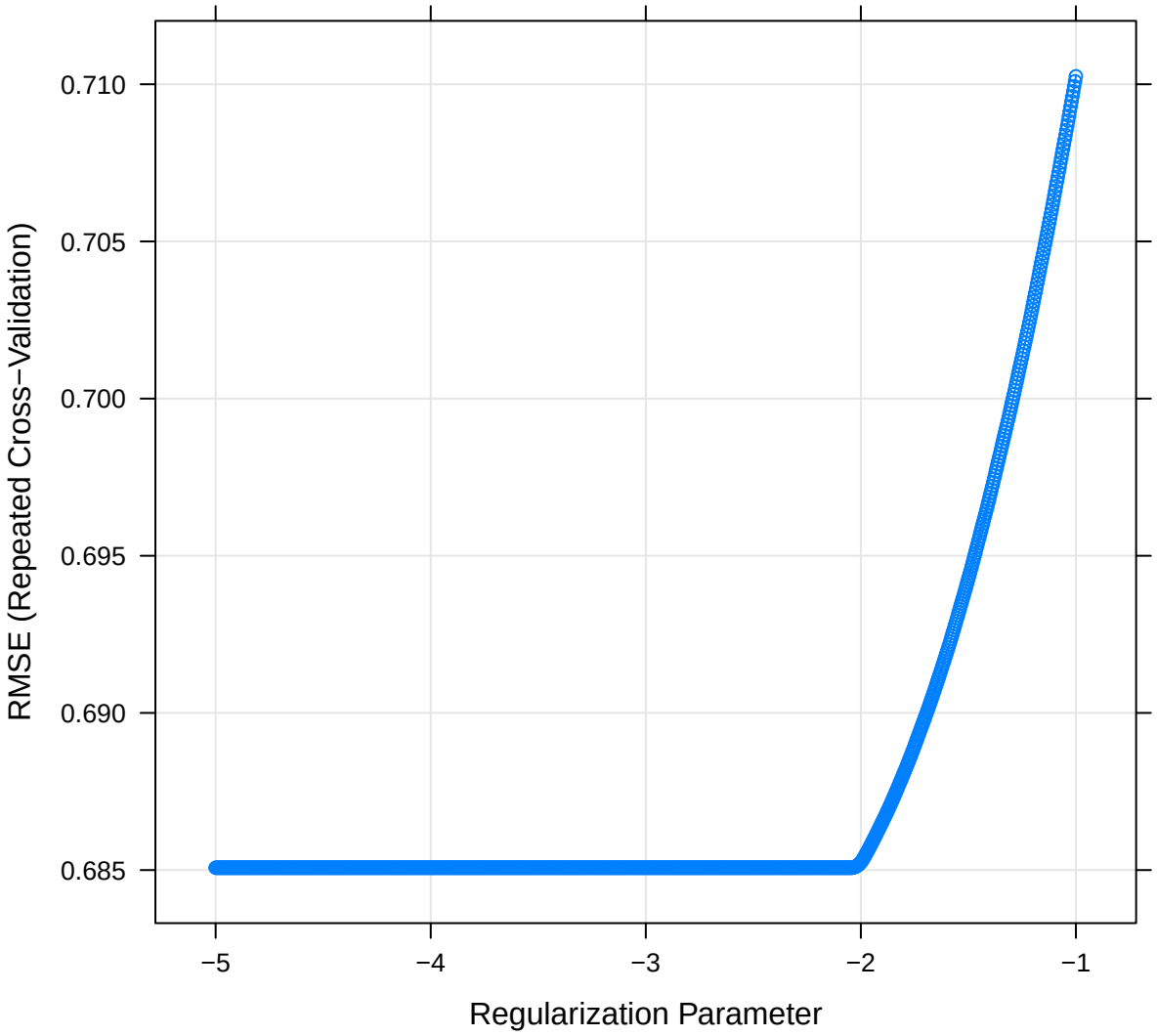
Question 1

```
set.seed(5)
fit.lm =
  train(
    solubility ~.,
    data = sol_train,
    method = "lm",
    trControl = ctr
  )

RMSE(predict(fit.lm, newdata = sol_test), sol_test$solubility)
```

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

Question 2

```r
set.seed(5)

fit.ridge =
  train(
    solubility ~.,
    data = sol_train,
    method = "glmnet",
    tuneGrid =
      expand.grid(
        alpha = 0,
        lambda = exp(seq(from = -1, to = -5, length = 1000))
        ),
    trControl = ctr,
    preProcess = c("center", "scale")
  )

plot(fit.ridge, xTrans = log)
```




```
fit.ridge$bestTune
```

```
##     alpha lambda
## 740     0   0.13
```

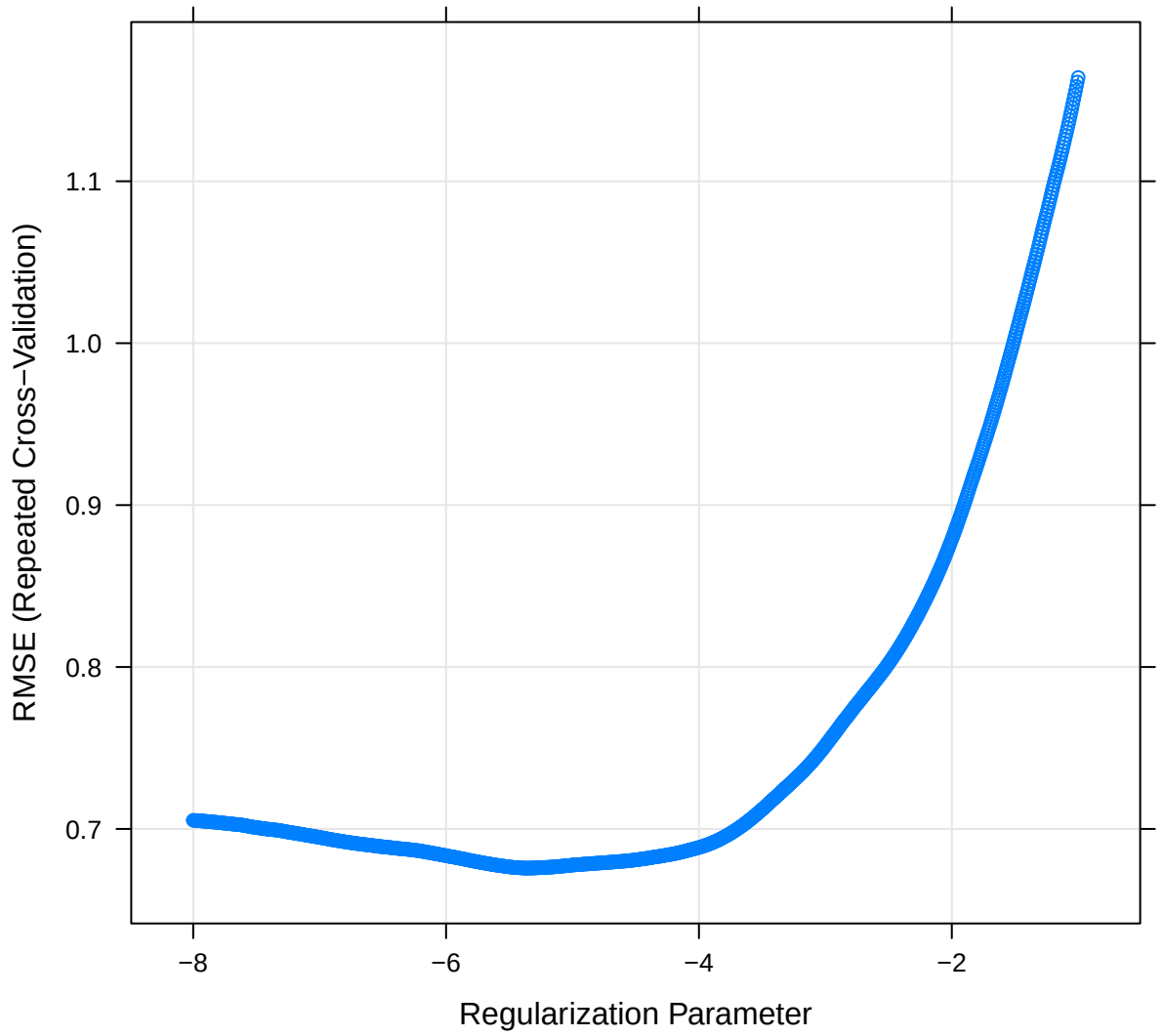
```
RMSE(predict(fit.ridge, s = "lamda.min", news = sol_test), sol_test$solubility)
```

```
## [1] 2.93
```

Question 3

```
set.seed(5)
fit.lasso =
```

```
  train(
    solubility ~.,
    data = sol_train,
    method = "glmnet",
    tuneGrid =
      expand.grid(
        alpha = 1,
        lambda = exp(seq(from = -1, to = -8, length = 1000))
      ),
    trControl = ctr,
    preProcess = c("center", "scale")
  )

plot(fit.lasso, xTrans = log)
```



```
fit.lasso$bestTune
```

```
##     alpha  lambda
## 378     1 0.00471
```

```
RMSE(predict(fit.lasso, s = "lambda.min", newx = sol_test), sol_test$solubility)
```

```
## [1] 2.95
```

```
sum(coef(fit.lasso$finalModel, s = fit.lasso$bestTune$lambda)!=0)
```

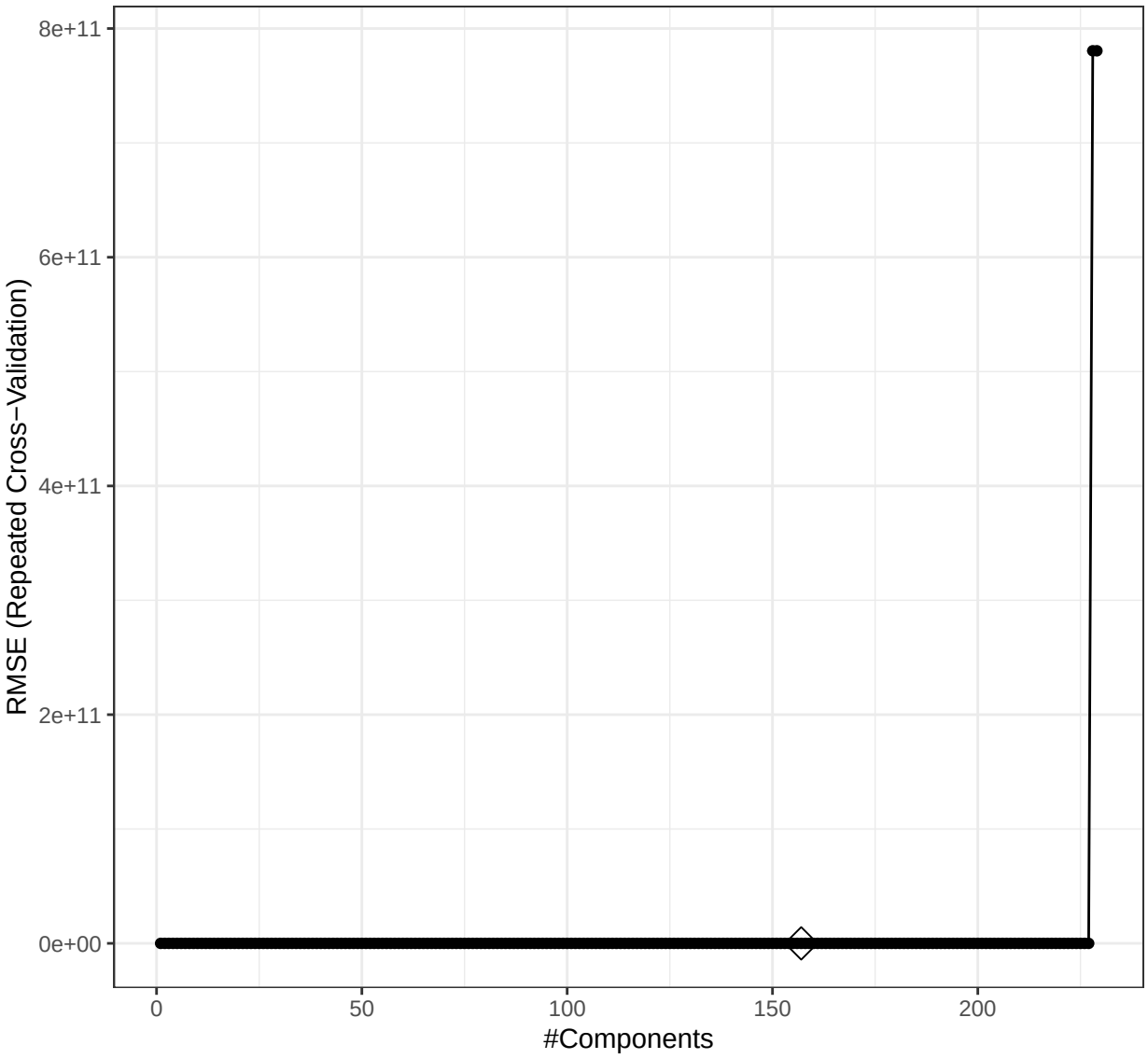
```
## [1] 144
```

Question 4

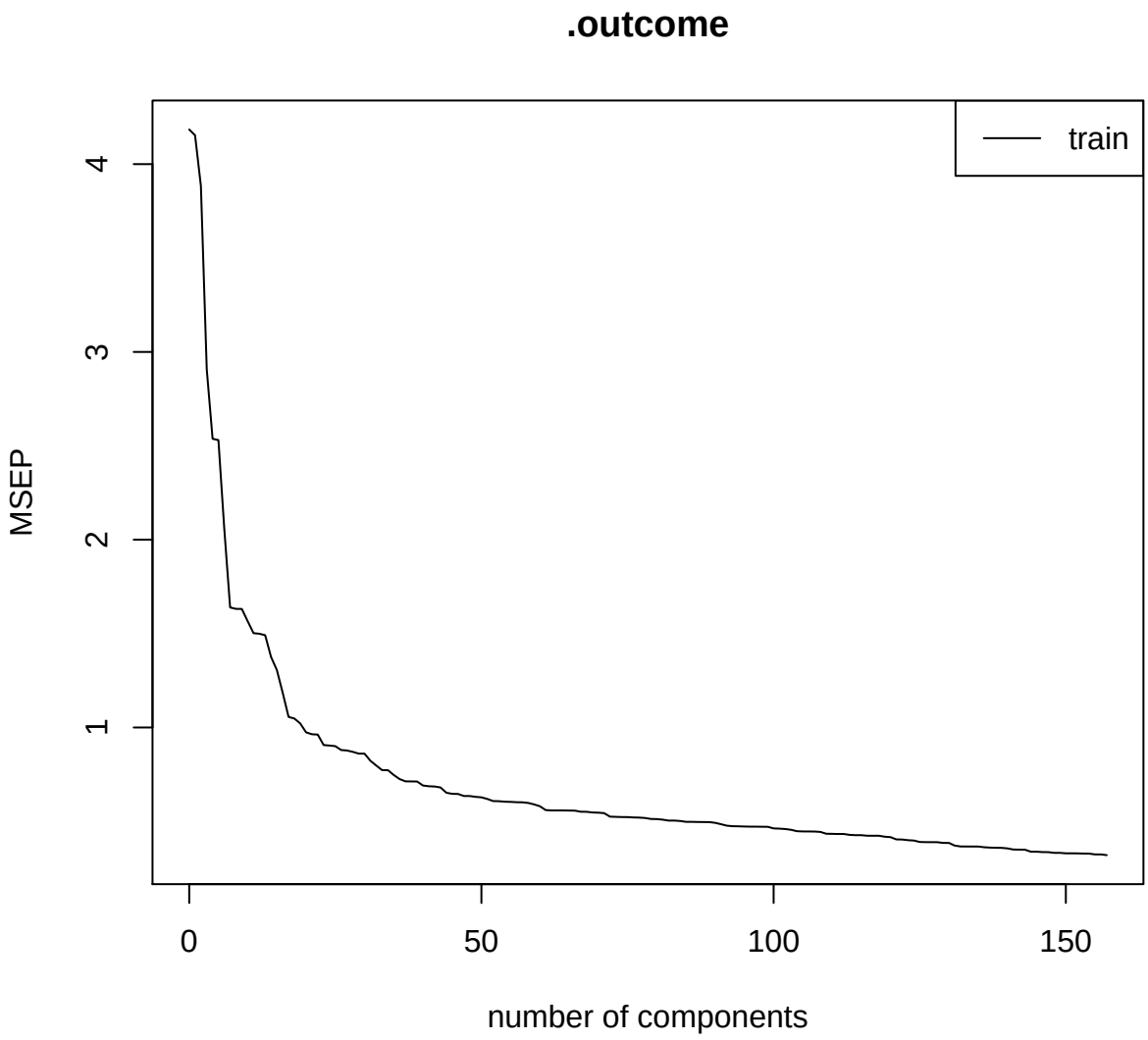
```
set.seed(5)
fit.pcr =
  train(
    solubility~.,
    data = sol_train,
    method = "pcr",
    tuneGrid =
      expand.grid(ncomp = seq(1,ncol(sol_train))),
    preProcess = c("center","scale"),
    trControl = ctr
  )

fit.pcr$bestTune
```

```
##     ncomp
## 157   157
```

```
ggplot(fit.pcr, highlight = TRUE) + theme_bw()
```




```
validationplot(fit.pcr$finalModel, val.type="MSEP", legendpos = "topright")
```




```
RMSE(predict(fit.pcr, x_test), y_test)
```

```
## [1] 0.742
```

```
mean((predict(fit.pcr, x_test) - y_test)^2)
```

```
## [1] 0.55
```

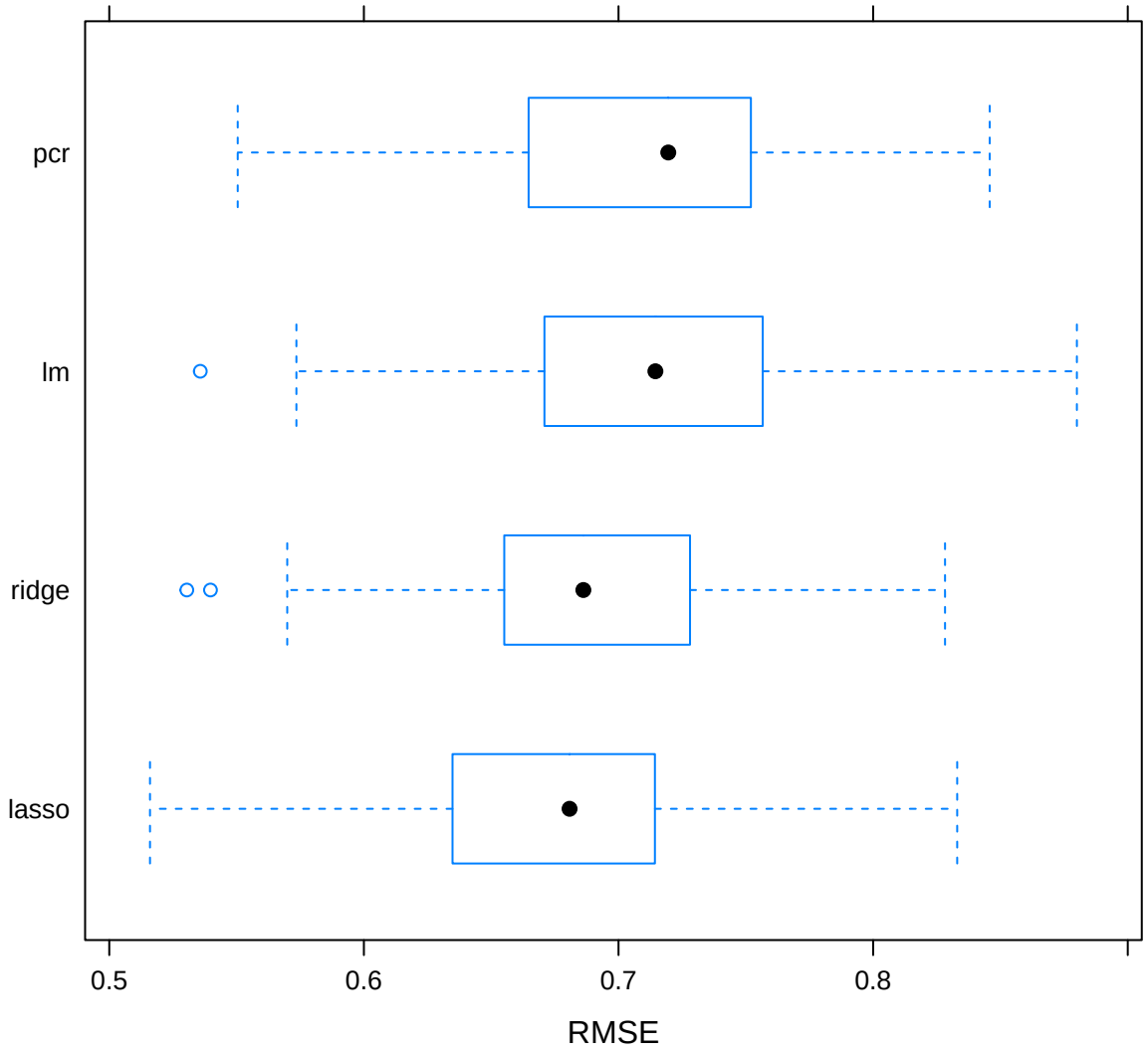
Question 5

```
resample =
  resamples(list(
    lm = fit.lm,
```

```
    ridge = fit.ridge,
    lasso = fit.lasso,
    pcr = fit.pcr
  ))

summary(resample)
```

```
##
## Call:
## summary.resamples(object = resample)
##
## Models: lm, ridge, lasso, pcr
## Number of resamples: 50
##
## MAE
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.401   0.499  0.536 0.530   0.564 0.607    0
## ridge 0.412   0.503  0.530 0.522   0.551 0.607    0
## lasso 0.416   0.498  0.518 0.518   0.544 0.605    0
## pcr   0.420   0.519  0.549 0.545   0.583 0.645    0
##
## RMSE
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.536   0.671  0.714 0.708   0.754 0.880    0
## ridge 0.530   0.656  0.686 0.685   0.727 0.828    0
## lasso 0.516   0.636  0.681 0.676   0.714 0.833    0
## pcr   0.550   0.666  0.720 0.709   0.752 0.846    0
##
## Rsquared
##        Min. 1st Qu. Median  Mean 3rd Qu.  Max. NA's
## lm    0.839   0.865  0.876 0.882   0.897 0.939    0
## ridge 0.821   0.871  0.885 0.887   0.905 0.943    0
## lasso 0.818   0.873  0.889 0.890   0.908 0.944    0
## pcr   0.821   0.858  0.880 0.880   0.903 0.937    0
```

```
bwplot(resample, metric = "RMSE")
```



From numeric result and boxplot, Lasso model has the smallest RMSE, and we will choose it for predicting solubility.