p8106_hw1_yg2625

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Import data

```
train_data = read.csv("./data/solubility_train.csv") %>%
  janitor::clean_names()
test_data = read.csv("./data/solubility_test.csv") %>%
  janitor::clean_names()
```

(a) Fit a linear model using least squares on the training data and calculate the mean square error using the test data.

Fit linear model on the training data

```
fit_lm_tr = lm(solubility ~ .  data = train_data)
summary(fit_lm_tr)
```

```
##
## Call:
## lm(formula = solubility ~ ., data = train_data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.75620 -0.28304  0.01165  0.30030  1.54887
##
## Coefficients:
##                      Estimate Std. Error t value Pr(>|t|)
## (Intercept)         2.431e+00  2.162e+00   1.124 0.261303
## fp001               3.594e-01  3.185e-01   1.128 0.259635
## fp002               1.456e-01  2.637e-01   0.552 0.580960
## fp003              -3.969e-02  1.314e-01  -0.302 0.762617
## fp004              -3.049e-01  1.371e-01  -2.223 0.026520 *
## fp005               2.837e+00  9.598e-01   2.956 0.003223 **
## fp006              -6.886e-02  2.041e-01  -0.337 0.735917
## fp007               4.044e-02  1.152e-01   0.351 0.725643
## fp008               1.121e-01  1.636e-01   0.685 0.493331
## fp009              -8.242e-01  8.395e-01  -0.982 0.326536
## fp010               4.193e-01  3.136e-01   1.337 0.181579
## fp011               5.158e-02  2.198e-01   0.235 0.814503
## fp012              -1.346e-02  1.611e-01  -0.084 0.933452
## fp013              -4.519e-01  5.473e-01  -0.826 0.409311
## fp014               3.281e-01  4.550e-01   0.721 0.471044
## fp015              -1.839e-01  1.521e-01  -1.209 0.226971
## fp016              -1.367e-01  1.548e-01  -0.883 0.377340
## fp017              -1.704e-01  1.386e-01  -1.230 0.219187
## fp018              -3.824e-01  2.388e-01  -1.602 0.109655
## fp019              -3.131e-01  3.863e-01  -0.811 0.417862
```

```
## fp020              2.072e-01  2.135e-01   0.971 0.332078
## fp021             -5.956e-02  2.632e-01  -0.226 0.821060
## fp022              2.336e-01  3.456e-01   0.676 0.499180
## fp023             -3.193e-01  1.909e-01  -1.672 0.094866 .
## fp024             -4.272e-01  2.827e-01  -1.511 0.131162
## fp025              4.376e-01  4.538e-01   0.964 0.335184
## fp026              2.068e-01  2.564e-01   0.806 0.420273
## fp027              2.424e-01  2.429e-01   0.998 0.318594
## fp028              1.070e-01  1.200e-01   0.892 0.372547
## fp029             -9.857e-02  2.199e-01  -0.448 0.654163
## fp030             -2.361e-01  2.468e-01  -0.957 0.339048
## fp031              8.690e-02  1.346e-01   0.646 0.518754
## fp032             -1.204e+00  7.772e-01  -1.550 0.121628
## fp033              5.766e-01  4.236e-01   1.361 0.173882
## fp034             -1.794e-01  2.618e-01  -0.685 0.493486
## fp035             -2.140e-01  1.704e-01  -1.256 0.209605
## fp036              7.701e-02  1.657e-01   0.465 0.642133
## fp037              1.098e-01  1.725e-01   0.636 0.524693
## fp038              2.721e-01  1.888e-01   1.441 0.150030
## fp039              2.011e-02  2.888e-01   0.070 0.944491
## fp040              5.477e-01  1.890e-01   2.898 0.003873 **
## fp041             -4.265e-01  3.004e-01  -1.420 0.156143
## fp042             -9.901e-01  7.078e-01  -1.399 0.162294
## fp043             -3.725e-02  2.096e-01  -0.178 0.859011
## fp044             -3.860e-01  2.184e-01  -1.768 0.077562 .
## fp045              2.120e-01  1.299e-01   1.631 0.103238
## fp046             -3.504e-02  2.733e-01  -0.128 0.898010
## fp047             -1.675e-02  1.414e-01  -0.118 0.905775
## fp048              2.610e-01  2.434e-01   1.073 0.283810
## fp049              1.241e-01  1.971e-01   0.630 0.529036
## fp050              9.087e-03  1.410e-01   0.064 0.948648
## fp051              1.050e-01  2.014e-01   0.521 0.602210
## fp052             -4.569e-01  2.482e-01  -1.841 0.066029 .
## fp053              2.994e-01  2.466e-01   1.214 0.225129
## fp054              2.734e-02  1.829e-01   0.149 0.881229
## fp055             -3.662e-01  1.970e-01  -1.858 0.063530 .
## fp056             -2.961e-01  2.979e-01  -0.994 0.320541
## fp057             -1.002e-01  1.379e-01  -0.727 0.467703
## fp058              3.100e-01  8.074e-01   0.384 0.701129
## fp059             -1.615e-01  1.690e-01  -0.956 0.339514
## fp060              2.350e-01  1.474e-01   1.595 0.111209
## fp061             -6.365e-01  1.440e-01  -4.421 1.13e-05 ***
## fp062             -5.224e-01  2.961e-01  -1.764 0.078078 .
## fp063             -2.001e+00  1.287e+00  -1.554 0.120553
## fp064              2.549e-01  1.221e-01   2.087 0.037207 *
## fp065             -2.844e-01  1.197e-01  -2.377 0.017714 *
## fp066              2.093e-01  1.264e-01   1.655 0.098301 .
## fp067             -1.406e-01  1.540e-01  -0.913 0.361631
## fp068              4.964e-01  2.028e-01   2.447 0.014630 *
## fp069              1.324e-01  8.824e-02   1.501 0.133885
## fp070              3.453e-03  8.088e-02   0.043 0.965963
## fp071              1.474e-01  1.237e-01   1.192 0.233775
## fp072             -9.773e-01  2.763e-01  -3.537 0.000431 ***
## fp073             -4.671e-01  2.072e-01  -2.254 0.024474 *
```

```
## fp074              1.793e-01  1.206e-01   1.487 0.137566
## fp075              1.231e-01  1.035e-01   1.188 0.235034
## fp076              5.166e-01  1.704e-01   3.031 0.002525 **
## fp077              1.644e-01  1.236e-01   1.331 0.183739
## fp078             -3.715e-01  1.588e-01  -2.339 0.019608 *
## fp079              4.254e-01  1.881e-01   2.262 0.023992 *
## fp080              3.101e-01  1.554e-01   1.996 0.046340 *
## fp081             -3.208e-01  1.117e-01  -2.873 0.004192 **
## fp082              1.243e-01  9.524e-02   1.305 0.192379
## fp083             -6.916e-01  2.134e-01  -3.241 0.001248 **
## fp084              3.626e-01  2.381e-01   1.523 0.128171
## fp085             -3.310e-01  1.428e-01  -2.317 0.020785 *
## fp086              1.169e-02  9.774e-02   0.120 0.904834
## fp087              4.559e-02  2.797e-01   0.163 0.870568
## fp088              2.416e-01  9.959e-02   2.425 0.015534 *
## fp089              5.999e-01  2.320e-01   2.586 0.009915 **
## fp090             -2.450e-02  1.154e-01  -0.212 0.831930
## fp091             -2.858e-01  3.185e-01  -0.897 0.369847
## fp092              2.665e-01  2.069e-01   1.288 0.198156
## fp093              1.974e-01  1.087e-01   1.816 0.069803 .
## fp094             -1.991e-01  1.441e-01  -1.381 0.167707
## fp095             -1.403e-01  1.124e-01  -1.248 0.212449
## fp096             -5.024e-01  1.459e-01  -3.445 0.000605 ***
## fp097             -2.635e-01  1.666e-01  -1.582 0.114020
## fp098             -2.865e-01  1.633e-01  -1.754 0.079863 .
## fp099              2.592e-01  2.568e-01   1.009 0.313136
## fp100             -4.008e-01  3.034e-01  -1.321 0.186949
## fp101             -1.760e-01  3.019e-01  -0.583 0.560147
## fp102              2.445e-01  3.449e-01   0.709 0.478579
## fp103             -1.493e-01  9.148e-02  -1.632 0.103176
## fp104             -1.428e-01  1.176e-01  -1.214 0.225238
## fp105             -6.912e-02  1.395e-01  -0.495 0.620482
## fp106              1.128e-01  1.288e-01   0.876 0.381495
## fp107              2.778e+00  8.247e-01   3.369 0.000796 ***
## fp108              8.836e-03  1.852e-01   0.048 0.961970
## fp109              8.200e-01  2.267e-01   3.617 0.000319 ***
## fp110              3.680e-01  3.311e-01   1.111 0.266811
## fp111             -5.565e-01  1.420e-01  -3.918 9.80e-05 ***
## fp112             -1.079e-01  2.705e-01  -0.399 0.690108
## fp113              1.511e-01  9.481e-02   1.594 0.111478
## fp114             -1.201e-01  1.891e-01  -0.635 0.525628
## fp115             -1.896e-01  1.405e-01  -1.349 0.177736
## fp116              7.778e-03  1.897e-01   0.041 0.967300
## fp117              2.583e-01  1.779e-01   1.452 0.147070
## fp118             -1.964e-01  1.230e-01  -1.596 0.110940
## fp119              7.515e-01  2.630e-01   2.857 0.004402 **
## fp120             -1.814e-01  1.794e-01  -1.011 0.312362
## fp121             -4.731e-02  3.957e-01  -0.120 0.904866
## fp122              1.048e-01  1.041e-01   1.007 0.314268
## fp123              3.926e-02  1.765e-01   0.222 0.824066
## fp124              1.235e-01  1.705e-01   0.724 0.469243
## fp125             -2.633e-04  1.151e-01  -0.002 0.998175
## fp126             -2.782e-01  1.177e-01  -2.363 0.018373 *
## fp127             -6.123e-01  1.739e-01  -3.521 0.000457 ***
```

```
## fp128            -5.424e-01  1.932e-01  -2.807 0.005136 **
## fp129            -6.731e-02  2.243e-01  -0.300 0.764167
## fp130            -1.034e+00  4.106e-01  -2.518 0.012009 *
## fp131             2.158e-01  1.617e-01   1.335 0.182405
## fp132            -1.976e-01  2.382e-01  -0.830 0.406998
## fp133            -1.573e-01  1.217e-01  -1.293 0.196319
## fp134             2.496e+00  1.196e+00   2.086 0.037310 *
## fp135             1.818e-01  1.319e-01   1.379 0.168460
## fp136            -7.763e-02  3.131e-01  -0.248 0.804237
## fp137            -4.613e-02  2.978e-01  -0.155 0.876947
## fp138            -9.392e-02  1.906e-01  -0.493 0.622251
## fp139             7.659e-02  4.063e-01   0.189 0.850517
## fp140             3.145e-01  2.149e-01   1.463 0.143784
## fp141             2.219e-01  2.765e-01   0.802 0.422532
## fp142             6.272e-01  1.488e-01   4.214 2.83e-05 ***
## fp143             9.981e-01  2.929e-01   3.407 0.000692 ***
## fp144             2.207e-01  2.839e-01   0.777 0.437195
## fp145            -1.146e-01  1.188e-01  -0.964 0.335169
## fp146            -2.324e-01  2.086e-01  -1.114 0.265716
## fp147             1.502e-01  1.228e-01   1.223 0.221703
## fp148            -1.600e-01  1.319e-01  -1.213 0.225560
## fp149             1.172e-01  1.650e-01   0.710 0.477770
## fp150             9.046e-02  1.577e-01   0.574 0.566368
## fp151             2.899e-01  3.120e-01   0.929 0.353202
## fp152            -2.544e-01  2.990e-01  -0.851 0.395087
## fp153            -3.765e-01  2.773e-01  -1.358 0.175029
## fp154            -1.027e+00  2.033e-01  -5.054 5.50e-07 ***
## fp155             4.888e-01  2.916e-01   1.676 0.094163 .
## fp156            -3.602e-02  3.636e-01  -0.099 0.921109
## fp157            -4.715e-01  2.468e-01  -1.910 0.056505 .
## fp158             1.669e-02  1.925e-01   0.087 0.930943
## fp159             1.800e-01  2.432e-01   0.740 0.459378
## fp160             1.525e-02  2.177e-01   0.070 0.944155
## fp161            -2.440e-01  1.433e-01  -1.703 0.089063 .
## fp162             4.910e-02  1.859e-01   0.264 0.791710
## fp163             4.785e-01  3.121e-01   1.533 0.125659
## fp164             5.096e-01  1.899e-01   2.684 0.007446 **
## fp165             5.793e-01  2.146e-01   2.700 0.007103 **
## fp166            -6.582e-02  2.185e-01  -0.301 0.763293
## fp167            -6.044e-01  2.515e-01  -2.403 0.016502 *
## fp168            -1.187e-01  1.872e-01  -0.634 0.526173
## fp169            -1.705e-01  8.312e-02  -2.051 0.040650 *
## fp170            -7.902e-02  1.560e-01  -0.506 0.612745
## fp171             4.651e-01  1.186e-01   3.922 9.64e-05 ***
## fp172            -4.426e-01  2.440e-01  -1.814 0.070120 .
## fp173             4.243e-01  1.657e-01   2.561 0.010634 *
## fp174            -1.010e-01  2.098e-01  -0.481 0.630311
## fp175            -4.657e-02  2.481e-01  -0.188 0.851136
## fp176             9.736e-01  2.644e-01   3.682 0.000249 ***
## fp177             1.386e-01  2.393e-01   0.579 0.562538
## fp178             6.497e-02  2.079e-01   0.313 0.754691
## fp179            -3.415e-02  2.232e-01  -0.153 0.878437
## fp180            -7.905e-01  5.523e-01  -1.431 0.152839
## fp181             4.925e-01  3.218e-01   1.531 0.126309
```

```
## fp182              -1.124e-01  1.310e-01  -0.858 0.391384
## fp183               2.998e-01  7.143e-01   0.420 0.674836
## fp184               4.876e-01  1.580e-01   3.087 0.002103 **
## fp185              -3.778e-01  2.037e-01  -1.854 0.064108 .
## fp186              -3.654e-01  1.953e-01  -1.871 0.061710 .
## fp187               4.457e-01  2.682e-01   1.662 0.097015 .
## fp188               1.475e-01  1.258e-01   1.172 0.241519
## fp189              -1.984e-02  3.468e-01  -0.057 0.954384
## fp190               2.629e-01  3.018e-01   0.871 0.383981
## fp191               2.799e-01  1.465e-01   1.911 0.056388 .
## fp192              -2.404e-01  2.751e-01  -0.874 0.382534
## fp193               1.502e-01  1.494e-01   1.005 0.315159
## fp194               8.029e-01  6.379e-01   1.259 0.208566
## fp195               5.967e-02  3.435e-01   0.174 0.862158
## fp196               1.091e-02  2.544e-01   0.043 0.965812
## fp197              -3.736e-02  1.569e-01  -0.238 0.811793
## fp198               1.896e-01  2.665e-01   0.712 0.476893
## fp199              -9.932e-02  1.797e-01  -0.553 0.580702
## fp200              -6.421e-02  2.161e-01  -0.297 0.766462
## fp201              -4.838e-01  1.980e-01  -2.444 0.014771 *
## fp202               5.664e-01  1.869e-01   3.031 0.002527 **
## fp203               2.586e-01  6.447e-01   0.401 0.688462
## fp204              -1.371e-01  2.543e-01  -0.539 0.590008
## fp205               7.177e-02  1.561e-01   0.460 0.645857
## fp206              -6.769e-02  1.860e-01  -0.364 0.716094
## fp207              -5.538e-03  2.060e-01  -0.027 0.978560
## fp208              -5.338e-01  6.324e-01  -0.844 0.398925
## mol_weight         -1.232e+00  2.296e-01  -5.365 1.09e-07 ***
## num_atoms          -1.478e+01  3.473e+00  -4.257 2.35e-05 ***
## num_non_h_atoms     1.795e+01  3.166e+00   5.670 2.07e-08 ***
## num_bonds           9.843e+00  2.681e+00   3.671 0.000260 ***
## num_non_h_bonds    -1.030e+01  1.793e+00  -5.746 1.35e-08 ***
## num_mult_bonds      2.107e-01  1.754e-01   1.201 0.229990
## num_rot_bonds      -5.213e-01  1.334e-01  -3.908 0.000102 ***
## num_dbl_bonds      -7.492e-01  3.163e-01  -2.369 0.018111 *
## num_aromatic_bonds -2.364e+00  6.232e-01  -3.794 0.000161 ***
## num_hydrogen        8.347e-01  1.880e-01   4.439 1.04e-05 ***
## num_carbon          1.730e-02  3.763e-01   0.046 0.963335
## num_nitrogen        6.125e+00  3.045e+00   2.011 0.044645 *
## num_oxygen          2.389e+00  4.523e-01   5.283 1.69e-07 ***
## num_sulfer         -8.508e+00  3.619e+00  -2.351 0.018994 *
## num_chlorine       -7.449e+00  1.989e+00  -3.744 0.000195 ***
## num_halogen         1.408e+00  2.109e+00   0.668 0.504615
## num_rings           1.276e+00  6.716e-01   1.901 0.057731 .
## hydrophilic_factor  1.099e-02  1.137e-01   0.097 0.922998
## surface_area1       8.825e-02  6.058e-02   1.457 0.145643
## surface_area2       9.555e-02  5.615e-02   1.702 0.089208 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5524 on 722 degrees of freedom
## Multiple R-squared:  0.9446, Adjusted R-squared:  0.9271
## F-statistic: 54.03 on 228 and 722 DF,  p-value: < 2.2e-16
```

Calculate the mean square error using the test data

```
pred_lm_tr = predict(fit_lm_tr, test_data)
mse_test = mean((pred_lm_tr - test_data$solubility)^2);mse_test
```

```
## [1] 0.5558898
```

Hence, the MSE using test data is 0.5558898.

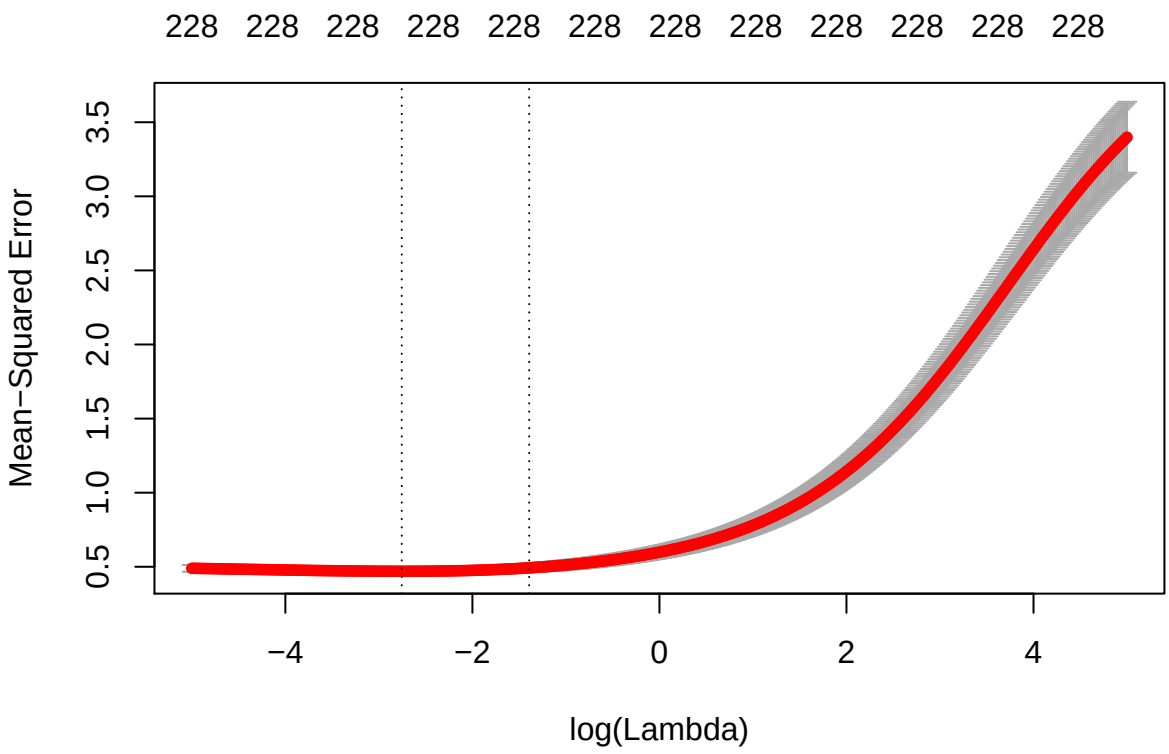
(b) Fit a ridge regression model on the training data, with lambda chosen by cross-validation. Report the test error.

Fit ridge regression model on the training data

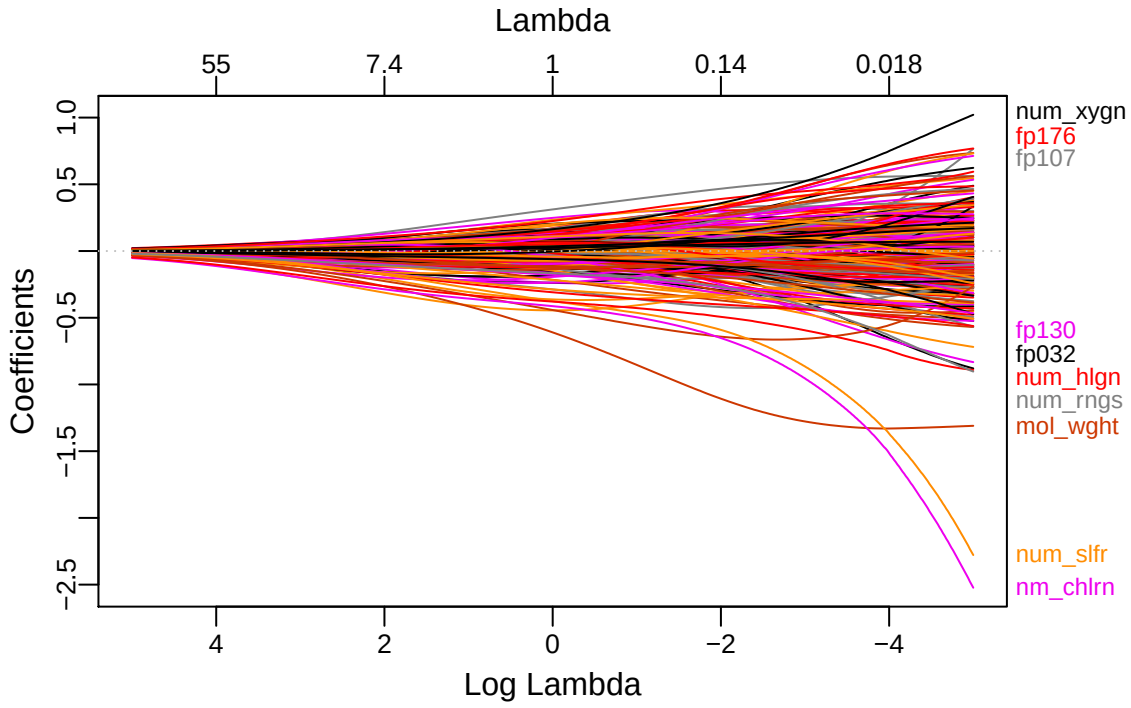
```
train_data = na.omit(train_data)
x = model.matrix(solubility ~ ., train_data)[, -1]
y = train_data$solubility

ridge_mod = glmnet(x, y, alpha = 0, lambda = exp(seq(-5, 5, length = 500)))
mat_coef = coef(ridge_mod)
dim(mat_coef)
```

```
## [1] 229 500
```

```
# Cross-validation
set.seed(1)
cv_ridge = cv.glmnet(x, y,
                     alpha = 0,
                     lambda = exp(seq(-5, 5, length = 500)),
                     type.measure = "mse")
plot(cv_ridge)
```




```
# Trace plot
plot_glmnet(ridge_mod, xvar = "rlambda")
```




```
# Predict response in final model
best_lambda = cv_ridge$lambda.min; best_lambda
```

```
## [1] 0.06357652
```

```
pred_resp_ridge = predict(ridge_mod, s = best_lambda, newx = model.matrix(solubility ~ ., test_data)[,
mse_ridge = mean((pred_resp_ridge - test_data$solubility)^2); mse_ridge
```

```
## [1] 0.5126573
```

Based on the result, the MSE for ridge regression is 0.5126573.

(c) Fit a lasso model on the training data, with lambda chosen by cross-validation. Report the test error, along with the number of non-zero coefficient estimates.

Fit lasso model on the training data