Sectional Project 1 - Regression

Group 3

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Introduction to the Boston Housing Dataset

The Boston Housing dataset considers housing values and their associated properties in suburbs of Boston, Massachusetts. The dataset contains 506 observations and 14 attributes. We acquired the dataset from the Machine Learning Database (MLDB), found here. In particular, we are interested in constructing a model through regression techniques to gain insight on housing values. As such, we will use the 13 features to model 'MEDV', the median value of owner occupied homes (in $1,000s). The following is metadata for for each attribute as given by the housing.names file:

1. CRIM:per capita crime rate by town
2. ZN:proportion of residential land zoned for lots over 25,000 sq.ft.
3. INDUS: proportion of non-retail business acres per town
4. CHAS: Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
5. NOX: nitric oxides concentration (parts per 10 million)
6. RM: average number of rooms per dwelling
7. AGE: proportion of owner-occupied units built prior to 1940
8. DIS: weighted distances to five Boston employment centres
9. RAD: index of accessibility to radial highways
10. TAX: full-value property-tax rate per $10,000
11. PTRATIO: pupil-teacher ratio by town
12. B: 1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
13. LSTAT: %lower status of the population
14. MEDV: Median value of owner-occupied homes in $1000's

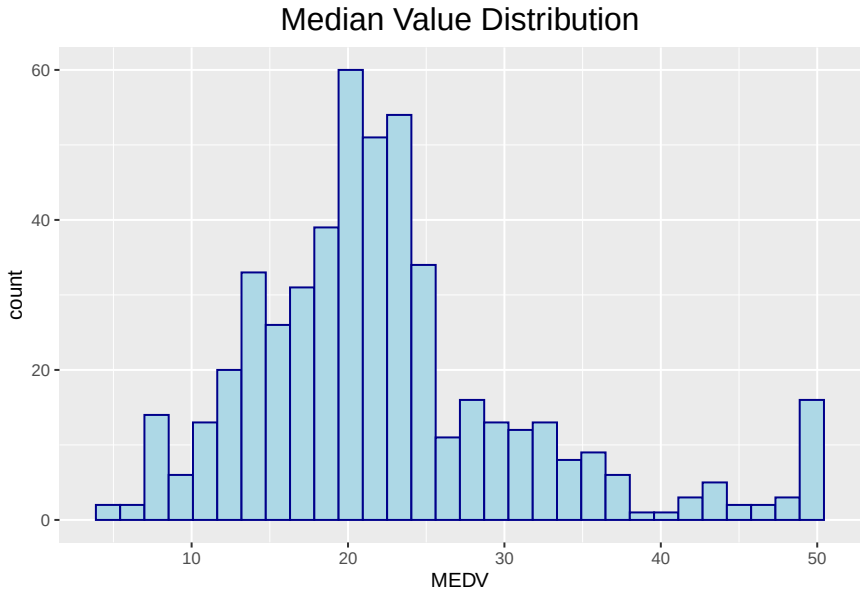
The data is displayed as follows.

```
##      CRIM ZN INDUS CHAS   NOX    RM  AGE    DIS RAD TAX PTRATIO      B LSTAT
## 1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900   1 296    15.3 396.90  4.98
## 2 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671   2 242    17.8 396.90  9.14
## 3 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671   2 242    17.8 392.83  4.03
## 4 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622   3 222    18.7 394.63  2.94
## 5 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622   3 222    18.7 396.90  5.33
## 6 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622   3 222    18.7 394.12  5.21
##   MEDV
## 1 24.0
## 2 21.6
```

```
## 3 34.7
## 4 33.4
## 5 36.2
## 6 28.7
```

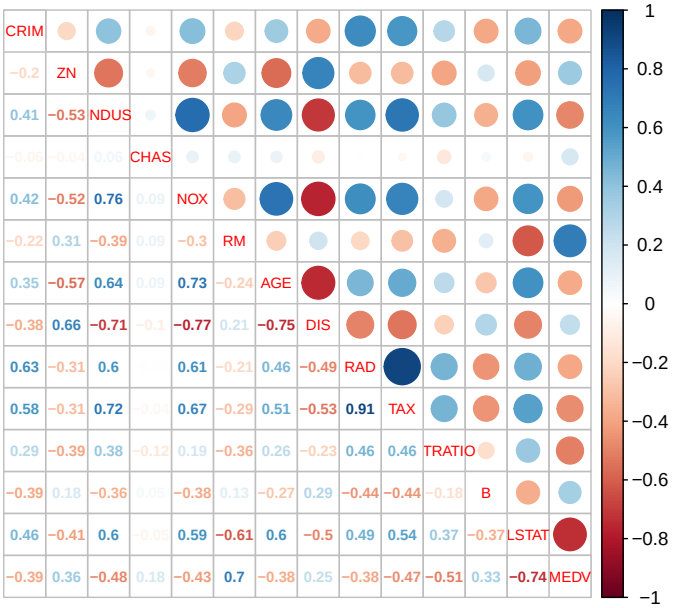
Exploratory Data Analysis

MEDV Distribution



The histogram demonstrates the values are not uniformly distributed. Rather, they follow a mostly normal distributions, with some outliers at the tail.

Correlation Matrix



While we produce many correlation values, we are firstly interested in how each attribute correlates to MEDV. This is represented by the bottom row or last column. We can immediately see the binary CHAS attribute does not correlate strongly with MEDV. However, it can be seen that RM (0.7) and LSTAT (-0.74) correlate with MEDV stronger than other attributes. Furthermore, the correlation between RM and LSTAT is -0.61. Since they do not correlate very strongly with one another, we can select both as predictor attributes without too much concern of collinearity for their case. The greatest correlation is between RAD and TAX of 0.91, and an R^2 of 0.82 thusly. Including both of these may raise some concerns regarding the minimal collinearity assumption of linear regression for these features.

Modelling and Regression

MedV takes the value for Y, along 13 feature attributes of the dataset, in the form of $Y = \beta_0 + \beta_1 x_1 + ... + \beta_n x_n$ + b.

Multiple Linear Regression

We chose to simply split the data in a 60/40 split for multiple Linear Regression.

```
#Setting seed for reproducible results
set.seed(1)

indices <-sample(1:nrow(data), 0.6 * nrow(data), replace = TRUE)
training <-data[indices,]
testing  <-data[-indices,]
```

Naively consider all features except the binary at onset for a MLR.

```
#Naively considering many attributes
multiModel1 <-lm(MEDV ~CRIM+ZN+INDUS+NOX+RM+AGE+DIS+RAD+TAX+PTRATIO+B+LSTAT, data=training)
summary(multiModel1)
```

```
##
## Call:
## lm(formula = MEDV ~ CRIM + ZN + INDUS + NOX + RM + AGE + DIS +
##     RAD + TAX + PTRATIO + B + LSTAT, data = training)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.7529  -2.3580  -0.3601   1.4662  25.0880
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  40.607269   6.933545   5.857 1.28e-08 ***
## CRIM         -0.117088   0.036419  -3.215  0.00145 **
## ZN            0.046371   0.016641   2.787  0.00568 **
## INDUS         0.098641   0.071828   1.373  0.17072
## NOX         -16.550316   5.088089  -3.253  0.00128 **
## RM            3.280962   0.577424   5.682 3.24e-08 ***
## AGE           0.013777   0.016774   0.821  0.41214
## DIS          -1.216793   0.250349  -4.860 1.92e-06 ***
## RAD           0.494834   0.078440   6.308 1.05e-09 ***
## TAX          -0.020556   0.004329  -4.749 3.22e-06 ***
## PTRATIO      -0.948615   0.160907  -5.895 1.04e-08 ***
## B             0.005826   0.003561   1.636  0.10289
## LSTAT        -0.635492   0.068081  -9.334  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.596 on 290 degrees of freedom
## Multiple R-squared:  0.7209, Adjusted R-squared:  0.7094
## F-statistic: 62.42 on 12 and 290 DF,  p-value: < 2.2e-16
```

Some initial insight is that LSTAT and RM indeed were strong predictors. Removing INDUS, AGE, and B, every attribute becomes a significant predictor, depending on alpha. Let's consider what happens if we remove RAD, which varies strongly with TAX.

```
##
## Call:
## lm(formula = MEDV ~ CRIM + ZN + NOX + RM + DIS + TAX + PTRATIO +
##     LSTAT, data = training)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -11.554  -2.727  -0.498   1.599  26.846
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.163e+01  6.530e+00   4.844 2.06e-06 ***
## CRIM        -7.328e-02  3.588e-02  -2.043   0.0420 *
## ZN           4.281e-02  1.755e-02   2.439   0.0153 *
## NOX         -1.114e+01  4.952e+00  -2.249   0.0252 *
## RM           3.799e+00  5.786e-01   6.566 2.34e-10 ***
## DIS         -1.247e+00  2.442e-01  -5.108 5.86e-07 ***
## TAX          5.472e-04  2.702e-03   0.203   0.8397
## PTRATIO     -8.010e-01  1.663e-01  -4.816 2.35e-06 ***
```

```
## LSTAT       -6.221e-01  6.418e-02  -9.693  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.886 on 294 degrees of freedom
## Multiple R-squared:  0.6802, Adjusted R-squared:  0.6715
## F-statistic: 78.16 on 8 and 294 DF,  p-value: < 2.2e-16
```

We can see that without RAD, TAX is no longer a strong predictor. As such, TAX adds predictive value in relation to RAD. The next model removes TAX and adds RAD back in.

```
##
## Call:
## lm(formula = MEDV ~ CRIM + ZN + NOX + RM + DIS + RAD + PTRATIO +
##     LSTAT, data = training)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -10.1059  -2.7763  -0.2535   1.3876  25.2754
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  39.92696    6.64060   6.013 5.41e-09 ***
## CRIM         -0.12935    0.03657  -3.537 0.000471 ***
## ZN            0.03885    0.01712   2.270 0.023954 *
## NOX         -18.55609    4.73339  -3.920 0.000110 ***
## RM            3.51728    0.56977   6.173 2.22e-09 ***
## DIS          -1.31761    0.23908  -5.511 7.80e-08 ***
## RAD           0.18688    0.04921   3.797 0.000178 ***
## PTRATIO      -0.97901    0.16325  -5.997 5.89e-09 ***
## LSTAT        -0.63314    0.06259 -10.116  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.771 on 294 degrees of freedom
## Multiple R-squared:  0.6951, Adjusted R-squared:  0.6868
## F-statistic: 83.77 on 8 and 294 DF,  p-value: < 2.2e-16
```

MSE and RMSE for model 1 and 3.

```
multiPredictions <-predict(multiModel1, testing)
RSS <- sum((testing$MEDV - multiPredictions)^2)
MSE1 <- mean((testing$MEDV - multiPredictions)^2)
RMSE1 <- sqrt(MSE1)

MSE1
```

```
## [1] 22.55438
```

```
RMSE1
```

```
## [1] 4.749145
```

```
multiPredictions <-predict(multiModel3, testing)
RSS3 <- sum((testing$MEDV - multiPredictions)^2)
MSE3 <- mean((testing$MEDV - multiPredictions)^2)
RMSE3 <- sqrt(MSE3)

MSE3
```

```
## [1] 23.02552
```

```
RMSE3
```

```
## [1] 4.798491
```

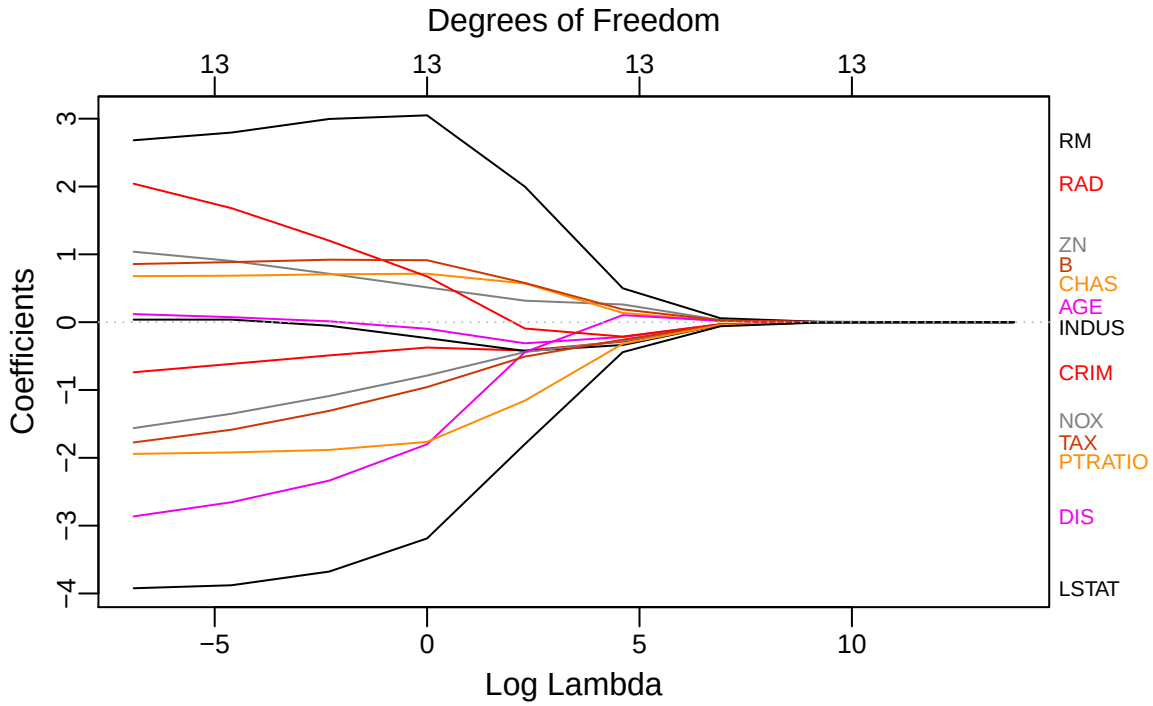
It seems we are left with 8 features. Lasso and Ridge will give us further insight into parameter selection.

It could also be noted that NOX has a much larger coefficient with larger error than the other predictors.

Ridge Regression

Constructing a Ridge model.

```
#lambda grid
grid <- 10^seq(6, -3, length=10)
#ridgeModel
ridge.mod <- glmnet(scale(x), y, alpha = 0, lambda = grid, thresh = 1e-2, standardize = TRUE)
#Plotting the ridge.mod
plot_glmnet(ridge.mod, xvar = "lambda", label = 13)
```

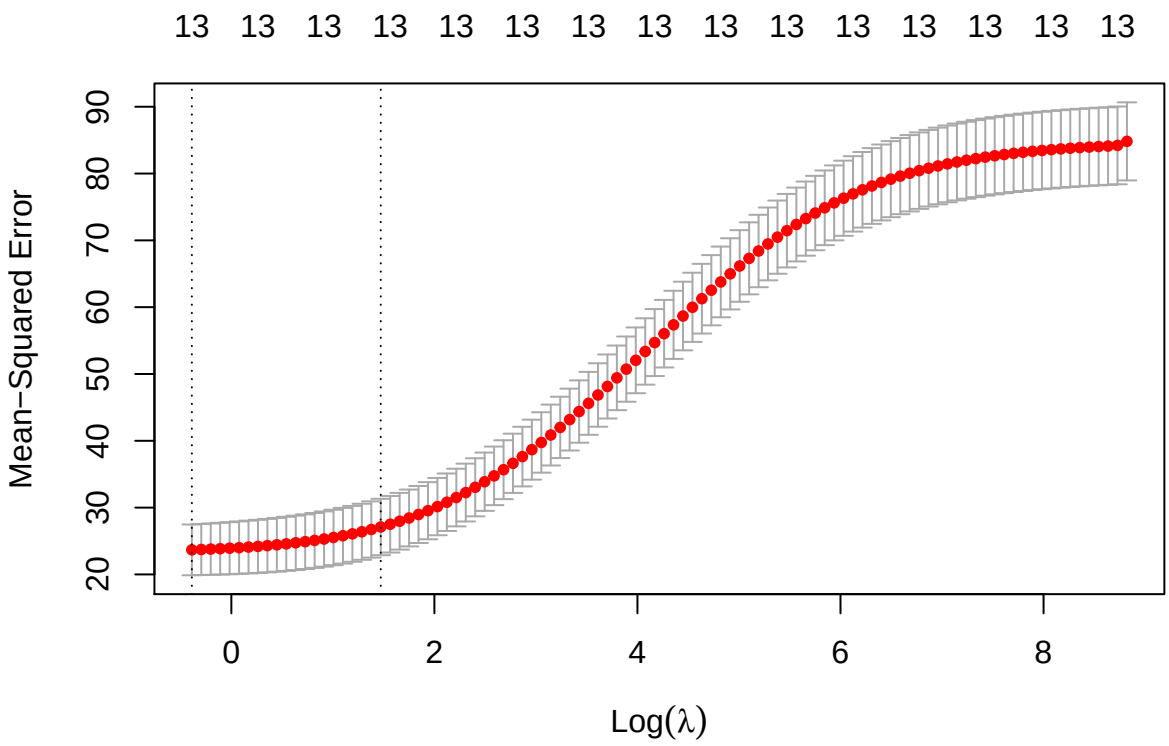


Considering a best lambda for the model and hyperparameter tuning.

```
cv.out <- cv.glmnet(x, y, alpha=0, nfolds = 10)
cv.out
```

```
##
## Call:  cv.glmnet(x = x, y = y, nfolds = 10, alpha = 0)
##
## Measure: Mean-Squared Error
##
##     Lambda Index Measure    SE Nonzero
## min  0.678   100   23.68 3.797      13
## 1se  4.357    80   27.10 4.220      13
```

```
plot(cv.out)
```




```
best.lambda <- cv.out$lambda.min
best.lambda
```

```
## [1] 0.6777654
```

Considering coefficients for Ridge.

```
#Viewing coefficients of scaled full ridge model
predict(ridge.mod, type="coefficients", s=best.lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                       1
## (Intercept) 22.53280632
## CRIM        -0.41568230
## ZN           0.58454162
## INDUS       -0.16968729
## CHAS         0.71113369
## NOX         -0.89496390
## RM           3.03015102
## AGE         -0.05816081
## DIS         -1.99196163
## RAD          0.86276996
## TAX         -1.08247269
## PTRATIO     -1.80779900
## B            0.91568362
## LSTAT       -3.36321495
```

```r
#Selecting above abs(1): NOX, DIS, PTRATIO, LSTAT, RM
newX = data.mat[, c(5,6,8,11,13)]
head(newX)
```

```
##     NOX    RM    DIS PTRATIO LSTAT
## 1 0.538 6.575 4.0900    15.3  4.98
## 2 0.469 6.421 4.9671    17.8  9.14
## 3 0.469 7.185 4.9671    17.8  4.03
## 4 0.458 6.998 6.0622    18.7  2.94
## 5 0.458 7.147 6.0622    18.7  5.33
## 6 0.458 6.430 6.0622    18.7  5.21
```

```r
#Final ridge with all coefficients
ridge.final1 <- glmnet(x, y, alpha = 0, lambda = best.lambda, thresh=1e-2, standardsize = TRUE)
predict(ridge.final1, type="coefficients", s=best.lambda)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                           1
## (Intercept)  24.811787388
## CRIM         -0.051540889
## ZN            0.025444744
## INDUS        -0.111469005
## CHAS          2.950592527
## NOX         -12.202495338
## RM            4.572000162
## AGE          -0.011122797
## DIS          -1.212875203
## RAD           0.096752050
## TAX          -0.004456126
## PTRATIO      -0.836004412
## B             0.009830260
## LSTAT        -0.405092069
```

```r
#Final ridge with only 5 coefficients
ridge.final2 <- glmnet(newX, y, alpha = 0, lambda = best.lambda, thresh=1e-2, standardsize = TRUE)
predict(ridge.final2, type="coefficients", s=best.lambda)
```

```
## 6 x 1 sparse Matrix of class "dgCMatrix"
##                          1
## (Intercept)  29.4519872
## NOX         -12.6387422
## RM            4.5085207
## DIS          -0.7280733
## PTRATIO      -1.0318123
## LSTAT        -0.5087480
```

Considering MSE and RMSE for Ridge using all coefficients.

```r
ridge.pred1 <- predict(ridge.final1, s=best.lambda, newx=x)
ridge.MSE = mean((ridge.pred1 -y)^2)
ridge.RMSE = sqrt(mean((ridge.pred1 - y)^2))

ridge.MSE
```

```
## [1] 22.89447
```

```
ridge.RMSE
```

```
## [1] 4.784817
```

Considering MSE and RMSE for Ridge using only 5 coefficients.

```
ridge.pred2 <- predict(ridge.final2, s=best.lambda, newx=newX)
ridge.MSE = mean((ridge.pred2 -y)^2)
ridge.RMSE = sqrt(mean((ridge.pred2 - y)^2))

ridge.MSE
```

```
## [1] 25.09644
```

```
ridge.RMSE
```

```
## [1] 5.009635
```

Considering R squared for each model manually

```
yBar = mean(y)
RSS1 = sum((ridge.pred1 - y)^2)
TSS1 = sum((y - yBar)^2)
rsq1 = 1 - (RSS1/TSS1)
rsq1
```

```
## [1] 0.7288013
```

```
RSS2 = sum((ridge.pred2 - y)^2)
TSS2 = sum((y - yBar)^2)
rsq2 = 1 - (RSS2/TSS2)
rsq2
```

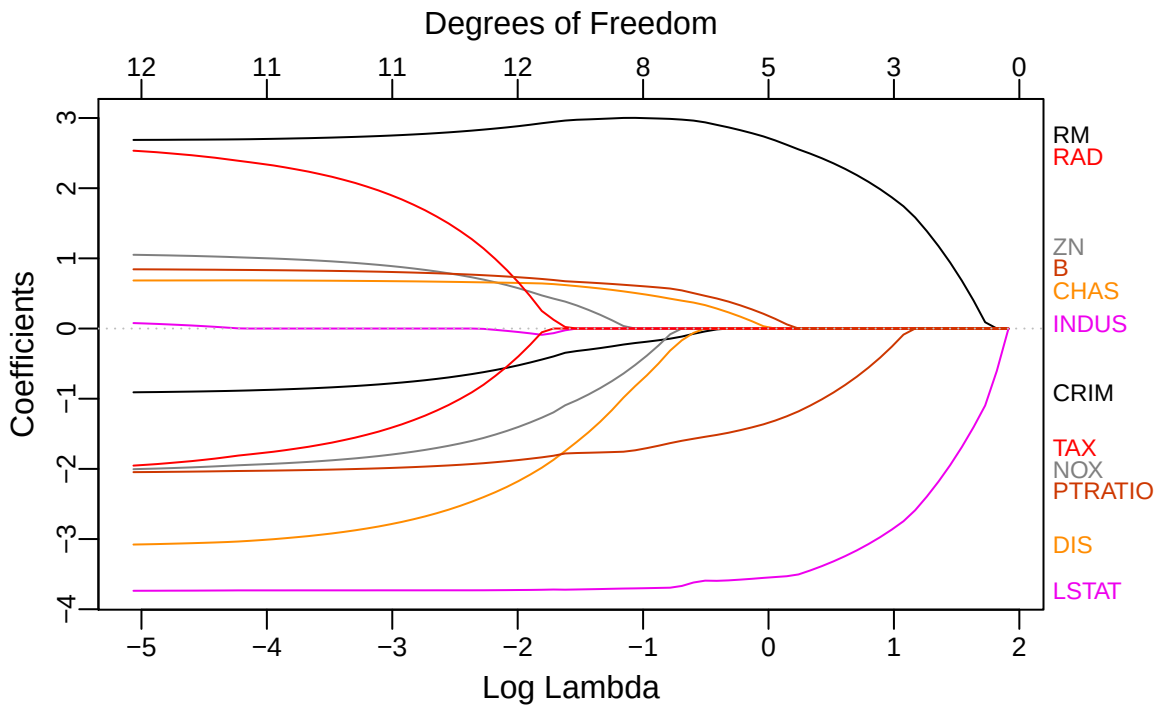
```
## [1] 0.7027177
```

Lasso Regression

The Lasso regression is using regularization method based on the ł1 norm of the regression coefficients vector. This regularization yields sparse models by forcing some regression coefficients exactly to zero when regularization parameter λ is sufficiently large. Thus, Lasso regression performs variables selection and produces simpler models, which are easier to interpret.

We use the same range of the regularization parameter, λ, values as for the Ridge regression, but sample this range more densely as it provided better results for selecting different numbers of non-zero input variables. The values of the Lasso regression coefficients for various λ are shown below. It is evident that with increasing λ some of the regression coefficients are forced to zero and the number of degrees of freedom is decreasing. Based on the Lasso variable selection results the most important predictors that have non-zero regression coefficients even for large λ are the RM and LSTAT variables. This observation is consistent with the conclusions of the exploratory data analysis section.

```
grid <- 10^seq(6, -3, length=100)
lasso.mod <- glmnet(scale(x), y) #default alpha=1
plot_glmnet(lasso.mod, xvar="lambda", label = 12)
```

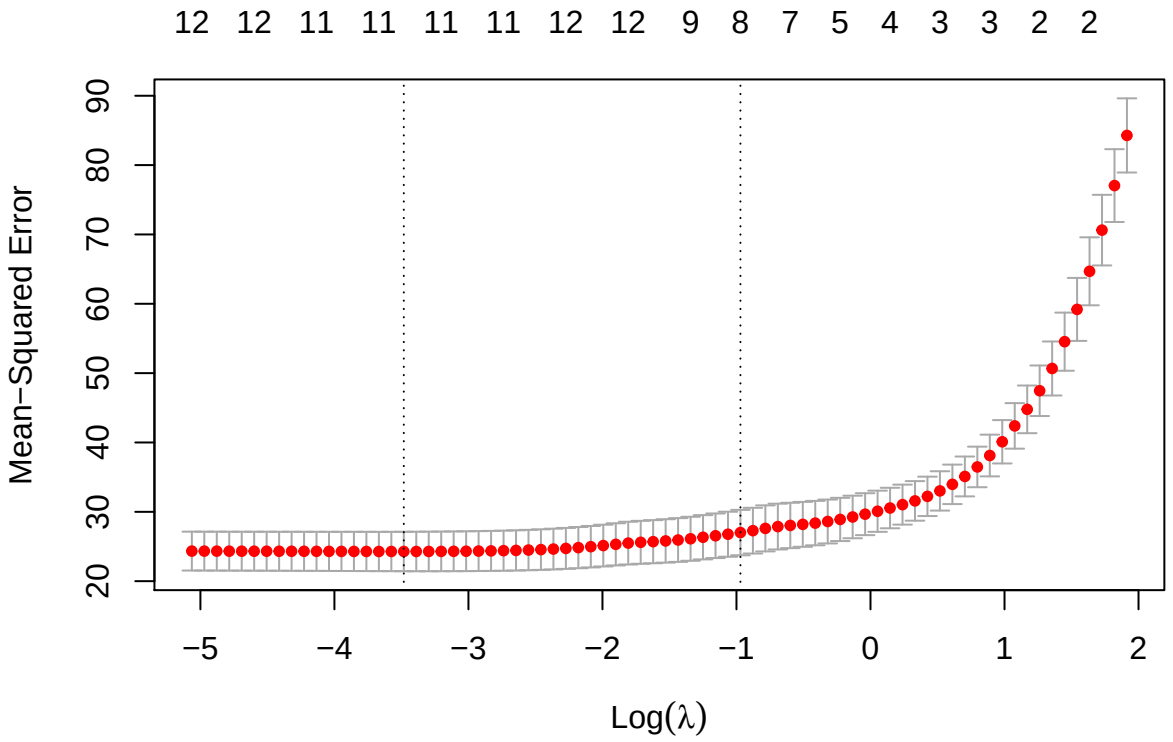


We use a 10-fold cross-validation approach to select the optimum value of λ. More detailed discussion on the cross-validation algorithm for the Lasso regression is given in the section " K-Fold Cross Validation ". The minimum MSE is produced for $\lambda = 0.0307$, which keeps 11 non-zero regression coefficients.

```
##cross-validation
lasso.cv.out <- cv.glmnet(scale(x), y, alpha=1, nfolds = 10)
lasso.cv.out
```

```
##
## Call:  cv.glmnet(x = scale(x), y = y, nfolds = 10, alpha = 1)
##
## Measure: Mean-Squared Error
##
##     Lambda Index Measure    SE Nonzero
## min 0.0307    59   24.28 2.844      11
## 1se 0.3789    32   27.01 3.275       8
```

```
plot(lasso.cv.out)
```



The coefficients of the Lasso regression for the optimum values of λ corresponding to the 11 non-zero regression coefficients is given below. We also plot the predicted home price values versus the true values and calculate the MSE and RMSE regression errors.

```
#keep few predictors in lasso
lasso.best.lambda <- lasso.cv.out$lambda[which.max(lasso.cv.out$nzero == 11)]
#lasso.final <- glmnet(scale(x), y, alpha=1, lambda=grid)
lasso.final <- glmnet(x, y, alpha=1, lambda=grid)
predict(lasso.final, type="coefficients", s=lasso.best.lambda )
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        1
## (Intercept) 23.512082531
## CRIM        -0.041774090
## ZN           0.016232882
## INDUS       -0.005184322
## CHAS         2.437746370
## NOX         -9.548458409
## RM           4.212602160
## AGE          .
## DIS         -0.829159065
## RAD          0.007102791
## TAX          .
## PTRATIO     -0.828101442
## B            0.007433893
## LSTAT       -0.520933847
```

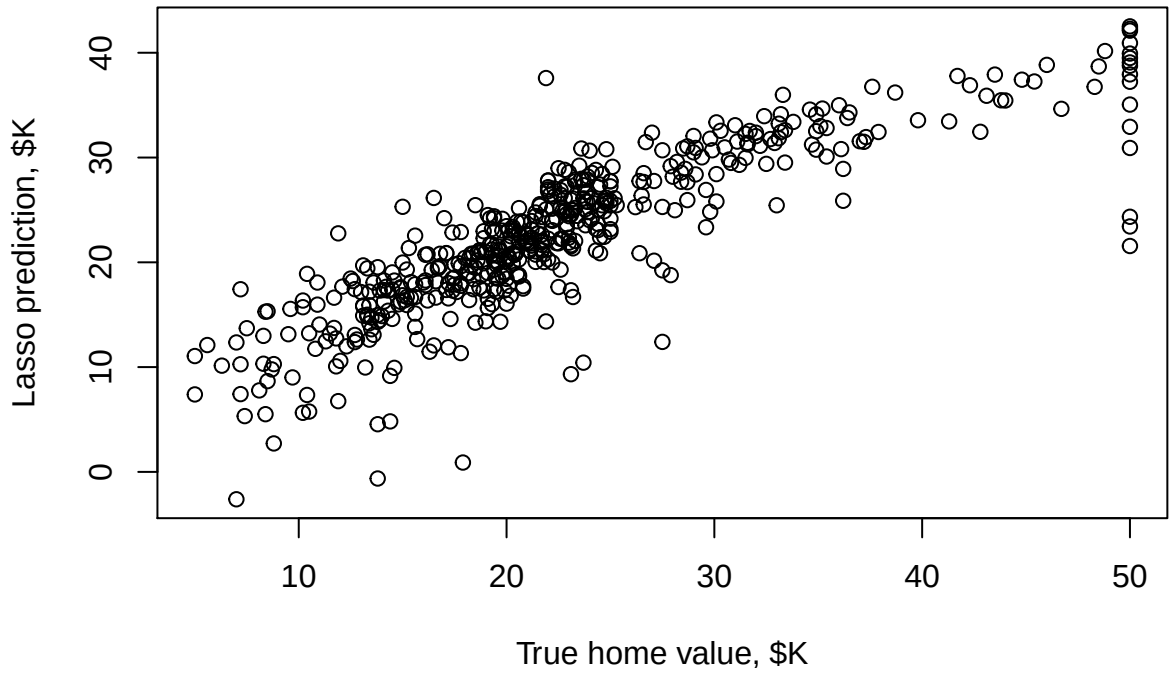
```
lasso.pred <- predict(lasso.final, s=lasso.best.lambda, newx=x)
print(paste('MSE:', mean((lasso.pred - y)^2)))
```

```
## [1] "MSE: 23.4455599763479"
```

```
print(paste('RMSE:', sqrt(mean((lasso.pred - y)^2))))
```

```
## [1] "RMSE: 4.84206154198271"
```

```
plot(y, lasso.pred,  xlab="True home value, $K", ylab="Lasso prediction, $K",)
```



Considering the R squared for the 11 selector Lasso model.

```
yBar = mean(y)
lassoRSS = sum((lasso.pred - y)^2)
lassoTSS = sum((y - yBar)^2)
rsq = 1 - (lassoRSS/lassoTSS)
rsq
```

```
## [1] 0.7222734
```

Next we further reduced the number of non-zero regression coefficients to keep only 5 most important predictors. The coefficients of the Lasso regression and the plot of the predicted home price versus the true

home prices are shown below. We also calculate the MSE and RMSE errors for the case of 5 predictors. As expected, the scatter of the plot and the MSE/RMSE errors are somewhat higher compared to the case of 11 predictors, but the Lasso model is still providing acceptable results in terms of predicting the home values based on only 5 predictors.

```
# check for fewer predictors
lasso.best.lambda <- lasso.cv.out$lambda[which.max(lasso.cv.out$nzero == 5)]
lasso.final <- glmnet(x, y, alpha=1, lambda=grid)
predict(lasso.final, type="coefficients", s=lasso.best.lambda )
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                         1
## (Intercept) 15.156492728
## CRIM         .
## ZN           .
## INDUS        .
## CHAS         0.130133129
## NOX          .
## RM           3.895113886
## AGE          .
## DIS          .
## RAD          .
## TAX          .
## PTRATIO     -0.630418762
## B            0.002297575
## LSTAT       -0.497652218
```

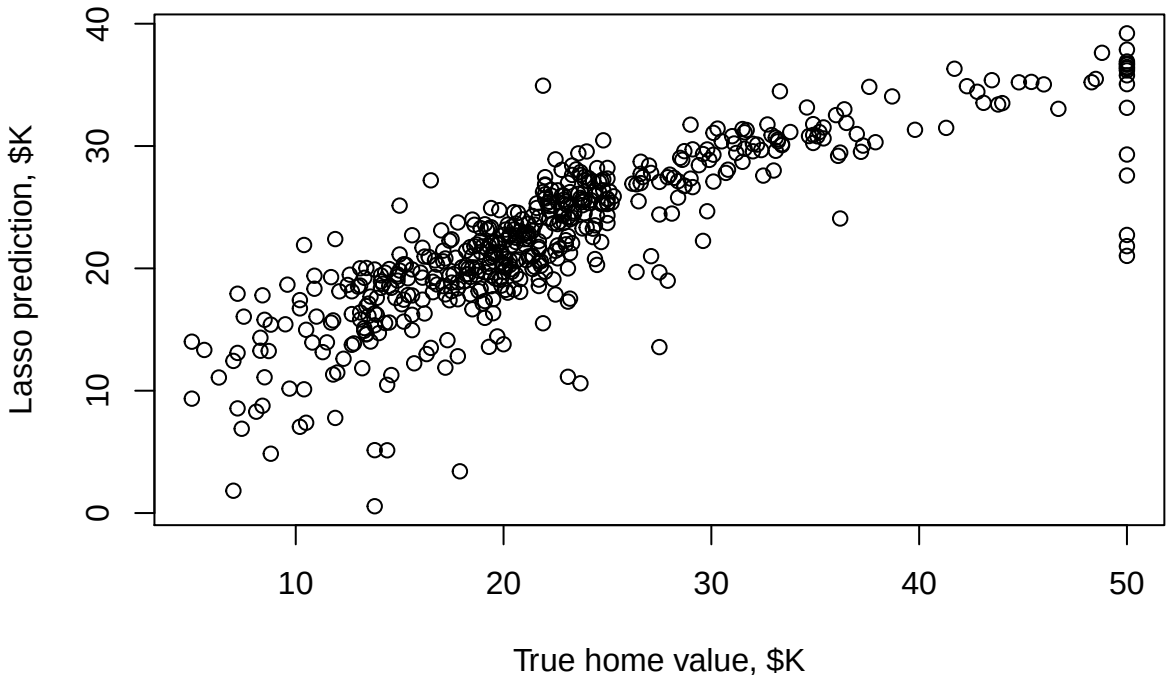
```
lasso.pred <- predict(lasso.final, s=lasso.best.lambda, newx=x)
print(paste('MSE:', mean((lasso.pred - y)^2)))
```

```
## [1] "MSE: 28.2507097708968"
```

```
print(paste('RMSE:', sqrt(mean((lasso.pred - y)^2))))
```

```
## [1] "RMSE: 5.31513967557738"
```

```
plot(y, lasso.pred, xlab="True home value, $K", ylab="Lasso prediction, $K",)
```



Considering the R squared for the 5 selector Lasso model.

```
yBar = mean(y)
lassoRSS = sum((lasso.pred - y)^2)
lassoTSS = sum((y - yBar)^2)
rsq = 1 - (lassoRSS/lassoTSS)
rsq
```

```
## [1] 0.6653535
```

K-Fold Cross Validation

In a standard for the analysis of the algorithm performace a part of the data is reserved as a test set and the rest of the data is used as a training set. This may lead to a highly variable test error depending on how the dataset was split. Moreover, the machine learning approaches tend to perform worse when less data are used for training, which happens when a part of the data has to be reserved for the test set.

For optimization of the Lasso regression we are employing a cross-validation (CV) technique as it helps to alleviate the above problems. Specifically, we use a K-fold cross validation where one fold is used as a test set while the remaining (K-1) folds are used as the training set. After a given data fold is tested the algorithm computes the obtained MSE for this fold and moves to another one. Thus, every data point in the set is a part of the training and the test set for some folds. The final K-fold CV mean squared error (MSE) error is computed as the mean of the MSE of individual folds.

In practice K = 5 or 10 tend to provide the best results as they yield a test error that does not suffer from excessively high bias, nor from very high variance. We chose to use the 10-fold cross-validation approach (K = 10).

The 10-fold CV MSE is computed for each value of λ on the grid that we have defined. Finally, the CV algorithm chooses the value of λ that minimizes the 10-fold CV MSE. In developing models based on the Lasso approach we also used higher values of λ to select the 5 most important predictors.

The final MSE's and RMSE's achieved by different regression approaches are given in the table below:

	MSE	RMSE	R^2
Multiple 12	22.554	4.749	0.720
Multiple 8	23.025	4.798	0.695
Ridge 13	22.894	4.784	0.728
Ridge 5	25.096	5.009	0.702
Lasso 11	23.445	4.842	0.722
Lasso 5	28.250	5.315	0.665

The above results suggest that having more independent variables as an input to regression provides overall smaller MSE and RMSE errors. However, the difference in errors between the Ridge regression and Lasso regression with 11 input variables is small. Furthermore, Lasso regression with only 5 most significant predictors still yields RMSE error, which is only 9.8 % higher compared to the results with 11 predictors. Thus, Lasso approach enables significant reduction in the model complexity and dataset requirements without significant loss of accuracy.

Explicit Regression Formula

The following display the regression formula more explicitly for each finalized model in which the parameters were tuned and selected. The coefficients for initial models with many more coefficients can still be seen above as output.

Multiple Linear Regression (8)

Top 8 were chosen by removing what was not statistically significant and observing if the leftover taken together were significant.

MEDV = (-0.12935)CRIM +(0.03885)ZN +(-18.55609)NOX +(3.51728)RM +(-1.31761)DIS +(0.18688)RAD +(-0.97901)PTRATIO +(-0.63314)LSTAT +39.92696

Ridge Regression (5)

Top 5 were chosen when selecting the greatest 5 coefficients when input was scaled.

MEDV = (-12.6387422)NOX +(4.5085207)RM +(-0.7280733)DIS +(-1.0318123)PTRATIO +(-0.5087480)LSTAT +(29.4519872)

Lasso Regression (11)

This Lasso had more parameters and a discretized lambda grid with larger intervals.

MEDV = (-0.041774090)CRIM + (0.016232882)ZN + (-0.005184322)INDUS + (2.437746370)CHAS + (-9.548458409)NOX + (4.212602160)RM + (-0.829159065)DIS + (0.007102791)RAD + (-0.828101442)PTRATIO + (0.007433893)B + (-0.520933847)LSTAT + 23.512082531

Lasso Regression (5)

MEDV = (0.130133129)CHAS+(3.895113886)RM+(-0.630418762)PTRATIO+(0.002297575)B +(-0.497652218)LSTAT +(15.156492728)

Summary

The goal was to model MEDV, the median value of owner occupied homes (in $1,000s), based on given features. MEDV follows a skewed normal distribution with some outliers at its tail. Three regression techniques were performed to model the data: multiple linear regression, Ridge, and Lasso. It was observed that TAX only became a predictor in MLR when RAD was included in, so TAX was removed. Removing insignificant predictors (to alpha) left 8 features. Ridge was performed using all features. Then Ridge was modified to include the 5 greatest predictors. This was determined by taking the greatest absolute value of the coefficients when input was scaled. Lasso was performed with 11 then 5 predictors. Among all methods, LSTAT, RM, and PTRatio remained as significant predictors for MEDV. Having more independent variables as an input to regression provides overall smaller MSE and RMSE errors. However, the difference in errors between Multiple Ridge and Lasso, each with mostly all input variables (11, 12, or 13), was small. This changed by different amounts when hyperparamater tuning or selection took place.

Citations

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