# Lab 5

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## 11:59PM March 16, 2019

Load the Boston housing data frame and create the vector y (the median value) and matrix X (all other features) from the data frame. Name the columns the same as Boston except for the first name it "(Intercept)".

```
data(Boston, package = "MASS")
y = Boston$medv
X = as.matrix(cbind(1, Boston[, 1 : 13]))
colnames(X)[1] = "(Intercept)"
```

Run the OLS linear model to get b, the vector of coefficients. Do not use lm.

```
b = solve(t(X) %*% X) %*% t(X) %*% y
```

Find the hat matrix for this regression H and find its rank. Is this rank expected?

```
H = X %*% solve(t(X) %*% X) %*% t(X)
dim(H)
```

```
## [1] 506 506
pacman::p_load(Matrix)
rankMatrix(H)
```

```
## [1] 14
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 1.123546e-13
```

Verify this is a projection matrix by verifying the two sufficient conditions. Use the testthat library's expect\_equal(matrix1, matrix2, tolerance = 1e-2).

```
pacman::p_load(testthat)
expect_equal(H, t(H), tolerance = 1e-2)
expect_equal(H %*% H, H, tolerance = 1e-2)
```

Find the matrix that projects onto the space of residuals H\_comp and find its rank. Is this rank expected?

```
I = diag(nrow(H))
H_comp = (I - H)
rankMatrix(H_comp)
```

```
## [1] 497
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 1.123546e-13
```

Verify this is a projection matrix by verifying the two sufficient conditions. Use the testthat library.

```
expect_equal(H_comp, t(H_comp), tolerance = 1e-2)
expect_equal(H_comp %*% H_comp, H_comp, tolerance = 1e-2)
Calculate \hat{y}.
yhat = H %*% y
#yhat
Calculate e as the difference of y and \hat{y} and the projection onto the space of the residuals. Verify the two
means of calculating the residuals provide the same results.
e = y - yhat
e_2 = H_{comp \% * \% y}
expect_equal(e, e_2)
Calculate \mathbb{R}^2 and RMSE.
sse = sum(e^2)
sst = sum((y - mean(y))^2)
Rsquared = 1 - sse / sst
Rsquared
## [1] 0.7406427
mse = sse / (nrow(X) - ncol(X))
rmse = sqrt(mse) #rmse is standard deviation of errors
rmse
## [1] 4.745298
Verify \hat{y} and e are orthogonal.
t(e) %*% yhat
##
                   [,1]
## [1,] -4.991142e-08
Verify \hat{y} - \bar{y} and e are orthogonal.
t(e) %*% (yhat - mean(y))
##
                  [,1]
## [1,] 2.832162e-09
Find the cosine-squared of y - \bar{y} and \hat{y} - \bar{y} and verify it is the same as R^2.
y_minus_y_bar = y - mean(y)
yhat_minus_y_bar = yhat - mean(y)
len_y_minus_y_bar = sqrt( sum(y_minus_y_bar^2) )
len_yhat_minus_y_bar = sqrt( sum(yhat_minus_y_bar^2) )
theta = acos( (t(y_minus_y_bar) %*% yhat_minus_y_bar) / (len_y_minus_y_bar * len_yhat_minus_y_bar) )
#cos_theta * (180 / pi)
cos_theta_sqrd = cos(theta)^2
cos_theta_sqrd
##
               [,1]
## [1,] 0.7406427
```

Verify the sum of squares identity which we learned was due to the Pythagorean Theorem (applies since the projection is specifically orthogonal).

```
len_y_minus_y_bar^2 - len_yhat_minus_y_bar^2 - sse
```

```
## [1] 5.666152e-09
```

Create a matrix that is  $(p+1) \times (p+1)$  full of NA's. Label the columns the same columns as X. Do not label the rows. For the first row, find the OLS estimate of the y regressed on the first column only and put that in the first entry. For the second row, find the OLS estimates of the y regressed on the first and second columns of X only and put them in the first and second entries. For the third row, find the OLS estimates of the y regressed on the first, second and third columns of X only and put them in the first, second and third entries, etc. For the last row, fill it with the full OLS estimates.

```
M = matrix(NA, nrow = ncol(X), ncol = ncol(X))
colnames(M) = colnames(X)
X_j = X[, 1, drop = FALSE]
b = solve(t(X_j) %*% X_j) %*% t(X_j) %*% y
M[1, 1] = b
X_{j_2} = X[, 1:2]
b = solve(t(X_j_2) %*% X_j_2) %*% t(X_j_2) %*% y
                       [,1]
##
## (Intercept) 24.0331062
## crim
                -0.4151903
for(j in 1 : ncol(M)){
  X_j = X[, 1 : j, drop = FALSE]
  b = solve(t(X_j) %*% X_j) %*% t(X_j) %*% y
  M[j, 1:j] = b
}
round(M, 2)
##
          (Intercept)
                       crim
                               zn indus chas
                                                 nox
                                                        rm
                                                             age
                                                                    dis
                                                                          rad
    [1,]
                22.53
                               NA
##
                         NA
                                     NA
                                           NA
                                                  NA
                                                        NA
                                                              NA
                                                                     NA
                                                                           NA
##
    [2,]
                24.03 -0.42
                               NA
                                                                     NA
                                                                           NA
                                     NA
                                           NA
                                                  NA
                                                        NA
                                                              NA
##
    [3,]
                22.49 -0.35 0.12
                                     NA
                                           NA
                                                  NA
                                                        NA
                                                              NA
                                                                     NA
                                                                           NA
##
    [4,]
                27.39 -0.25 0.06 -0.42
                                                  NA
                                           NA
                                                        NA
                                                              NA
                                                                     NA
                                                                           NA
##
    [5,]
                27.11 -0.23 0.06 -0.44 6.89
                                                  NA
                                                        NA
                                                              NA
                                                                     NA
                                                                           NA
##
    [6,]
                29.49 -0.22 0.06 -0.38 7.03
                                               -5.42
                                                                     NA
                                                                           NA
                                                        NA
                                                              NA
##
    [7,]
               -17.95 -0.18 0.02 -0.14 4.78
                                               -7.18 7.34
                                                              ΝA
                                                                     NA
                                                                           NA
##
    [8,]
               -18.26 -0.17 0.01 -0.13 4.84
                                               -4.36 7.39 -0.02
                                                                     NA
                                                                           NA
    [9,]
                 0.83 -0.20 0.06 -0.23 4.58 -14.45 6.75 -0.06 -1.76
                                                                           NA
##
  [10,]
                 0.16 -0.18 0.06 -0.21 4.54 -13.34 6.79 -0.06 -1.75
                                                                        -0.05
   [11,]
                 2.99 -0.18 0.07 -0.10 4.11 -12.59 6.66 -0.05 -1.73
##
                                                                         0.16
                27.15 -0.18 0.04 -0.04 3.49 -22.18 6.08 -0.05 -1.58
##
   [12,]
                                                                         0.25
                20.65 -0.16 0.04 -0.03 3.22 -20.48 6.12 -0.05 -1.55
## [13,]
                                                                         0.28
                36.46 -0.11 0.05 0.02 2.69 -17.77 3.81 0.00 -1.48
## [14,]
                                                                         0.31
           tax ptratio black lstat
##
##
            NA
                     NA
                            NA
                                  NA
    [1,]
    [2,]
##
             NA
                     NA
                            NA
                                  NA
    [3,]
##
             NA
                     NA
                            NA
                                  NA
##
    [4,]
             NA
                     NA
                            NA
                                  NA
##
    [5,]
             NA
                     NA
                            NA
                                  NA
##
    [6,]
             NA
                     NA
                            NA
                                  NA
##
    [7,]
             NA
                     NA
                            NA
                                  NA
```

```
[8,]
             NA
##
                       NA
                              NA
                                    NA
##
    [9,]
                              NA
             NA
                       NA
                                    NA
  [10,]
             NA
                       NA
                              NA
                                    NA
## [11,] -0.01
                              NA
                       NA
                                    NA
## [12,] -0.01
                   -1.00
                              NA
                                    NA
                   -1.01
                           0.01
## [13,] -0.01
                                    NA
## [14,] -0.01
                   -0.95
                           0.01 - 0.52
```

Examine this matrix. Why are the estimates changing from row to row as you add in more predictors? As we add more predictors the estimates change because of the different associations between the variables, its effect makes the stimators to chance as we add more and more.

Clear the workspace and load the diamonds dataset.

```
pacman::p_load(ggplot2)
data(diamonds, package = "ggplot2")
```

Extract y, the price variable and "c", the nominal variable "color" as vectors.

#### summary(diamonds)

```
##
        carat
                               cut
                                           color
                                                         clarity
##
    Min.
                                                      SI1
            :0.2000
                       Fair
                                 : 1610
                                           D: 6775
                                                              :13065
    1st Qu.:0.4000
                       Good
                                 : 4906
                                           E: 9797
                                                      VS2
                                                              :12258
##
    Median :0.7000
                       Very Good: 12082
                                           F: 9542
                                                      SI2
                                                              : 9194
##
            :0.7979
                       Premium
                                :13791
                                           G:11292
                                                      VS1
                                                              : 8171
    Mean
                                                      VVS2
##
    3rd Qu.:1.0400
                       Ideal
                                 :21551
                                           H: 8304
                                                              : 5066
##
    Max.
            :5.0100
                                           I: 5422
                                                      VVS1
                                                              : 3655
##
                                           J: 2808
                                                      (Other): 2531
                                            price
##
                          table
        depth
                                                                x
##
    Min.
            :43.00
                              :43.00
                                                  326
                                                                 : 0.000
                      Min.
                                       Min.
                                                         Min.
##
    1st Qu.:61.00
                      1st Qu.:56.00
                                        1st Qu.:
                                                  950
                                                         1st Qu.: 4.710
    Median :61.80
                      Median :57.00
                                       Median: 2401
                                                         Median : 5.700
##
##
    Mean
            :61.75
                      Mean
                              :57.46
                                       Mean
                                               : 3933
                                                         Mean
                                                                 : 5.731
                      3rd Qu.:59.00
                                        3rd Qu.: 5324
##
    3rd Qu.:62.50
                                                         3rd Qu.: 6.540
##
    Max.
            :79.00
                      Max.
                              :95.00
                                       Max.
                                               :18823
                                                         Max.
                                                                 :10.740
##
##
           у
                             z
                               : 0.000
            : 0.000
##
    Min.
                       Min.
                       1st Qu.: 2.910
##
    1st Qu.: 4.720
##
    Median : 5.710
                       Median : 3.530
##
    Mean
            : 5.735
                               : 3.539
                       Mean
    3rd Qu.: 6.540
                       3rd Qu.: 4.040
##
    Max.
            :58.900
                               :31.800
                       Max.
##
y = diamonds$price
c = diamonds$color
table(c)
```

```
## c
## D E F G H I J
## 6775 9797 9542 11292 8304 5422 2808
```

Convert the "c" vector to X which contains an intercept and an appropriate number of dummies. Let the color G be the reference category as it is the modal color. Name the columns of X appropriately. The first should be "(Intercept)". Delete G.

```
X = rep(1, nrow(diamonds))
X = cbind(X, diamonds$color == 'D')
X = cbind(X, diamonds$color == 'E')
X = cbind(X, diamonds$color == 'F')
X = cbind(X, diamonds$color == 'H')
X = cbind(X, diamonds$color == 'I')
X = cbind(X, diamonds$color == 'J')
colnames(X) = c("Intercept", "is_D", "is_E", "is_F", "is_H", "is_I", "is_J")
head(X)
        Intercept is_D is_E is_F is_H is_I is_J
##
## [1,]
                1
                      0
                           1
                                0
                                     0
## [2,]
                 1
                      0
                           1
                                      0
                                                0
## [3,]
                                0
                                     0
                      0
                           1
                                           0
                                                0
                 1
## [4,]
                      0
                           0
                                0
                                     0
                1
                                           1
                                                0
## [5,]
                      0
                           0
                                0
                                      0
                                                1
                1
## [6,]
Repeat the iterative exercise above we did for Boston here.
b = solve(t(X) %*% X) %*% t(X) %*% y
M = matrix(NA, nrow = ncol(X), ncol = ncol(X))
colnames(M) = colnames(X)
X_j = X[, 1, drop = FALSE]
b = solve(t(X_j) %*% X_j) %*% t(X_j) %*% y
M[1, 1] = b
X_{j_2} = X[, 1:2]
b = solve(t(X_j_2) %*% X_j_2) %*% t(X_j_2) %*% y
                   [,1]
## Intercept 4042.3784
             -872.4243
## is D
for(j in 1 : ncol(M)){
  X_j = X[, 1 : j, drop = FALSE]
  b = solve(t(X_j) %*% X_j) %*% t(X_j) %*% y
 M[j, 1:j] = b
}
round(M, 2)
##
        Intercept
                                is_E
                                         is_F
                                                is_H
                                                        is_I
                                                                 is_J
                       is_D
## [1,]
          3932.80
                         NA
                                  NA
                                           NA
                                                  NA
                                                           NA
                                                                   NA
## [2,]
          4042.38 -872.42
                                  NA
                                           NA
                                                  NA
                                                           NA
                                                                   NA
## [3,]
          4295.54 -1125.59 -1218.79
                                                  NA
                                                           NA
                                                                   NA
## [4,]
          4491.23 -1321.28 -1414.48 -766.34
                                                           NA
                                                                   NA
                                                  NA
## [5,]
          4493.17 -1323.22 -1416.42 -768.28
                                              -6.50
                                                           NA
                                                                   NA
## [6,]
          4262.94 -1092.99 -1186.19 -538.06 223.72 828.93
                                                                   NΑ
```

Why didn't the estimates change as we added more and more features?

3999.14 -829.18 -922.38 -274.25 487.53 1092.74 1324.68

## [7,]

# TO-DO

Create a vector y by simulating n = 100 standard iid normals. Create a matrix of size  $100 \times 2$  and populate the first column by all ones (for the intercept) and the second column by 100 standard iid normals. Find the  $R^2$  of an OLS regression of  $y \sim X$ . Use matrix algebra.

```
y = rnorm(100, mean = 0, sd = 1)
intercept = rep(1, 100)
X = cbind(intercept, rnorm(100, mean = 0, sd = 1))
##
        intercept
## [1,]
                1 -1.66074889
## [2,]
                1 0.51295296
## [3,]
                1 -1.67630958
## [4,]
                1 0.09649496
## [5,]
                1 1.37781493
## [6,]
                1 1.09246027
H = X \% *\% solve(t(X) \% *\% X) \% *\% t(X)
yhat = H %*% y
e = y - yhat
sse = sum(e^2)
sst = sum((y - mean(y))^2)
Rsquared = 1 - sse / sst
Rsquared
## [1] 0.008503835
reg = lm(y \sim X)
```

from the last problem. Find the  $\mathbb{R}^2$  of an OLS regression of y ~ X. You can use the summary function of an lm model.

Write a for loop to each time bind a new column of 100 standard iid normals to the matrix X and find the  $R^2$  each time until the number of columns is 100. Create a vector to save all  $R^2$ 's. What happened??

```
n = 100
N = 100 - 2
v = rep(NA, 98)
for (i in 1 : N ){
    colm = rnorm(100, mean = 0, sd = 1)
    X = cbind(X, colm)
    v[i] = summary(lm(y ~ X))$r.squared
}
## [1] 0.01383835 0.01385991 0.03577735 0.04105826 0.04549885 0.05058290
## [7] 0.05100189 0.05105692 0.06681203 0.08915309 0.08940169 0.09102598
## [13] 0.09780512 0.10047727 0.11274099 0.15662943 0.15751082 0.15756278
```

## [19] 0.15758803 0.16113063 0.16183604 0.16597154 0.16608310 0.18643102 ## [25] 0.21324908 0.21433170 0.22104419 0.23411068 0.25626521 0.26335643 ## [31] 0.27022129 0.30848908 0.31191956 0.32994215 0.33951773 0.33966708

```
## [37] 0.34962502 0.34993271 0.35946771 0.36687123 0.37567581 0.37756223
## [43] 0.38237060 0.41564266 0.44811207 0.44879482 0.45013788 0.45989823
## [49] 0.48033404 0.48054209 0.48122316 0.48815230 0.49153052 0.51384314
## [55] 0.51554800 0.55312335 0.55532299 0.55590615 0.56768176 0.57594817
## [61] 0.57709206 0.60321189 0.60899763 0.61329779 0.63585036 0.66232084
## [67] 0.66232758 0.69135509 0.69165978 0.69635956 0.75480313 0.76186222
## [73] 0.76497154 0.77540703 0.78487752 0.78539204 0.78543561 0.78775387
## [79] 0.79749909 0.80248751 0.81382792 0.84392093 0.84417039 0.88196292
## [85] 0.88614137 0.92665087 0.93847845 0.94239110 0.94451417 0.94597553
## [91] 0.96298585 0.96749943 0.96947658 0.96951561 0.97237536 0.97459568
## [97] 0.97584503 1.00000000
```

## ## [1] 100 100

Add one final column to X to bring the number of columns to 101. Then try to compute  $\mathbb{R}^2$ . What happens and why?

```
newX = cbind(X, rnorm(100, mean = 0, sd = 1) )
summary(lm(y ~ newX))$r.squared
```

#### ## [1] 1

As we add more and more p features to the matrix  $R^2$  becomes 1. Little by little p+1 gets closer and closer to n. We are overfitting.