Lab 4

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Load up the famous iris dataset. We are going to do a different prediction problem. Imagine the only input x is Species and you are trying to predict y which is Petal.Length. A reasonable prediction is the average petal length within each Species. Prove that this is the OLS model by fitting an appropriate `lm` and then using the predict function to verify.

```
data(iris)
mod = lm(Petal.Length ~ Species, iris)
#head(mod, 20)

mean(iris$Petal.Length[iris$Species == "setosa"])
```

```
## [1] 1.462
```

```
mean(iris$Petal.Length[iris$Species == "versicolor"])
```

```
## [1] 4.26
```

```
mean(iris$Petal.Length[iris$Species == "virginica"])
```

```
## [1] 5.552
```

```
predict(mod, data.frame(Species = c("setosa")))
```

```
##     1
## 1.462
```

```
predict(mod, data.frame(Species = c("versicolor")))
```

```
##    1
## 4.26
```

```
predict(mod, data.frame(Species = c("virginica")))
```

```
##     1
## 5.552
```

Construct the design matrix with an intercept, X, without using `model.matrix`.

```r
X = cbind(1, iris$Species == "versicolor", iris$Species == "virginica")
head(X)
```

```
##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    1    0    0
## [3,]    1    0    0
## [4,]    1    0    0
## [5,]    1    0    0
## [6,]    1    0    0
```

Find the hat matrix H for this regression.

```r
H = X %*% solve(t(X) %*% X) %*% t(X)
Matrix::rankMatrix(H)
```

```
## [1] 3
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 3.330669e-14
```

Verify this hat matrix is symmetric using the `expect_equal` function in the package `testthat`.

```r
#install.packages("pacman")
pacman::p_load(testthat)
expect_equal(H, t(H))
```

Verify this hat matrix is idempotent using the `expect_equal` function in the package `testthat`.

```r
expect_equal(H, H %*% H)
```

Using the `diag` function, find the trace of the hat matrix.

```r
sum(diag(H))
```

```
## [1] 3
```

It turns out the trace of a hat matrix is the same as its rank! But we don't have time to prove these interesting and useful facts..

For masters students: create a matrix $X_\perp$.

```r
I = diag(nrow(H))
x_perp = (I - H) %*% X

t(x_perp) %*% X
```

```
##                [,1]          [,2]          [,3]
## [1,] -6.835157e-14 -6.952772e-15 -2.600697e-14
## [2,] -1.600109e-14 -1.600109e-14  0.000000e+00
## [3,] -3.494427e-14  0.000000e+00 -3.494427e-14
```

Using the hat matrix, compute the $\hat{y}$ vector and using the projection onto the residual space, compute the e vector and verify they are orthogonal to each other.

```r
y = iris$Petal.Length
y_hat = H %*% y
table(y_hat)
```

```
## y_hat
## 1.462  4.26 5.552
##    50    50    50
```

```r
I = diag(nrow(iris))
e = (I - H) %*% y
head(e)
```

```
##        [,1]
## [1,] -0.062
## [2,] -0.062
## [3,] -0.162
## [4,]  0.038
## [5,] -0.062
## [6,]  0.238
```

```r
expect_equal(t(e) %*% y_hat, as.matrix(0))
Matrix::rankMatrix(I - H)
```

```
## [1] 147
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 3.330669e-14
```

Compute SST, SSR and SSE and R^2 and then show that SST = SSR + SSE.

```r
SSE = t(e) %*% e
y_bar = mean(y)
SST = t(y - y_bar) %*% (y - y_bar)

Rsq = 1 - SSE/SST
Rsq
```

```
##           [,1]
## [1,] 0.9413717
```

```r
SSR = t(y_hat - y_bar) %*% (y_hat - y_bar)
SSR
```

```
##          [,1]
## [1,] 437.1028
```

```r
expect_equal(SSR+SSE, SST)

var(y)
```

```
## [1] 3.116278
```

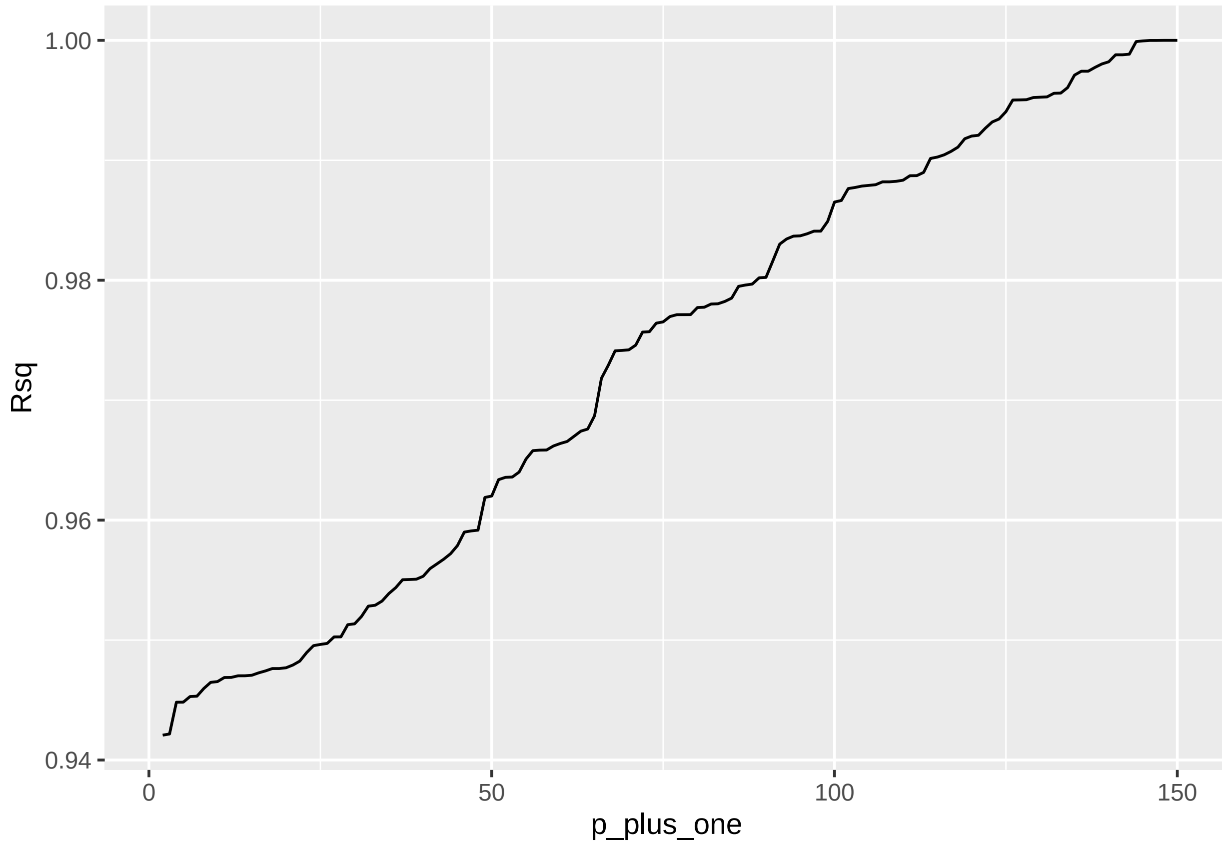
```r
var(e)
```

```
##          [,1]
## [1,] 0.182702
```

```r
n = 150
Rsqs = array(NA, n)
for (p_plus_one in 2 : n){
  X = cbind(X, rnorm(n))
  Rsqs[p_plus_one] = summary(lm(y ~ X))$r.squared
}

pacman::p_load(ggplot2)
base = ggplot(data.frame(p_plus_one = 1 : n, Rsq = Rsqs))
base + geom_line(aes(x = p_plus_one, y = Rsq))
```

```
## Warning: Removed 1 row(s) containing missing values (geom_path).
```



Find the angle θ between y - $\bar{y}1$ and $\hat{y} - \bar{y}1$ and then verify that its cosine squared is the same as the R^2 from the previous problem.

```
theta = acos(t(y - y_bar) %*% (y_hat - y_bar) / sqrt(SST*SSR))
theta = theta *180/ pi
theta
```

```
##           [,1]
## [1,] 14.01245
```

Project the y vector onto each column of the X matrix and test if the sum of these projections is the same as yhat.

```
proj1 = (X[,1] %*% t(X[,1]) / as.numeric(t(X[,1]) %*% X[,1])) %*% y
proj2 = (X[,2] %*% t(X[,2]) / as.numeric(t(X[,2]) %*% X[,2])) %*% y
proj3 = (X[,3] %*% t(X[,3]) / as.numeric(t(X[,3]) %*% X[,3])) %*% y


#expect_equal(proj1 + proj2 + proj3, y_hat)
# Not supposed to be equal. We can only add the projections if the vectors are orthogonal
```

Construct the design matrix without an intercept, X, without using `model.matrix`.

```r
X2 = cbind(iris$Species == "setosa", as.numeric(iris$Species == "versicolor"), iris$Species == "virgini
y = iris$Petal.Length
head(X2)
```

```
##      [,1] [,2] [,3]
## [1,]    1    0    0
## [2,]    1    0    0
## [3,]    1    0    0
## [4,]    1    0    0
## [5,]    1    0    0
## [6,]    1    0    0
```

Find the OLS estimates using this design matrix. It should be the sample averages of the petal lengths within species.

```r
# Hat matrix AKA Projection matrix
H2 = X2 %*% solve(t(X2) %*% X2) %*% t(X2)
y_hat2 = H2 %*% y

unique(y_hat2)
```

```
##       [,1]
## [1,] 1.462
## [2,] 4.260
## [3,] 5.552
```

```r
unique(y_hat)
```

```
##       [,1]
## [1,] 1.462
## [2,] 4.260
## [3,] 5.552
```

```r
# Actual means
mean(iris$Petal.Length[iris$Species == "setosa"])
```

```
## [1] 1.462
```

```r
mean(iris$Petal.Length[iris$Species == "versicolor"])
```

```
## [1] 4.26
```

```r
mean(iris$Petal.Length[iris$Species == "virginica"])
```

```
## [1] 5.552
```

Verify the hat matrix constructed from this design matrix is the same as the hat matrix constructed from the design matrix with the intercept. (Fact: orthogonal projection matrices are unique).

```
pacman::p_load(testthat)
expect_equal(H, H2)
```

Project the y vector onto each column of the X matrix and test if the sum of these projections is the same as yhat.

```
Hy = H2 %*% y
expect_equal(Hy, y_hat2)
```

Convert this design matrix into Q, an orthonormal matrix.

```
qrX = qr(X2)
Q = qr.Q(qrX)
R = qr.R(qrX)
dim(Q)
```

```
## [1] 150   3
```

```
dim(R)
```

```
## [1] 3 3
```

```
Matrix::rankMatrix(Q)
```

```
## [1] 3
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 3.330669e-14
```

```
Matrix::rankMatrix(R)
```

```
## [1] 3
## attr(,"method")
## [1] "tolNorm2"
## attr(,"useGrad")
## [1] FALSE
## attr(,"tol")
## [1] 6.661338e-16
```

```
#verification
sum(Q[, 1]^2) #normalized?
```

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

```r
sum(Q[, 2]^2) #normalized?
```

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

```r
sum(Q[, 3]^2) #normalized?
```

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

```r
Q[, 1] %*% Q[, 2] #orthogonal?
```

```
##      [,1]
## [1,]    0
```

```r
Q[, 1] %*% Q[, 3] #orthogonal?
```

```
##      [,1]
## [1,]    0
```

```r
Q[, 2] %*% Q[, 3] #orthogonal?
```

```
##      [,1]
## [1,]    0
```

Project the y vector onto each column of the Q matrix and test if the sum of these projections is the same as yhat.

```r
proj1 = (Q[,1] %*% t(Q[,1]) / as.numeric(t(Q[,1]) %*% Q[,1])) %*% y
proj2 = (Q[,2] %*% t(Q[,2]) / as.numeric(t(Q[,2]) %*% Q[,2])) %*% y
proj3 = (Q[,3] %*% t(Q[,3]) / as.numeric(t(Q[,3]) %*% Q[,3])) %*% y

yhat_Q = Q %*% t(Q) %*% y
head(y_hat2)
```

```
##       [,1]
## [1,] 1.462
## [2,] 1.462
## [3,] 1.462
## [4,] 1.462
## [5,] 1.462
## [6,] 1.462
```

```r
head(yhat_Q)
```

```
##       [,1]
## [1,] 1.462
## [2,] 1.462
## [3,] 1.462
## [4,] 1.462
## [5,] 1.462
## [6,] 1.462
```

```r
expect_equal(yhat_Q, y_hat2)
```

Find the $p = 3$ linear OLS estimates if Q is used as the design matrix using the `lm` method. Is the OLS solution the same as the OLS solution for X?

```r
mod_Q= lm(Petal.Length ~ 0 + Q, iris)
mod_Q
```

```
##
## Call:
## lm(formula = Petal.Length ~ 0 + Q, data = iris)
##
## Coefficients:
##     Q1      Q2      Q3
## -10.34  -30.12  -39.26
```

```r
mod_X = lm(y ~ X2, iris)
mod_X
```

```
##
## Call:
## lm(formula = y ~ X2, data = iris)
##
## Coefficients:
## (Intercept)          X21          X22          X23
##       5.552       -4.090       -1.292           NA
```

Use the predict function and ensure that the predicted values are the same for both linear models: the one created with X as its design matrix and the one created with Q as its design matrix.

```r
predict(mod_Q, data.frame(Q))
```

```
##     1     2     3     4     5     6     7     8     9    10    11    12    13
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    14    15    16    17    18    19    20    21    22    23    24    25    26
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    27    28    29    30    31    32    33    34    35    36    37    38    39
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    40    41    42    43    44    45    46    47    48    49    50    51    52
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 4.260 4.260
##    53    54    55    56    57    58    59    60    61    62    63    64    65
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    66    67    68    69    70    71    72    73    74    75    76    77    78
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    79    80    81    82    83    84    85    86    87    88    89    90    91
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    92    93    94    95    96    97    98    99   100   101   102   103   104
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 5.552 5.552 5.552 5.552
##   105   106   107   108   109   110   111   112   113   114   115   116   117
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   118   119   120   121   122   123   124   125   126   127   128   129   130
```

```
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   131   132   133   134   135   136   137   138   139   140   141   142   143
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   144   145   146   147   148   149   150
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552
```

```r
predict(mod_X, data.frame(X2[1]))
```

```
## Warning: 'newdata' had 1 row but variables found have 150 rows
```

```
## Warning in predict.lm(mod_X, data.frame(X2[1])): prediction from a rank-
## deficient fit may be misleading
```

```
##     1     2     3     4     5     6     7     8     9    10    11    12    13
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    14    15    16    17    18    19    20    21    22    23    24    25    26
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    27    28    29    30    31    32    33    34    35    36    37    38    39
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462
##    40    41    42    43    44    45    46    47    48    49    50    51    52
## 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 1.462 4.260 4.260
##    53    54    55    56    57    58    59    60    61    62    63    64    65
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    66    67    68    69    70    71    72    73    74    75    76    77    78
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    79    80    81    82    83    84    85    86    87    88    89    90    91
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260
##    92    93    94    95    96    97    98    99   100   101   102   103   104
## 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 4.260 5.552 5.552 5.552 5.552
##   105   106   107   108   109   110   111   112   113   114   115   116   117
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   118   119   120   121   122   123   124   125   126   127   128   129   130
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   131   132   133   134   135   136   137   138   139   140   141   142   143
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552 5.552
##   144   145   146   147   148   149   150
## 5.552 5.552 5.552 5.552 5.552 5.552 5.552
```

Clear the workspace and load the boston housing data and extract X and y. The dimensions are $n = 506$ and $p = 13$. 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.

```r
boston <- MASS::Boston
y = MASS::Boston$medv
X = as.matrix(cbind(1, MASS::Boston[, 1 : 13]))
n = nrow(X)
p_plus_one = ncol(X)
matrix <- matrix(NA, nrow = p_plus_one, ncol = p_plus_one, dimnames = list(NULL,colnames(X)))
```

```r
for (i in 1:ncol(matrix)){
  b=array(NA, dim = ncol(matrix))
  X_star = X[, 1:i]
  X_star = as.matrix(X_star)
  XTX_inv = solve(t(X_star) %*% X_star)
  b[1:i] = XTX_inv %*% t(X_star) %*% y
  matrix[i, ] <- b
}
matrix
```

```
##                 1       crim         zn       indus     chas        nox
##  [1,]  22.5328063         NA         NA          NA       NA         NA
##  [2,]  24.0331062 -0.4151903         NA          NA       NA         NA
##  [3,]  22.4856281 -0.3520783 0.11610909          NA       NA         NA
##  [4,]  27.3946468 -0.2486283 0.05850082 -0.41557782       NA         NA
##  [5,]  27.1128031 -0.2287981 0.05928665 -0.44032511 6.894059         NA
##  [6,]  29.4899406 -0.2185190 0.05511047 -0.38348055 7.026223  -5.424659
##  [7,] -17.9546350 -0.1769135 0.02128135 -0.14365267 4.784684  -7.184892
##  [8,] -18.2649261 -0.1727607 0.01421402 -0.13089918 4.840730  -4.357411
##  [9,]   0.8274820 -0.1977868 0.06099257 -0.22573089 4.577598 -14.451531
## [10,]   0.1553915 -0.1780398 0.06095248 -0.21004328 4.536648 -13.342666
## [11,]   2.9907868 -0.1795543 0.07145574 -0.10437742 4.110667 -12.591596
## [12,]  27.1523679 -0.1840321 0.03909990 -0.04232450 3.487528 -22.182110
## [13,]  20.6526280 -0.1599391 0.03887365 -0.02792186 3.216569 -20.484560
## [14,]  36.4594884 -0.1080114 0.04642046  0.02055863 2.686734 -17.766611
##             rm          age       dis         rad         tax    ptratio
##  [1,]       NA           NA        NA          NA          NA         NA
##  [2,]       NA           NA        NA          NA          NA         NA
##  [3,]       NA           NA        NA          NA          NA         NA
##  [4,]       NA           NA        NA          NA          NA         NA
##  [5,]       NA           NA        NA          NA          NA         NA
##  [6,]       NA           NA        NA          NA          NA         NA
##  [7,] 7.341586           NA        NA          NA          NA         NA
##  [8,] 7.386357 -0.0236248493        NA          NA          NA         NA
##  [9,] 6.752352 -0.0556354540 -1.760312          NA          NA         NA
## [10,] 6.791184 -0.0562612189 -1.748296 -0.04529059          NA         NA
## [11,] 6.664084 -0.0546675064 -1.727933  0.15926305 -0.01434060         NA
## [12,] 6.075744 -0.0451880522 -1.583852  0.25472196 -0.01221262 -0.9962062
## [13,] 6.123072 -0.0459320518 -1.554912  0.28157503 -0.01173838 -1.0142228
## [14,] 3.809865  0.0006922246 -1.475567  0.30604948 -0.01233459 -0.9527472
##             black       lstat
##  [1,]          NA          NA
##  [2,]          NA          NA
##  [3,]          NA          NA
##  [4,]          NA          NA
##  [5,]          NA          NA
##  [6,]          NA          NA
##  [7,]          NA          NA
##  [8,]          NA          NA
##  [9,]          NA          NA
## [10,]          NA          NA
## [11,]          NA          NA
## [12,]          NA          NA
```

```
## [13,] 0.013620833          NA
## [14,] 0.009311683 -0.5247584
```

Why are the estimates changing from row to row as you add in more predictors?

Every row is a different model, with a different number of features. The first row represents a model with no features, only a y-intercept. The second row represents a model with the y-intercept, and a single feature crim, with its associated weight. We find that the values of the weights of a single feature may vary as we change the number of features we fit the model on. This is because the estimates of the weights

Create a vector of length $p + 1$ and compute the R^2 values for each of the above models.

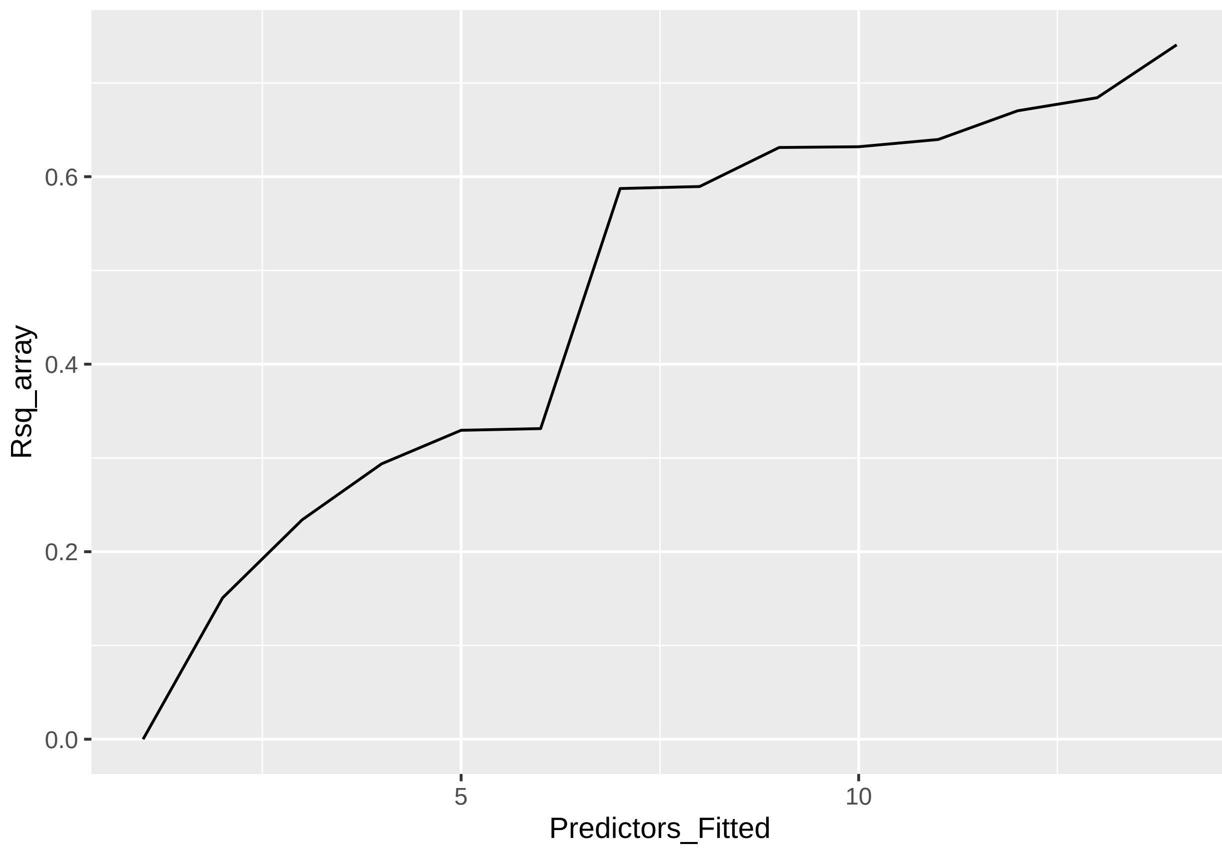
```r
Rsq_array = array(dim = p_plus_one)
ybar = mean(y)
SST = sum((y - ybar)^2)


for(i in 1:nrow(matrix)){
  b = c(matrix[i, 1:i], rep(0, nrow(matrix) - i))

  # Calculating SSR for every row in matrix
  yhat = X %*% b
  SSR = sum((yhat - ybar)^2)
  Rsq = SSR/SST
  Rsq_array[i] = Rsq
}
Rsq_array
```

```
##  [1] 5.382448e-30 1.507805e-01 2.339884e-01 2.937136e-01 3.295277e-01
##  [6] 3.313127e-01 5.873770e-01 5.894902e-01 6.311488e-01 6.319479e-01
## [11] 6.396628e-01 6.703141e-01 6.842043e-01 7.406427e-01
```

```r
pacman::p_load(ggplot2)
base = ggplot(data.frame(Predictors_Fitted = 1 : nrow(matrix), Rsq = Rsq_array)) + geom_line(aes(x = Pre
base
```



Is R^2 monotonically increasing? Why? Yes! R^2 is increasing because we are fitting more features on the model with every iteration. Does this mean that the model becomes better as R^2 increases? Not necessarily, we are likely over-fitting the model with these addition features.