

## Lab 5

Amy Butler

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#Create a 2x2 matrix with the first column 1's and the next column iid normals. Find the absolute value of the angle (in degrees, not radians) between the two columns.

```
norm_vec=function(v){
  sqrt(sum(v^2))
}
X=matrix(1:1,nrow=2,ncol=2)
X[,2]=rnorm(2)
cos_theta= t(X[,1]%*%X[,2]) / (norm_vec(X[,1])*norm_vec(X[,2]))
cos_theta

##           [,1]
## [1,] 0.7370102

abs(90-acos(cos_theta)*180/pi)

##           [,1]
## [1,] 47.47735
```

#Repeat this exercise Nsim = 1e5 times and report the average absolute angle.

```
Nsim = 1e5
angles=array(NA,Nsim)
for (i in 1:Nsim){
  X=matrix(1:1,nrow=2,ncol=2)
  X[,2]=rnorm(2)
  cos_theta= t(X[,1]%*%X[,2]) / (norm_vec(X[,1])*norm_vec(X[,2]))
  angles[i]=abs(90-acos(cos_theta)*180/pi)
}
mean(angles)

## [1] 45.14763
```

#Create a 2xn matrix with the first column 1's and the next column iid normals. Find the absolute value of the angle (in degrees, not radians) between the two columns. For n = 10, 50, 100, 200, 500, 1000, report the average absolute angle over Nsim = 1e5 simulations.

```
N_s=c(2,5,10, 50, 100, 200, 500, 1000)
Nsim = 1e5
angles=matrix(NA,nrow=Nsim,ncol=length(N_s))
for (j in 1:length(N_s)){
  for (i in 1:Nsim){
    X=matrix(1,nrow=N_s[j],ncol=2)
```

```

    X[,2]=rnorm(N_s[j])
    cos_theta= t(X[,1])%*%X[,2]) / (norm_vec(X[,1])*norm_vec(X[,2]))
    angles[i,j]=abs(90-acos(cos_theta)*180/pi)
  }
}
colMeans(angles)

## [1] 44.975187 23.206373 15.352776 6.512916 4.596174 3.254262 2.046538
## [8] 1.443217

```

#What is this absolute angle converging to? Why does this make sense?

The absolute angle difference from ninety is converging to zero. This makes sense because in a high dimensional space random directions are orthogonal.

#Create a vector y by simulating n = 100 standard iid normals. Create a matrix of size 100 x 2 and populate the first column by all ones (for the intercept) and the second column by 100 standard iid normals. Find the R<sup>2</sup> of an OLS regression of y ~ X. Use matrix algebra.

```

n=100
X=cbind(1,rnorm(n))
y=rnorm(n)

H=X %*% solve((t(X)%*% X)) %*% t(X)
y_hat= H%*% y
y_bar= mean(y)

SSR=sum((y_hat-y_bar)^2)
SST=sum((y-y_bar)^2)

Rsqr=(SSR/SST)
Rsqr

## [1] 0.0006872124

```

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

```

Rsqr_s=array(NA,dim=n-2)
for (j in 1:(n-2)){
  X= cbind(X,rnorm(n))
  H=X %*% solve((t(X) %*% X)) %*% t(X)
  y_hat= H %*% y
  y_bar= mean(y)
  SSR=sum((y_hat-y_bar)^2)
  SST=sum((y-y_bar)^2)
  Rsqr_s[j]=(SSR/SST)
}
Rsqr_s

```

```
## [1] 0.0007389075 0.0060698005 0.0124403810 0.0156202066 0.0173855688
## [6] 0.0174309724 0.0198342760 0.0439464716 0.0441725038 0.0442132082
## [11] 0.0669590225 0.0736459674 0.0865487111 0.0865558153 0.0871539189
## [16] 0.1585263306 0.1615464305 0.1684894368 0.2586822230 0.2735748259
## [21] 0.2740060139 0.2821029857 0.2949488743 0.2953542491 0.2963664553
## [26] 0.2964021237 0.2964853823 0.2984531653 0.3179491299 0.3180605332
## [31] 0.3318574173 0.3410024326 0.3423887451 0.3424038273 0.3467535305
## [36] 0.3622493473 0.3624735695 0.3630034965 0.3731853577 0.3749901323
## [41] 0.3754271601 0.3878920151 0.3960800544 0.4170297343 0.4172912501
## [46] 0.4225410067 0.4420243375 0.4420751456 0.4441167122 0.4475500025
## [51] 0.5254704342 0.5302888506 0.5307700046 0.5985103039 0.5985953201
## [56] 0.5986833179 0.6106209167 0.6157035436 0.6159066897 0.6188085355
## [61] 0.6224860466 0.6522302115 0.6726604738 0.6866731187 0.6866739608
## [66] 0.6886858756 0.6914217282 0.7168473184 0.7198930407 0.7391515964
## [71] 0.7391534880 0.7593055052 0.7781554545 0.7885030204 0.7928726143
## [76] 0.7946673467 0.7999369637 0.8040434041 0.8040632051 0.8460649367
## [81] 0.8506447594 0.8855042311 0.8907876074 0.8918577060 0.8936762775
## [86] 0.8957954296 0.8961222460 0.9203886513 0.9645464397 0.9684620063
## [91] 0.9767741647 0.9805354289 0.9842280686 0.9856367686 0.9920010926
## [96] 0.9934796406 0.9967833070 1.0000000000
```

```
diff(Rsq_s)
```

```
## [1] 5.330893e-03 6.370580e-03 3.179826e-03 1.765362e-03 4.540365e-05
## [6] 2.403304e-03 2.411220e-02 2.260321e-04 4.070448e-05 2.274581e-02
## [11] 6.686945e-03 1.290274e-02 7.104163e-06 5.981036e-04 7.137241e-02
## [16] 3.020100e-03 6.943006e-03 9.019279e-02 1.489260e-02 4.311880e-04
## [21] 8.096972e-03 1.284589e-02 4.053749e-04 1.012206e-03 3.566841e-05
## [26] 8.325859e-05 1.967783e-03 1.949596e-02 1.114033e-04 1.379688e-02
## [31] 9.145015e-03 1.386312e-03 1.508220e-05 4.349703e-03 1.549582e-02
## [36] 2.242222e-04 5.299270e-04 1.018186e-02 1.804775e-03 4.370278e-04
## [41] 1.246485e-02 8.188039e-03 2.094968e-02 2.615158e-04 5.249757e-03
## [46] 1.948333e-02 5.080814e-05 2.041567e-03 3.433290e-03 7.792043e-02
## [51] 4.818416e-03 4.811540e-04 6.774030e-02 8.501619e-05 8.799779e-05
## [56] 1.193760e-02 5.082627e-03 2.031462e-04 2.901846e-03 3.677511e-03
## [61] 2.974416e-02 2.043026e-02 1.401264e-02 8.421569e-07 2.011915e-03
## [66] 2.735853e-03 2.542559e-02 3.045722e-03 1.925856e-02 1.891583e-06
## [71] 2.015202e-02 1.884995e-02 1.034757e-02 4.369594e-03 1.794732e-03
## [76] 5.269617e-03 4.106440e-03 1.980101e-05 4.200173e-02 4.579823e-03
## [81] 3.485947e-02 5.283376e-03 1.070099e-03 1.818572e-03 2.119152e-03
## [86] 3.268165e-04 2.426641e-02 4.415779e-02 3.915567e-03 8.312158e-03
## [91] 3.761264e-03 3.692640e-03 1.408700e-03 6.364324e-03 1.478548e-03
## [96] 3.303666e-03 3.216693e-03
```

#Test that the projection matrix onto this X is the same as I\_n. You may have to vectorize the matrices in the expect\_equal function for the test to work.

```
pacman::p_load(testthat)
#dim(X)
#H=X %%% solve((t(X)%% X)) %%% t(X)
#H[1:10,1:10]
```

```
I=diag(n)
expect_equal(H,I)
```

#Add one final column to X to bring the number of columns to 101. Then try to compute  $R^2$ . What happens?

```
X= cbind(X,rnorm(n)) H=X %% solve((t(X) %% X)) %% t(X) y_hat= H %% y y_bar= mean(y)
SSR=sum((y_hat-y_bar)^2) SST=sum((y-y_bar)^2) Rsq=SSR/SST
```

#Why does this make sense?

It fails because  $X$ -transpose- $X$  is rank deficient making it impossible to invert.

#Write a function spec'd as follows:

```
## Orthogonal Projection
##
## Projects vector a onto v.
##
## @param a the vector to project
## @param v the vector projected onto
##
## @returns a list of two vectors, the orthogonal projection parallel to v
named a_parallel,
## and the orthogonal error orthogonal to v called a_perpendicular
orthogonal_projection = function(a, v){
  H=v %% t(v) / norm_vec(v)^2
  a_parallel=H %% a
  a_perpendicular=a-a_parallel
  list(a_parallel = a_parallel, a_perpendicular = a_perpendicular)
}
```

#Provide predictions for each of these computations and then run them to make sure you're correct.

```
orthogonal_projection(c(1,2,3,4), c(1,2,3,4))

## $a_parallel
##      [,1]
## [1,]    1
## [2,]    2
## [3,]    3
## [4,]    4
##
## $a_perpendicular
##      [,1]
## [1,]    0
## [2,]    0
## [3,]    0
## [4,]    0
```

```

#prediction: This makes sense.
orthogonal_projection(c(1, 2, 3, 4), c(0, 2, 0, -1))

## $a_parallel
##      [,1]
## [1,]    0
## [2,]    0
## [3,]    0
## [4,]    0
##
## $a_perpendicular
##      [,1]
## [1,]    1
## [2,]    2
## [3,]    3
## [4,]    4

#prediction: The dot product is zero so the two vectors are perpendicular.
The parallel vector should be zero and the perpendicular vector should be
itself.
result = orthogonal_projection(c(2, 6, 7, 3), c(1, 3, 5, 7)*37)
t(result$a_parallel) %*% result$a_perpendicular

##      [,1]
## [1,] -3.552714e-15

#prediction:
result$a_parallel + result$a_perpendicular

##      [,1]
## [1,]    2
## [2,]    6
## [3,]    7
## [4,]    3

#prediction: tHIS should be reconstructed the original vector.
result$a_parallel / c(1, 3, 5, 7)*37

##      [,1]
## [1,] 33.47619
## [2,] 33.47619
## [3,] 33.47619
## [4,] 33.47619

#prediction: The scalar.

```

#Let's use the Boston Housing Data for the following exercises

```

y = MASS::Boston$medv
X = model.matrix(medv ~ ., MASS::Boston)
p_plus_one = ncol(X)

```

```

n = nrow(X)
head(X)

## (Intercept)    crim zn indus chas    nox    rm  age    dis rad tax
ptratio
## 1          1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900    1 296
15.3
## 2          1 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671    2 242
17.8
## 3          1 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671    2 242
17.8
## 4          1 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622    3 222
18.7
## 5          1 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622    3 222
18.7
## 6          1 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622    3 222
18.7
##    black lstat
## 1 396.90  4.98
## 2 396.90  9.14
## 3 392.83  4.03
## 4 394.63  2.94
## 5 396.90  5.33
## 6 394.12  5.21

```

#Using your function `orthogonal_projection` orthogonally project onto the column space of X by projecting y on each vector of X individually and adding up the projections and call the sum `yhat_naive`.

```

yhat_naive = rep(0,n)
for(j in 1:p_plus_one){
  yhat_naive= yhat_naive+orthogonal_projection(y,X[,j])$a_parallel
}

```

#How much double counting occurred? Measure the magnitude relative to the true LS orthogonal projection.

```

yhat = X %%% solve((t(X) %%% X)) %%% t(X) %%% y
sqrt(sum(yhat_naive^2)) / sqrt(sum(yhat^2))

## [1] 8.997118

```

#Is this ratio expected? Why or why not?

It is expected to be different from one.

#Convert X into V where V has the same column space as X but has orthogonal columns. You can use the function `orthogonal_projection`. This is the Gram-Schmidt orthogonalization algorithm.

```

V = matrix(NA, nrow = n, ncol = p_plus_one)
V[, 1] = X[, 1]
for(j in 2:p_plus_one){
  V[,j] = X[,j]
  for(k in 1:(j-1)){
    V[,j] = V[,j] - orthogonal_projection(X[,j], V[,k])$a_parallel
  }
}

V[,7] %*% V[,9]

##           [,1]
## [1,] -2.140346e-11

```

#Convert V into Q whose columns are the same except normalized

```

Q = matrix(NA, nrow = n, ncol = p_plus_one)
for (j in 1:p_plus_one){
  Q[,j] = V[,j] / norm_vec(V[,j])
}

```

#Verify  $Q^T Q$  is  $I_{\{p+1\}}$  i.e. Q is an orthonormal matrix.

```
expect_equal(t(Q) %*% Q, diag(p_plus_one)) expect_equal(Q, Q_from_Rs_builtin)
```

#Is your Q the same as what results from R's built-in QR-decomposition function?

```
Q_from_Rs_builtin = qr.Q(qr(X))
```

#Is this expected? Why did this happen?

There are infinite orthonormal bases of any column space. The projection will be exactly the same.

#Project y onto  $\text{colsp}[Q]$  and verify it is the same as the OLS fit. You may have to use the function `unname` to compare the vectors since they the entries will likely have different names.

```

y_hat = lm(y~X)$fitted.values
expect_equal(c(unname(Q %*% t(Q) %*% y)), unname(y_hat))

```

Project y onto  $\text{colsp}[Q]$  one by one and verify it sums to be the projection onto the whole space.

```

yhat_naive = rep(0,n)
for(j in 1:p_plus_one){
  yhat_naive = yhat_naive + orthogonal_projection(y, Q[,j])$a_parallel
}
H = Q %*% solve(t(Q) %*% Q) %*% t(Q)
expect_equal(H %*% y, yhat_naive)

```

Split the Boston Housing Data into a training set and a test set where the training set is 80% of the observations. Do so at random.

```
K = 5
n_test = round(n * 1 / K)
n_train = n - n_test
test_ind = sample(1:n, n_test)
train_ind = setdiff(1:n, test_ind)
X_test = X[test_ind,]
X_train = X[train_ind]
Y_test = y[test_ind]
Y_train = y[train_ind]
```

Fit an OLS model. Find the  $s_e$  in sample and out of sample. Which one is greater? Note: we are now using  $s_e$  and not RMSE since RMSE has the  $n - (p + 1)$  in the denominator not  $n - 1$  which attempts to de-bias the error estimate by inflating the estimate when overfitting in high  $p$ . Again, we're just using  $sd(e)$ , the sample standard deviation of the residuals.

```
mod = lm(Y_train ~ . + 0, data.frame(X_train))
sd(mod$residuals)

## [1] 9.2823

y_hat = predict(mod, data.frame(X_test))

## Warning: 'newdata' had 101 rows but variables found have 405 rows

e = Y_test - y_hat

## Warning in Y_test - y_hat: longer object length is not a multiple of
## shorter
## object length

oos_SE = sd(e)
oos_SE

## [1] 8.751189
```

Do these two exercises  $N_{sim} = 1000$  times and find the average difference between  $s_e$  and  $ooss_e$ .

```
Nsim = 1000 sum = 0 for (i in 1:Nsim) { test_indices = sample(1 : n, n_test) train_indices =
setdiff(1 : n, test_indices) X_train = X[train_indices,] y_train = y[train_indices] X_test =
X[test_indices,] y_test = y[test_indices] ols_mod = lm(y_train ~ .+0, data.frame(X_train)) s_e
= sd(ols_mod$residuals) y_oos = predict(ols_mod, data.frame(X_test)) residuals = y_test -
y_oos ooss_e = sd(residuals) sum = sum + abs(s_e - ooss_e) } avg_diff = sum / Nsim avg_diff
```

#We'll now add random junk to the data so that  $p_{plus\_one} = n_{train}$  and create a new data matrix  $X_{with\_junk}$ .

```
X_with_junk = cbind(X, matrix(rnorm(n * (n_train - p_plus_one)), nrow = n))
dim(X)
```



```
## [1] 506 14
dim(X_with_junk)
## [1] 506 405
```

Repeat the exercise above measuring the average `s_e` and `ooss_e` but this time record these metrics by number of features used. That is, do it for the first column of `X_with_junk` (the intercept column), then do it for the first and second columns, then the first three columns, etc until you do it for all columns of `X_with_junk`. Save these in `s_e_by_p` and `ooss_e_by_p`.

```
test_indices = sample(1 : n, n_test) train_indices = setdiff(1 : n, test_indices) s_e_by_p =
rep(NA, ncol(X_with_junk)) ooss_e_by_p = rep(NA, ncol(X_with_junk)) sum_by_p = 0
oos_sum_by_p = 0 Nsim = 100 for (i in 1 : Nsim) { for (j in 1 : ncol(X_with_junk)) { X_train =
X_with_junk[train_indices, 1 : j, drop = FALSE] y_train = y[train_indices] X_test =
X_with_junk[test_indices, 1 : j, drop = FALSE] y_test = y[test_indices] in_mod = lm(y_train ~
.+0, data.frame(X_train)) oos_y = predict(in_mod, data.frame(X_test)) s_e_by_p[j] =
sd(in_mod$residuals) ooss_e_by_p[j] = sd(y_test - oos_y) } sum_by_p = sum_by_p +
sum(s_e_by_p) oos_sum_by_p = oos_sum_by_p + sum(ooss_e_by_p) } sum_by_p /
(ncol(X_with_junk) * Nsim) oos_sum_by_p / (ncol(X_with_junk) * Nsim)
```

#You can graph them here:

```
pacman::p_load(ggplot2) ggplot( rbind( data.frame(s_e = s_e_by_p, p = 1 : n_train, series =
"in-sample"), data.frame(s_e = ooss_e_by_p, p = 1 : n_train, series = "out-of-sample") )) +
geom_line(aes(x = p, y = s_e, col = series))
```

#Is this shape expected? Explain.

Yes this shape is expected because we added more features.