HW2.5_Mary_Futey

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```
library(ggplot2)
library(MASS)

## Warning: package 'MASS' was built under R version 3.6.2
library(cluster)
library(fpc)
```

load data and explore

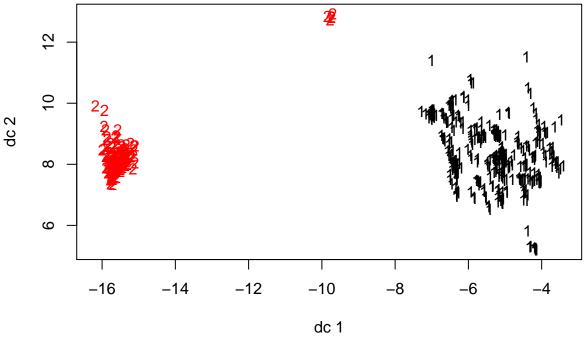
```
boston <- Boston
```

kmeans

```
set.seed(4)
# the result printed is the best result of 20 tries
# clustering vector: information on each observation (what cluster it is assigned)
# sum of squares: measure of variance inside the cluster
km_res <- kmeans(boston, centers = 2, nstart = 20)</pre>
km_res
## K-means clustering with 2 clusters of sizes 369, 137
##
## Cluster means:
##
          crim
                      zn
                             indus
                                         chas
                                                    nox
                                                                      age
## 1 0.3887744 15.58266 8.420894 0.07317073 0.5118474 6.388005 60.63225 4.441272
tax ptratio
                                    black
                                             lstat
## 1 4.455285 311.9268 17.80921 381.0426 10.41745 24.85718
## 2 23.270073 667.6423 20.19635 291.0391 18.67453 16.27226
##
## Clustering vector:
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  381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400
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## 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420
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## 501 502 503 504 505 506
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##
## Within cluster sum of squares by cluster:
## [1] 2868770 2896224
    (between_SS / total_SS = 70.3 %)
##
##
## Available components:
##
## [1] "cluster"
                        "centers"
                                        "totss"
                                                         "withinss"
                                                                          "tot.withinss"
## [6] "betweenss"
                                        "iter"
                        "size"
                                                         "ifault"
# withinss: sum of squares within each cluster
# tot.withins: what we are trying to minimize
```

```
str(km_res)
## List of 9
    $ cluster
                  : Named int [1:506] 1 1 1 1 1 1 1 1 1 1 ...
     ..- attr(*, "names")= chr [1:506] "1" "2" "3" "4" ...
                 : num [1:2, 1:14] 0.389 12.299 15.583 0 8.421 ...
##
    $ centers
##
    ..- attr(*, "dimnames")=List of 2
     ....$ : chr [1:2] "1" "2"
##
     ....$ : chr [1:14] "crim" "zn" "indus" "chas" ...
##
                  : num 19401064
    $ totss
    $ withinss
                  : num [1:2] 2868770 2896224
##
  $ tot.withinss: num 5764994
  $ betweenss
                 : num 13636070
                  : int [1:2] 369 137
##
    $ size
##
    $ iter
                  : int 1
   $ ifault
                  : int 0
##
## - attr(*, "class")= chr "kmeans"
# vizualize results of clustering by kmeans
plotcluster(boston, km_res$cluster)
```



try with different cluster sizes

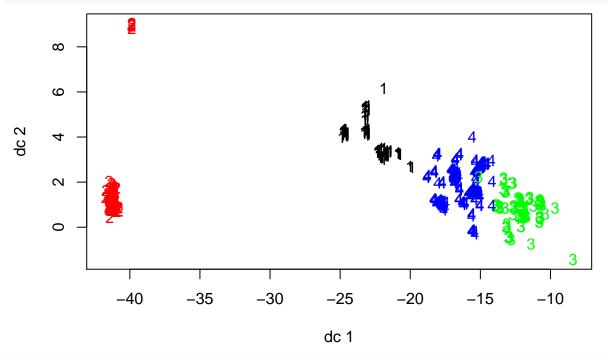
```
set.seed(4)

# 4 cluster sizes produces good results based on plot and tot.withinss,
# but has outliers in 2nd cluster
km_res3 <- kmeans(boston, 4, nstart = 3)
km_res3</pre>
## K-means clustering with 4 clusters of sizes 96, 137, 81, 192
```

```
## Cluster means:
##
                              indus
            crim
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                                                                        age
## 1 0.81874729 7.96875 13.589896 0.07291667 0.5962187 6.169427 75.68750
0.08724728 24.11728 6.198642 0.08641975 0.4659494 6.588148 49.26790
## 4 0.30099479 15.78906 6.773906 0.06770833 0.4890250 6.412859 57.89896
          dis
                    rad
                             tax ptratio
                                             black
                                                        lstat
## 1 3.054214 4.864583 408.4167 17.70417 362.3918 13.009062 22.18125
## 2 2.054470 23.270073 667.6423 20.19635 291.0391 18.674526 16.27226
## 3 4.916821 3.567901 225.9259 17.83210 391.3574 8.404444 28.91358
##
##
  Clustering vector:
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## 501 502 503 504 505 506
         4
## Within cluster sum of squares by cluster:
## [1] 604434.9 2896224.4 186507.3 458666.1
  (between_SS / total_SS = 78.6 %)
##
## Available components:
##
                                      "totss"
## [1] "cluster"
                      "centers"
                                                     "withinss"
                                                                     "tot.withinss"
## [6] "betweenss"
                                      "iter"
                      "size"
                                                     "ifault"
```

plotcluster(boston, km_res3\$cluster)



```
# check res
str(km res3)
```

```
## List of 9
## $ cluster
                 : Named int [1:506] 4 3 3 3 3 4 4 4 4 ...
    ..- attr(*, "names")= chr [1:506] "1" "2" "3" "4" ...
                 : num [1:4, 1:14] 0.8187 12.2992 0.0872 0.301 7.9688 ...
   $ centers
##
   ..- attr(*, "dimnames")=List of 2
    ....$ : chr [1:4] "1" "2" "3" "4"
    ....$ : chr [1:14] "crim" "zn" "indus" "chas" ...
##
```

```
## $ totss : num 19401064
## $ withinss : num [1:4] 604435 2896224 186507 458666
## $ tot.withinss: num 4145833
## $ betweenss : num 15255231
## $ size : int [1:4] 96 137 81 192
## $ iter : int 3
## $ ifault : int 0
## - attr(*, "class")= chr "kmeans"
```

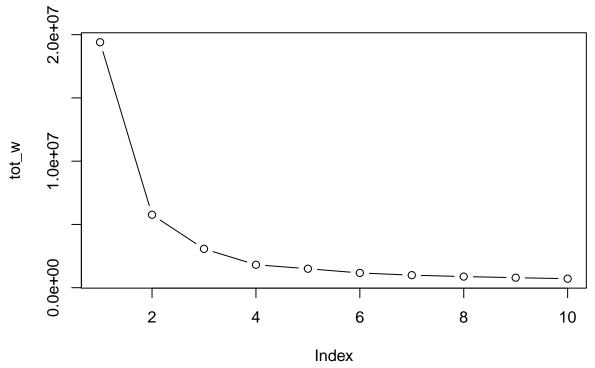
scree plot

```
# scree plot

tot_w <- rep(0,10)

# perform k means with 1 to 10 clusters
# total withinss is measure of quality for clustering
set.seed(8)
for (k in 1:10) {
   tot_w[k] <- kmeans(boston, k, nstart = 20)$tot.withinss
}

# see that 3, maybe 4, is optimal
plot(tot_w, type = "b")</pre>
```



```
boston_F <- boston

# create categorical medv (Median house value) to use as class for pca and hc
quant_00 = min(boston$medv)
quant_25 = quantile(boston$medv, 0.25)
quant_50 = quantile(boston$medv, 0.50)</pre>
```

```
quant_75 = quantile(boston$medv, 0.75)
quant_100 = max(boston$medv)
rb = rbind(quant_00, quant_25, quant_50, quant_75, quant_100)
dimnames(rb)[[2]] = "Value"
boston_F$medv_F[boston$medv >= quant_00 &
                     boston$medv < quant 25] = "FirstQ"</pre>
boston_F$medv_F[boston$medv >= quant_25 &
                     boston$medv < quant_50] = "SecondQ"</pre>
boston_F$medv_F[boston$medv >= quant_50 &
                     boston$medv <= quant_75] = "ThirdQ"</pre>
boston_F$medv_F[boston$medv >= quant_75 &
                     boston$medv <= quant_100] = "FourthQ"</pre>
boston_F$medv_F = factor(boston_F$medv_F,
levels=c("FirstQ", "SecondQ", "ThirdQ", "FourthQ"))
# remove median house value from boston housing dataset
boston_pca <- subset(boston, select = -medv)</pre>
```

hierarchical clustering

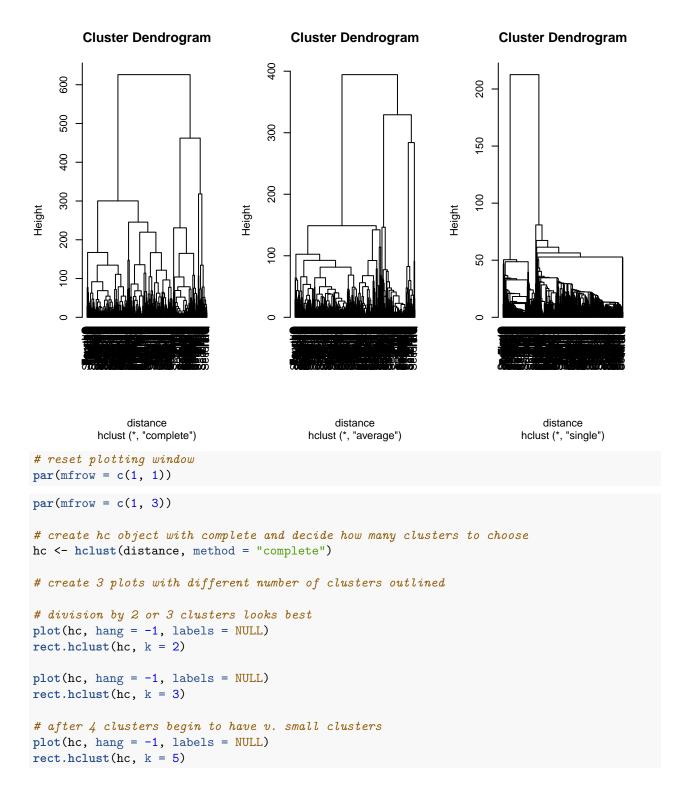
```
distance <- dist(boston)

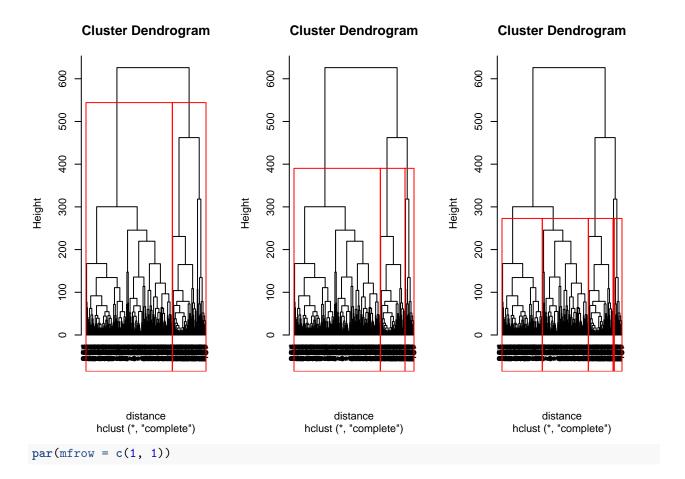
# takes max distance
hc_comp <- hclust(distance, method = "complete")
# takes average distance
hc_avg <- hclust(distance, method = "average")
# minimal distance
hc_sing <- hclust(distance, method = "single")</pre>
```

hc dendrograms

```
# organzine plotting window with 3 cells aligned as columns
par(mfrow = c(1, 3))

# complete and average look similar
plot(hc_comp, hang = -1, labels = boston_F$medv_F)
plot(hc_avg, hang = -1, labels = boston_F$medv_F)
plot(hc_sing, hang = -1, labels = boston_F$medv_F)
```





PCA

```
# check column means
colMeans(boston)
##
                                     indus
                                                    chas
           crim
                           zn
                                                                  nox
                                                                                 rm
##
     3.61352356
                 11.36363636
                               11.13677866
                                              0.06916996
                                                           0.55469506
                                                                         6.28463439
##
                                                              ptratio
                                                                              black
            age
                          dis
                                       rad
                                                     tax
##
    68.57490119
                  3.79504269
                                9.54940711 408.23715415 18.45553360 356.67403162
##
          lstat
                         medv
   12.65306324 22.53280632
##
# check sd
apply(boston, 2, sd)
##
          crim
                         zn
                                  indus
                                               chas
                                                             nox
                                                                           rm
##
     8.6015451 23.3224530
                              6.8603529
                                          0.2539940
                                                       0.1158777
                                                                    0.7026171
##
                       dis
                                    rad
                                                         ptratio
                                                                        black
           age
                                                 tax
    28.1488614
                 2.1057101
                              8.7072594 168.5371161
                                                       2.1649455
                                                                  91.2948644
##
##
         lstat
                      medv
                 9.1971041
     7.1410615
# perform PCA with scaled data based on the above checks
pca <- prcomp(x = boston_pca, center = TRUE, scale = TRUE)</pre>
## Standard deviations (1, .., p=13):
```

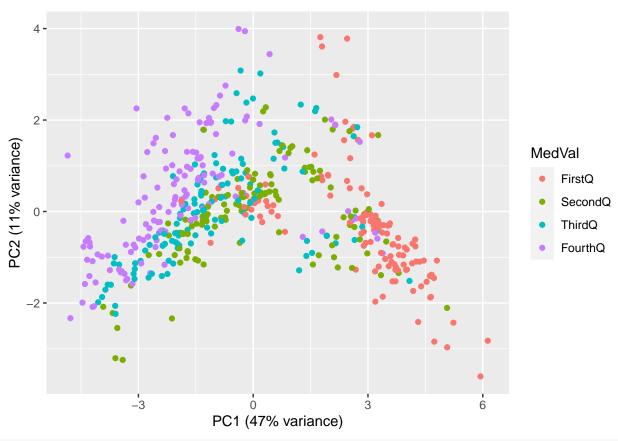
```
[1] 2.4752472 1.1971947 1.1147272 0.9260535 0.9136826 0.8108065 0.7316803
   [8] 0.6293626 0.5262541 0.4692950 0.4312938 0.4114644 0.2520104
##
##
## Rotation (n x k) = (13 \times 13):
##
                  PC1
                            PC2
                                       PC3
                                                  PC4
          0.250951397 - 0.31525237 \ 0.24656649 - 0.06177071
## crim
                                                      0.082156919
## zn
          -0.256314541 -0.32331290 0.29585782 -0.12871159
## indus
          ## chas
          0.005042434 0.45482914 0.28978082 -0.81594136
                                                       0.086530945
## nox
          0.342852313 0.21911553 0.12096411 0.12822614
                                                      0.136853557
## rm
          -0.189242570 0.14933154 0.59396117
                                           0.28059184 -0.423447195
          age
         -0.321543866 -0.34907000 -0.04973627 -0.21543585 0.098592247
##
  dis
## rad
          0.319792768 -0.27152094 0.28725483 -0.13234996 -0.204131621
          ## tax
## ptratio 0.204942258 -0.30589695 -0.32344627 -0.28262198 -0.584002232
          -0.202972612 0.23855944 -0.30014590 -0.16849850 -0.345606947
## black
## lstat
          0.309759840 -0.07432203 -0.26700025 -0.06941441 0.394561129
                            PC7
##
                 PC6
                                        PC8
                                                   PC9
                                                              PC10
## crim
                                             0.26039028 -0.019369130
          -0.21965961 0.777607207 -0.153350477
## zn
         -0.32338810 -0.274996280 0.402680309 0.35813749 -0.267527234
          -0.07613790 -0.339576454 -0.173931716 0.64441615 0.363532262
## indus
          0.16749014 \quad 0.074136208 \quad 0.024662148 \quad -0.01372777 \quad 0.006181836
## chas
          -0.15298267 -0.199634840 -0.080120560 -0.01852201 -0.231056455
## nox
## rm
          ## age
          -0.07170914 0.116010713 0.600822917 -0.06756218 -0.362778957
          0.02343872 - 0.103900440 \quad 0.121811982 - 0.15329124 \quad 0.171213138
## dis
## rad
          -0.14319401 -0.137942546 -0.080358311 -0.47089067 -0.021909452
         -0.19293428 -0.314886835 -0.082774347 -0.17656339 0.035168348
## tax
## ptratio 0.27315330 0.002323869 0.317884202 0.25442836 -0.153430488
## black
          -0.80345454
                     0.070294759
                                0.004922915 -0.04489802
                                                       0.096515117
## lstat
          -0.05321583
                     0.087011169  0.424352926  -0.19522139  0.600711409
##
                PC11
                            PC12
                                       PC13
          -0.10964435 -0.086761070
                                0.045952304
## crim
          0.26275629
                     0.071425278 -0.080918973
## indus
         ## chas
          0.01392667 0.003982683
                                0.035921715
          0.11131888 -0.804322567
## nox
                                 0.043630446
          0.05316154 -0.152872864
## rm
                                0.045567096
         -0.45915939 0.211936074 -0.038550683
## age
## dis
         -0.69569257 -0.390941129 -0.018298538
          ## rad
## tax
          -0.10483575 0.215191126
                                0.720233448
## ptratio 0.17450534 -0.209598826 0.023398052
## black
          0.01927490 -0.041723158 -0.004463073
          0.27138243 -0.055225960 0.024431677
## 1stat
# first 4 components explain ~75% of variance
summary(pca)
## Importance of components:
                          PC1
                                PC2
                                       PC3
                                               PC4
                                                      PC5
                                                             PC6
                                                                    PC7
##
```

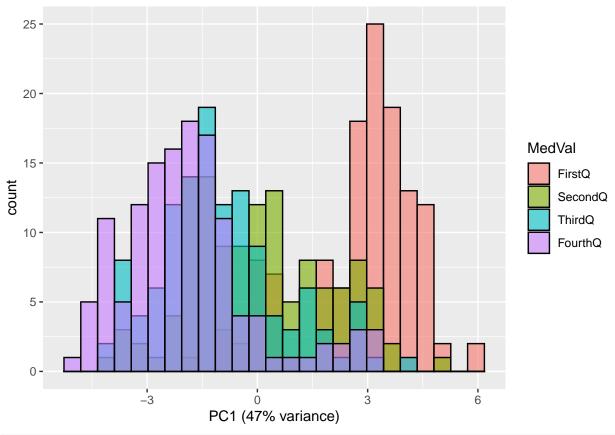
Proportion of Variance 0.4713 0.1103 0.09559 0.06597 0.06422 0.05057 0.04118 ## Cumulative Proportion 0.4713 0.5816 0.67713 0.74310 0.80732 0.85789 0.89907

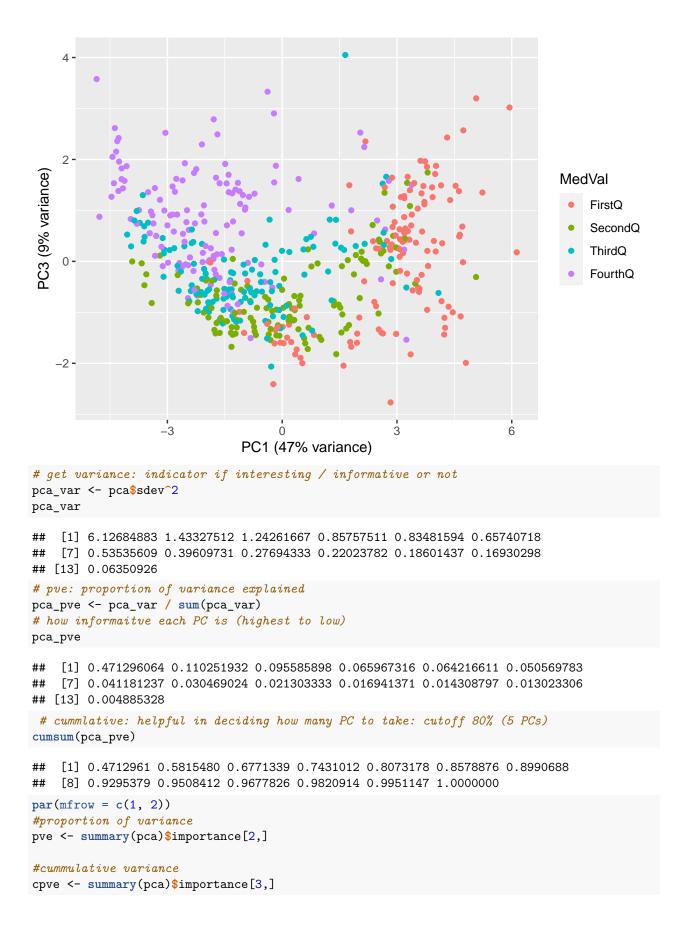
Standard deviation

2.4752 1.1972 1.11473 0.92605 0.91368 0.81081 0.73168

```
##
                               PC8
                                      PC9
                                             PC10
                                                     PC11
                                                              PC12
                                                                      PC13
## Standard deviation
                          0.62936 0.5263 0.46930 0.43129 0.41146 0.25201
## Proportion of Variance 0.03047 0.0213 0.01694 0.01431 0.01302 0.00489
## Cumulative Proportion 0.92954 0.9508 0.96778 0.98209 0.99511 1.00000
# chas is co-directed with PC1
biplot(pca)
                 -10
                                     10
                                              20
                            0
                                                   20
                                           age
                                             nox
                                            indu
     0.00
                                                    0
             -0.10
                          0.00
                                       0.10
                           PC1
# data frame with MedVal
pca_adj <- data.frame(pca$x, MedVal = boston_F$medv_F)</pre>
```

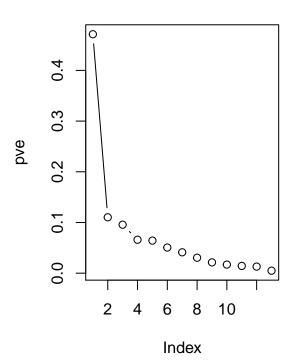




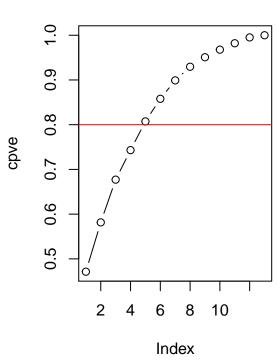


```
plot(pve, type = "b", main = "Proportion of Var. Explained")
# 5 features explain 80%
plot(cpve, type = "b", main = "Cumulative Prop. of Var. Explained")
abline(h = 0.8, col = "red")
```

Proportion of Var. Explained Cumulative Prop. of Var. Explaine



0



```
par(mfrow = c(1, 1))
plot(pca)
```

pca

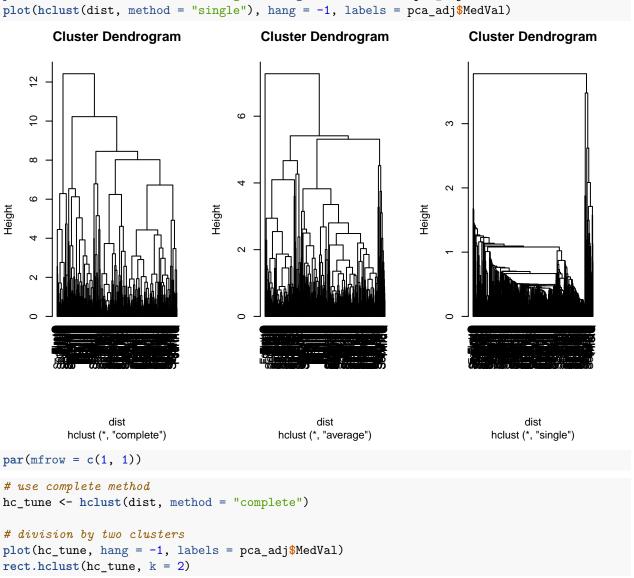


```
par(mfrow = c(1, 3))

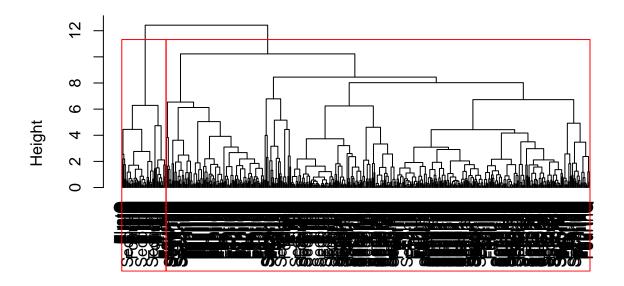
# based on above, decided to use first 5 PCs
# clustering visually looks better than initial

pca_tune <- pca_adj[, 1:5]
dist <- dist(pca_tune)

# complete looks best, single terrible
plot(hclust(dist, method = "complete"), hang = -1, labels = pca_adj$MedVal)
plot(hclust(dist, method = "average"), hang = -1, labels = pca_adj$MedVal)
plot(hclust(dist, method = "single"), hang = -1, labels = pca_adj$MedVal)</pre>
```



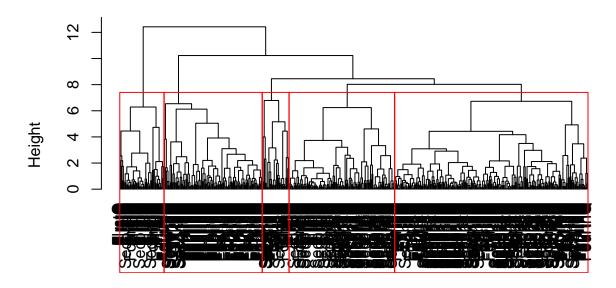
Cluster Dendrogram



dist hclust (*, "complete")

```
plot(hc_tune, hang = -1, labels = pca_adj$MedVal)
rect.hclust(hc_tune, k = 5)
```

Cluster Dendrogram



dist hclust (*, "complete")

```
# check intersection of clusters (k = 2-5) and
# compare with original hc without tuning: improved
table(pca_adj$MedVal, cutree(hc_tune, 2))
##
##
              1
                  2
##
    FirstQ
             85
                 42
##
    SecondQ 121
                  3
##
    ThirdQ 122
    FourthQ 130
##
table(pca_adj$MedVal, cutree(hc, 2))
##
##
              1
                  2
##
    FirstQ 36 91
     SecondQ 98 26
##
     ThirdQ 109 14
##
##
    FourthQ 121 11
table(pca_adj$MedVal, cutree(hc_tune, 3))
##
##
              1
                  2
                      3
##
    FirstQ
              0 85 42
              7 114
##
     SecondQ
                      3
##
     ThirdQ
             29 93
                      1
                      2
##
     FourthQ 70 60
table(pca_adj$MedVal, cutree(hc, 3))
##
##
              1
                 2
                      3
##
     FirstQ
             36 33 58
##
     SecondQ 98
                     22
##
     ThirdQ 109
                 1 13
    FourthQ 121
                  0 11
table(pca_adj$MedVal, cutree(hc_tune, 4))
##
##
              1 2
                      3
                          4
##
    FirstQ
              0 80
                      5 42
##
              7 110
    SecondQ
                      4
                          3
##
     ThirdQ
             29 83 10
    FourthQ 70 50 10
##
                          2
table(pca_adj$MedVal, cutree(hc, 4))
##
##
                      3
##
    FirstQ
             36
                  4 58
                         29
##
     SecondQ 98
                  1
                     22
                          3
##
    ThirdQ 109
                  0 13
                          1
    FourthQ 121
                  0 11
# difficult to make a call as they are not cleanly clustered,
# but 4 looks best to me (above)
```

```
table(pca_adj$MedVal, cutree(hc_tune, 5))
##
##
             1 2 3 4 5
##
             0 22 58 5 42
    FirstQ
     SecondQ 7 73 37 4 3
##
##
     ThirdQ 29 70 13 10 1
##
    FourthQ 70 44 6 10 2
table(pca_adj$MedVal, cutree(hc, 5))
##
##
             1 2 3 4 5
##
    FirstQ 20 16 4 58 29
##
     SecondQ 56 42 1 22 3
     ThirdQ 67 42 0 13 1
##
    FourthQ 51 70 0 11 0
##
# graphical analysis of pca data with clustering with 5 priniciple components
# create data frame with first 2 PCs
data_pca_clust <- data.frame(pca$x[, 1:2], # use 2 PCs even tho use 5 for clustering
                             # create factored columns with cluster assignment with 5 PCs
                            k2 = factor(cutree(hc_tune, 2)),
                            k3 = factor(cutree(hc_tune, 3)),
                            k4 = factor(cutree(hc_tune, 4)),
                            k5 = factor(cutree(hc_tune, 5)),
                            label = pca_adj$MedVal)
# plot k = 2
p4 <- ggplot(data_pca_clust,
      aes(x = PC1,
          y = PC2,
          color = k2,
          label = pca_adj$MedVal)) +
 geom_point() +
 geom_label() +
 theme_bw()
p4
```

