Wine Quality Clustering

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Libraries

Reading in data set

```
wine = read_delim("winequality-red.csv", delim = ";", escape_double = FALSE, trim_ws = T
## Rows: 1599 Columns: 12
## -- Column specification -------
## Delimiter: ";"
## dbl (12): fixed acidity, volatile acidity, citric acid, residual sugar, chlo...
##
## i Use 'spec()' to retrieve the full column specification for this data.
## i Specify the column types or set 'show_col_types = FALSE' to quiet this message.
head(wine, 5)
```

```
## # A tibble: 5 x 12
     'fixed acidity' 'volatile acidity' 'citric acid' 'residual sugar' chlorides
##
               <dbl>
                                   <dbl>
                                                 <dbl>
                                                                  <dbl>
                                                                             <dbl>
## 1
                 7.4
                                    0.7
                                                  0
                                                                    1.9
                                                                             0.076
## 2
                 7.8
                                    0.88
                                                                    2.6
                                                  0
                                                                             0.098
## 3
                 7.8
                                    0.76
                                                  0.04
                                                                    2.3
                                                                             0.092
## 4
                                    0.28
                                                                    1.9
                11.2
                                                  0.56
                                                                             0.075
## 5
                 7.4
                                    0.7
                                                                    1.9
                                                                             0.076
                                                  0
## # i 7 more variables: 'free sulfur dioxide' <dbl>,
       'total sulfur dioxide' <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,
## #
       alcohol <dbl>, quality <dbl>
```

Looking at correlation matrix

```
wine %>%
select(-quality) %>%
cor(use="pairwise.complete.obs") %>%
round(2)
```

##		fixed acidity	volatile acidity	citric acid	residual	sugar
##	fixed acidity	1.00	-0.26	0.67		0.11
##	volatile acidity	-0.26	1.00	-0.55		0.00
##	citric acid	0.67	-0.55	1.00		0.14
##	residual sugar	0.11	0.00	0.14		1.00
##	chlorides	0.09	0.06	0.20		0.06
##	free sulfur dioxide	-0.15	-0.01	-0.06		0.19
##	${\tt total \ sulfur \ dioxide}$	-0.11	0.08	0.04		0.20
##	density	0.67	0.02	0.36		0.36
##	рН	-0.68	0.23	-0.54		-0.09
##	sulphates	0.18	-0.26	0.31		0.01
##	alcohol	-0.06	-0.20	0.11		0.04
##		chlorides free	sulfur dioxide t	total sulfur	dioxide	density
##	fixed acidity	0.09	-0.15		-0.11	0.67
##	volatile acidity	0.06	-0.01		0.08	0.02
##	citric acid	0.20	-0.06		0.04	0.36
##	residual sugar	0.06	0.19		0.20	0.36
##	chlorides	1.00	0.01		0.05	0.20
##	free sulfur dioxide	0.01	1.00		0.67	-0.02
##	total sulfur dioxide	0.05	0.67		1.00	0.07
	density	0.20	-0.02		0.07	1.00
##	рН	-0.27	0.07		-0.07	-0.34
##	sulphates	0.37	0.05		0.04	0.15
##	alcohol	-0.22	-0.07		-0.21	-0.50
##		pH sulphate	s alcohol			

```
## fixed acidity
                       -0.68
                                  0.18
                                         -0.06
## volatile acidity
                                 -0.26
                                         -0.20
                        0.23
## citric acid
                       -0.54
                                  0.31
                                         0.11
## residual sugar
                       -0.09
                                  0.01
                                         0.04
## chlorides
                                  0.37
                                        -0.22
                       -0.27
## free sulfur dioxide
                                  0.05
                                         -0.07
                       0.07
## total sulfur dioxide -0.07
                                  0.04
                                        -0.21
## density
                                  0.15
                                        -0.50
                       -0.34
## pH
                                 -0.20
                                        0.21
                        1.00
## sulphates
                       -0.20
                                  1.00
                                        0.09
## alcohol
                        0.21
                                  0.09 1.00
```

i 6 more variables: 'free sulfur dioxide' <dbl>,

Normalizing the data

```
predictors = wine %>%
  select(-quality)
predictors[, c("fixed acidity", "volatile acidity", "citric acid", "residual sugar", "ch
head(predictors, 5)
## # A tibble: 5 x 11
     'fixed acidity' 'volatile acidity' 'citric acid' 'residual sugar' chlorides
##
##
               <dbl>
                                   <dbl>
                                                 <dbl>
                                                                   <dbl>
                                                                             <dbl>
## 1
              -0.528
                                   0.962
                                                 -1.39
                                                                -0.453
                                                                           -0.244
## 2
              -0.298
                                   1.97
                                                 -1.39
                                                                 0.0434
                                                                            0.224
## 3
              -0.298
                                   1.30
                                                 -1.19
                                                                -0.169
                                                                            0.0963
                                  -1.38
## 4
               1.65
                                                  1.48
                                                                -0.453
                                                                           -0.265
## 5
              -0.528
                                   0.962
                                                 -1.39
                                                                -0.453
                                                                           -0.244
```

'total sulfur dioxide' <dbl>, density <dbl>, pH <dbl>, sulphates <dbl>,

Fitting and Evaluating

#

alcohol <dbl>

```
kmodel = kmeans(predictors, centers = 3, nstart = 20)
kmodel

## K-means clustering with 3 clusters of sizes 724, 502, 373
##
## Cluster means:
```

```
fixed acidity volatile acidity citric acid residual sugar
##
                            chlorides
## 1
   -0.64949027
          0.45482336 -0.7591418
                     -0.22780950 -0.188575893
## 2
   1.00367463
          -0.68547433
                1.0204527
                      0.03104004 0.276076371
## 3
   -0.09011718
          0.03972118
                0.1001378
                      0.40040745 -0.005526519
  free sulfur dioxide total sulfur dioxide
                     density
                            pH sulphates
## 1
      -0.2216967
               -0.3492025 -0.4505506 0.6139437 -0.2873116
## 2
      -0.4767114
               -0.4815366   0.4383036   -0.7518363   0.5544470
## 3
               1.3258820 0.2846387 -0.1798214 -0.1885221
      1.0718969
##
   alcohol
  0.06851232
## 1
## 2 0.28250279
## 3 -0.51318854
##
## Clustering vector:
  [1] \ 1 \ 3 \ 1 \ 2 \ 1 \ 1 \ 1 \ 1 \ 1 \ 3 \ 1 \ 3 \ 1 \ 2 \ 3 \ 3 \ 2 \ 1 \ 2 \ 3 \ 3 \ 2 \ 3 \ 1 \ 1 \ 1 \ 2 \ 1 \ 1 \ 1 \ 1 \ 3 \ 3 \ 1 \ 1 \ 1
  ##
  ##
##
 ##
##
 ##
##
 ##
##
 ##
 [371] 1 2 2 3 2 2 2 2 2 3 2 2 2 2 3 1 3 1 3 2 1 2 2 3 2 2 3 2 2 1 3 1 2 2 1 2 2
##
 ##
 ##
 ##
 ##
 ##
 [593] 3 2 1 3 2 2 1 2 1 2 1 2 3 1 2 3 2 1 3 2 1 2 2 3 3 2 2 2 3 3 2 1 3 3 1 1 1
##
 [667] \ 2 \ 2 \ 2 \ 2 \ 3 \ 1 \ 3 \ 1 \ 2 \ 2 \ 2 \ 1 \ 3 \ 2 \ 2 \ 1 \ 3 \ 1 \ 1 \ 3 \ 1 \ 2 \ 1 \ 3 \ 2 \ 3 \ 3 \ 1 \ 1 \ 1 \ 3 \ 2 \ 3 \ 1 \ 1
##
##
 ##
 ##
##
 ##
 ##
 [889] \ 1\ 3\ 3\ 1\ 2\ 1\ 1\ 1\ 2\ 1\ 2\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 2\ 2\ 2\ 2\ 1\ 2\ 1\ 3\ 3\ 1\ 2\ 3\ 1\ 3\ 2
 ##
  [963] \ 1 \ 2 \ 2 \ 2 \ 3 \ 2 \ 1 \ 2 \ 2 \ 1 \ 2 \ 3 \ 3 \ 1 \ 2 \ 2 \ 1 \ 3 \ 3 \ 1 \ 2 \ 1 \ 3 \ 1 \ 3 \ 1 \ 1 \ 1 \ 1 
##
```

```
## [1370] 1 2 2 2 3 1 3 1 1 1 1 1 1 3 3 3 3 3 1 1 1 3 1 1 1 1 3 1 1 3 1 1 3 1 2 2 1 2
## [1592] 1 1 1 1 1 1 1 1
##
## Within cluster sum of squares by cluster:
## [1] 4195.309 5040.596 3386.103
## (between_SS / total_SS = 28.2 %)
##
## Available components:
##
## [1] "cluster"
      "centers"
                   "tot.withinss"
          "totss"
              "withinss"
## [6] "betweenss"
      "size"
          "iter"
              "ifault"
```

The SS proportion is not very great, now its time to test different possible cluster amounts:

```
max_clusters = 10

# Within sum of squares
wss = numeric(max_clusters)

# Reproducibility
set.seed(321)

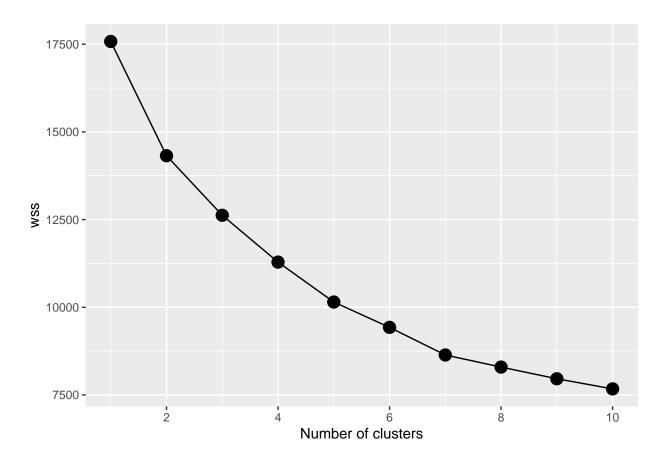
# Look over 1 -> n clusters
for (i in 1:max_clusters) {
    km = kmeans(predictors, centers = i, nstart = 20)

    wss[i] = km$tot.withinss
}

# Produce a scree plot to visualize wss vs clusters
wss_df = tibble(clusters = 1:max_clusters, wss = wss)

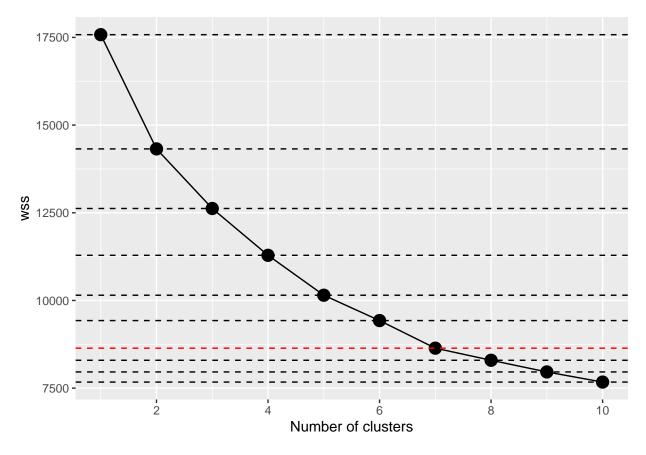
scree_plot = ggplot(wss_df, aes(x = clusters, y = wss, group = 1)) +
    geom_point(size = 4) +
```

```
geom_line() +
scale_x_continuous(breaks = c(2, 4, 6, 8, 10)) +
xlab("Number of clusters")
scree_plot
```



It's hard to tell where the drop off happens so I'll add lines in the graph.

```
scree_plot +
  geom_hline(
    yintercept = wss,
    linetype = "dashed",
    col = c(rep("#000000", 6), "#FF0000", rep("#000000", 3))
)
```



There is a significant reduction in model improvement after the 7th cluster, so we'll build a model based on this result.

```
k = 7
set.seed(321)
km = kmeans(predictors, centers = k, nstart = 20)
km
## K-means clustering with 7 clusters of sizes 335, 34, 246, 497, 29, 267, 191
##
## Cluster means:
##
     fixed acidity volatile acidity citric acid residual sugar
                                                                  chlorides
       -0.10300336
                         0.05409899
                                    0.05352831
                                                   -0.01164417 -0.03293559
## 1
## 2
      -0.08560643
                        -0.03464133 0.41472600
                                                     4.96021580 0.29629520
## 3
        0.05035896
                        -1.03768918 0.70824781
                                                    -0.18148350 -0.28949306
       -0.40951062
                         0.63621199 -0.78204789
                                                    -0.20640683 -0.03782882
## 4
## 5
        0.08180575
                         0.01794915 1.14382029
                                                    -0.39927103 5.60297844
        1.64680959
                        -0.60790045
                                    1.23778419
                                                     0.14965815 0.03321812
## 6
## 7
       -1.11788120
                         0.43935979 -0.94891620
                                                    -0.24029985 -0.42083775
     free sulfur dioxide total sulfur dioxide
                                                   density
                                                                        sulphates
                                                                   рΗ
                                    1.2318849 0.22367883 -0.1077529 -0.18807595
## 1
              0.99407806
```

```
## 2
            1.74964380
                               1.6953018 1.22461740 -0.3253578 -0.02378189
## 3
           -0.26318636
                              -0.5055549 -0.68017199 -0.1230637 0.39462568
## 4
           -0.48364728
                              -0.4113709 0.02578926 0.3178251 -0.38981527
           -0.07045695
                               0.4742672 0.18574466 -1.6868288 3.71944476
## 5
## 6
           -0.52906451
                              -0.4704402 1.08624118 -0.9962650 0.29506721
                              -0.1552359 -1.34804889 1.2271977 -0.13702903
## 7
            0.29275382
##
       alcohol
## 1 -0.57245599
## 2 -0.36379918
## 3 1.01179431
## 4 -0.51438888
## 5 -0.88228685
## 6 0.02435629
## 7 1.20405754
##
## Clustering vector:
##
     [1] 4 4 4 6 4 4 4 4 4 1 4 1 7 5 1 1 1 5 4 5 1 1 4 4 4 4 4 4 4 4 4 4 1 2 4 4 4
##
    ##
    [75] 1 3 3 4 4 1 4 5 1 5 3 4 5 4 1 4 1 5 5 4 7 7 4 4 4 4 4 4 4 4 4 5 4 1 1 4
   ##
   [149] 4 3 3 5 1 1 1 1 1 1 4 1 4 4 4 2 2 1 1 4 4 5 4 4 4 7 4 4 4 4 4 4 4 5 4 4 4
##
##
   [186] 1 1 4 1 1 1 4 1 4 4 1 4 6 7 7 3 1 4 4 4 6 6 1 1 6 3 4 6 1 4 1 4 4 4 1 1 1
   [223] 4 4 4 1 5 4 1 4 7 4 1 4 4 4 4 4 4 5 6 1 6 6 4 4 4 4 4 6 4 6 1 4 1 6 4 5
##
##
   [260] 6 1 4 4 1 6 6 4 3 4 6 1 6 6 4 2 1 4 6 6 6 6 5 4 6 1 1 6 1 4 6 4 5 6 4 6 6
##
   [297] 1 4 4 4 4 6 4 4 1 6 4 6 6 4 6 1 1 1 1 3 1 1 1 1 1 1 1 1 2 2 6 6 6 6 6 6 1
   [334] 4 7 6 3 1 6 6 6 6 6 6 6 6 1 7 6 6 4 6 4 4 6 1 7 6 6 6 6 6 1 1 6 6 6 6 6 6 6 3
##
   [371] 1 3 3 1 6 6 6 3 6 1 3 6 3 3 1 4 1 4 1 6 7 6 6 1 6 6 2 6 6 4 2 3 6 6 4 3 6
##
   [408] 6 6 6 1 1 4 6 1 2 6 1 6 4 1 7 4 6 4 7 7 4 4 6 6 1 6 6 6 6 1 6 6 4 6 6 6 3
##
   [445] 7 4 6 3 4 6 6 5 4 6 3 6 4 1 6 6 3 4 6 1 6 6 6 3 6 1 6 3 6 6 6 4 6 6 4 4 2
##
##
   [482] 3 6 6 6 6 6 6 6 6 6 1 3 3 1 2 6 4 1 6 1 4 2 2 6 6 3 6 6 1 6 6 1 6 6 6 2 6 6
   [519] 6 1 6 1 1 1 1 1 1 1 1 4 3 6 6 3 6 3 4 4 6 6 1 6 4 6 6 1 4 6 6 6 4 6 6 7 6
##
##
   [556] 6 6 6 6 6 6 1 1 1 6 6 4 4 6 7 6 7 6 6 6 6 4 1 1 6 6 6 6 6 1 4 6 1 7 6 1 1
   [593] 1 6 4 2 6 6 4 6 4 6 4 6 1 4 3 1 6 7 1 6 4 3 5 1 1 6 6 6 1 1 4 3 4 4 4 4 4
##
##
   [630] 1 4 6 4 4 1 4 1 1 4 3 6 1 6 1 6 4 4 4 3 2 6 1 6 6 6 1 6 6 4 4 4 4 4 6 6 1
   ##
##
   [741] 4 1 4 6 6 4 1 1 4 4 4 4 1 4 5 7 7 4 4 1 1 4 4 4 4 4 1 1 1 4 1 1 1 4 4 4 4
##
##
   [778] 4 4 1 4 4 1 4 4 6 6 1 1 1 1 1 4 4 3 6 1 3 6 6 1 4 7 4 4 3 3 3 4 4 4 6 6 3
##
   [815] 6 6 4 3 4 4 4 7 4 4 4 4 3 4 7 7 4 7 1 1 4 4 7 7 3 4 6 4 1 1 3 4 4 4 4 4 6
   [852] 6 1 1 1 7 1 3 6 7 4 7 4 4 4 4 7 7 7 7 7 7 1 3 6 3 4 7 1 4 4 7 3 4 1 4 4 3
##
##
   [889] 7 2 1 4 6 4 4 7 3 7 3 4 3 4 4 4 4 1 1 7 7 3 3 2 3 3 3 3 7 2 1 7 6 1 7 2 3
##
   ##
   [963] 4 3 3 3 3 1 3 4 3 3 3 3 1 1 1 3 6 4 4 7 4 6 7 3 1 4 3 4 1 1 1 1 4 7 7 4
  [1000] 7 3 3 3 3 1 3 3 3 3 1 3 3 4 4 4 3 3 3 3 4 6 6 4 3 4 4 3 7 1 4 7 4 4 4 4 6
  [1037] 3 4 3 3 4 4 3 2 3 7 4 1 3 3 1 5 7 3 4 4 3 1 3 3 6 3 3 3 7 4 7 6 6 1 3 2 1
```

```
## [1074] 4 2 1 3 6 6 2 3 2 1 3 1 1 3 3 6 6 3 3 7 3 4 6 4 4 3 4 3 3 7 3 3 7 3 3 4 6
## [1111] 4 7 3 6 7 7 7 7 7 7 7 3 7 7 6 7 3 7 7 1 1 4 1 3 4 3 3 6 6 1 1 1 3 7 3 1 3 4
## [1148] 6 3 3 3 7 4 3 7 4 3 7 3 6 6 3 3 4 4 5 6 3 3 3 3 7 3 1 1 7 7 7 7 3 3 3 1 1 4
## [1185] 1 3 7 3 1 4 3 4 3 4 4 4 1 4 3 1 4 3 3 1 3 3 3 1 3 3 4 1 4 3 6 3 1 3 3 3 6
## [1222] 6 1 3 6 1 1 4 7 1 3 1 1 6 7 2 4 7 4 7 1 1 3 1 2 4 4 4 3 7 7 1 4 4 4 7 1 1
## [1259] 7 7 5 7 1 4 3 4 4 3 1 7 7 7 7 1 4 1 3 4 1 3 1 1 4 1 7 6 3 7 1 1 4 1 7 4 1
## [1296] 1 1 7 7 4 7 7 3 3 1 1 1 7 1 1 1 7 4 1 1 1 7 3 1 5 1 7 3 3 7 7 7 7 4 1 1 1
## [1333] 4 4 4 7 4 4 4 4 4 4 4 4 6 4 7 4 4 7 1 7 4 4 4 4 4 7 1 6 4 4 6 4 7 4 4 1 1
## [1370] 4 5 3 5 1 4 1 4 7 4 4 4 4 1 1 1 1 4 4 4 1 7 4 4 1 1 4 4 1 4 7 1 1 3 3 4 3
## [1407] 3 7 3 7 7 3 3 1 6 4 6 3 4 1 4 1 7 4 3 3 3 3 4 3 3 1 7 4 2 2 1 7 4 1 3 1 4
## [1444] 7 1 1 4 4 1 3 3 3 7 1 6 7 7 1 3 3 1 4 4 4 1 1 1 7 1 4 4 7 3 7 2 7 2 7 4 3
## [1481] 7 3 4 3 4 4 4 7 7 7 3 7 7 1 7 7 1 7 4 7 4 1 4 3 3 4 4 3 3 3 1 4 4 7 4 4 3
## [1518] 7 3 4 7 4 3 1 7 4 4 4 1 1 7 4 4 1 7 4 7 7 7 1 7 3 7 6 3 4 4 7 6 3 4 4 7 4
## [1555] 7 7 4 7 2 1 1 1 4 4 4 7 3 4 4 7 3 7 1 7 2 3 3 7 7 7 3 7 7 1 3 3 3 7 7 2 7
## [1592] 7 7 4 7 7 7 7 3
##
## Within cluster sum of squares by cluster:
## [1] 1853.1985 627.7512 1111.1525 2013.9315 462.0344 1502.8903 1068.2468
## (between_SS / total_SS = 50.9 %)
##
## Available components:
##
## [1] "cluster"
                      "centers"
                                     "totss"
                                                    "withinss"
                                                                   "tot.withinss"
## [6] "betweenss"
                      "size"
                                     "iter"
                                                    "ifault"
```