# Assignment5_Bonus

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## Neural networks (seeds data)

seeds data set from UCI repository1

Explore the data.

Measurements of geometrical properties of kernels belonging to three different varieties of wheat. A soft X-ray technique and GRAINS package were used to construct all seven, real-valued attributes.

```r
library(tidyverse)
```

```
## -- Attaching packages --------------------------------------- tidyverse 1.3.0 --
```

```
## v ggplot2 3.3.3     v purrr   0.3.4
## v tibble  3.0.6     v dplyr   1.0.4
## v tidyr   1.1.2     v stringr 1.4.0
## v readr   1.4.0     v forcats 0.5.0
```

```
## -- Conflicts ------------------------------------------ tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```r
seeds <- read.table(
  "https://archive.ics.uci.edu/ml/machine-learning-databases/00236/seeds_dataset.txt"
  )
colnames(seeds) <- c("area",
                     "perimeter",
                     "compactness",
                     "length_of_kernel",
                     "width_of_kernel",
                     "asy_coeff",
                     "length_of_kernel_groove",
                     "Class")
summary(seeds)
```

```
##       area         perimeter      compactness     length_of_kernel
##  Min.   :10.59   Min.   :12.41   Min.   :0.8081   Min.   :4.899
##  1st Qu.:12.27   1st Qu.:13.45   1st Qu.:0.8569   1st Qu.:5.262
##  Median :14.36   Median :14.32   Median :0.8734   Median :5.524
##  Mean   :14.85   Mean   :14.56   Mean   :0.8710   Mean   :5.629
##  3rd Qu.:17.30   3rd Qu.:15.71   3rd Qu.:0.8878   3rd Qu.:5.980
##  Max.   :21.18   Max.   :17.25   Max.   :0.9183   Max.   :6.675
##  width_of_kernel   asy_coeff      length_of_kernel_groove     Class
##  Min.   :2.630   Min.   :0.7651   Min.   :4.519           Min.   :1
##  1st Qu.:2.944   1st Qu.:2.5615   1st Qu.:5.045           1st Qu.:1
##  Median :3.237   Median :3.5990   Median :5.223           Median :2
```

| area | perimeter | compactness | length_of_kernel | width_of_kernel | asy_coeff | length_of_kernel_groove | Class |
|---|---|---|---|---|---|---|---|
| 15.26 | 14.84 | 0.8710 | 5.763 | 3.312 | 2.221 | 5.220 | 1 |
| 14.88 | 14.57 | 0.8811 | 5.554 | 3.333 | 1.018 | 4.956 | 1 |
| 14.29 | 14.09 | 0.9050 | 5.291 | 3.337 | 2.699 | 4.825 | 1 |
| 13.84 | 13.94 | 0.8955 | 5.324 | 3.379 | 2.259 | 4.805 | 1 |
| 16.14 | 14.99 | 0.9034 | 5.658 | 3.562 | 1.355 | 5.175 | 1 |
| 14.38 | 14.21 | 0.8951 | 5.386 | 3.312 | 2.462 | 4.956 | 1 |

```
##  Mean   :3.259   Mean   :3.7002   Mean   :5.408           Mean   :2
##  3rd Qu.:3.562   3rd Qu.:4.7687   3rd Qu.:5.877           3rd Qu.:3
##  Max.   :4.033   Max.   :8.4560   Max.   :6.550           Max.   :3
```

```
cor(dplyr::select(seeds, -Class))
```

```
##                               area  perimeter compactness length_of_kernel
## area                     1.0000000  0.9943409   0.6082884        0.9499854
## perimeter                0.9943409  1.0000000   0.5292436        0.9724223
## compactness              0.6082884  0.5292436   1.0000000        0.3679151
## length_of_kernel         0.9499854  0.9724223   0.3679151        1.0000000
## width_of_kernel          0.9707706  0.9448294   0.7616345        0.8604149
## asy_coeff               -0.2295723 -0.2173404  -0.3314709       -0.1715624
## length_of_kernel_groove  0.8636927  0.8907839   0.2268248        0.9328061
##                         width_of_kernel   asy_coeff length_of_kernel_groove
## area                          0.9707706 -0.22957233              0.86369275
## perimeter                     0.9448294 -0.21734037              0.89078390
## compactness                   0.7616345 -0.33147087              0.22682482
## length_of_kernel              0.8604149 -0.17156243              0.93280609
## width_of_kernel               1.0000000 -0.25803655              0.74913147
## asy_coeff                    -0.2580365  1.00000000             -0.01107902
## length_of_kernel_groove       0.7491315 -0.01107902              1.00000000
```

```
library(tidyverse)
library(kableExtra)
```

```
##
## Attaching package: 'kableExtra'

## The following object is masked from 'package:dplyr':
##
##     group_rows
```

```
library(knitr)
dim(seeds)
```

```
## [1] 210   8
```

```
knitr::kable(head(seeds)) %>%
  kable_styling(latex_options="scale_down")
```

```
x <- seeds %>%
  dplyr::select(-Class) %>%
  scale()
```

```
library(tidyverse)
set.seed(1)

seeds_train_index <- seeds %>%
  mutate(ind = 1:nrow(seeds)) %>%
```

```r
  group_by(Class) %>%
  mutate(n = n()) %>%
  sample_frac(size = .75, weight = n) %>%
  ungroup() %>%
  print(pull(ind))
```

```
## # A tibble: 156 x 10
##     area perimeter compactness length_of_kernel width_of_kernel asy_coeff
##    <dbl>     <dbl>       <dbl>            <dbl>           <dbl>     <dbl>
##  1  12.7      13.6       0.869             5.23            3.05      4.10
##  2  12.7      13.7       0.856             5.40            2.96      2.50
##  3  13.5      13.8       0.885             5.35            3.16      2.25
##  4  12.8      13.6       0.872             5.26            3.03      1.18
##  5  13.7      14.0       0.874             5.48            3.11      2.93
##  6  13.2      13.8       0.868             5.40            3.07      4.16
##  7  14.0      14.3       0.862             5.61            3.16      2.22
##  8  15.4      14.8       0.886             5.70            3.39      1.37
##  9  15.1      14.5       0.899             5.58            3.46      3.13
## 10  16.1      15.0       0.903             5.66            3.56      1.36
## # ... with 146 more rows, and 4 more variables: length_of_kernel_groove <dbl>,
## #   Class <int>, ind <int>, n <int>
```

```r
library(nnet)
set.seed(1)

seeds_train_index <- seeds %>%
  mutate(ind = 1:nrow(seeds)) %>%
  group_by(Class) %>%
  mutate(n = n()) %>%
  sample_frac(size = .75, weight = n) %>%
  ungroup() %>%
  pull(ind)

class_labels <- pull(seeds, Class) %>%
  class.ind()
knitr::kable(head(class_labels)) %>%
  kable_styling(latex_options="scale_down")
```

```r
seeds_train <- x[seeds_train_index, ]
train_class <- class_labels[seeds_train_index,]
seeds_test <- x[-seeds_train_index, ]
test_class <- class_labels[-seeds_train_index,]

nn_seeds <- nnet(
  x = seeds_train,
  y = train_class,
  size = 4,
  decay = 0,
  softmax = TRUE,
  maxit=500)
```

```
## # weights:  47
## initial  value 179.079752
## iter  10 value 10.357187
## iter  20 value 0.304073
```

| | | |
|---|---|---|
| 1 | 2 | 3 |
| 1 | 0 | 0 |
| 1 | 0 | 0 |
| 1 | 0 | 0 |
| 1 | 0 | 0 |
| 1 | 0 | 0 |
| 1 | 0 | 0 |

```
## iter  30 value 0.002143
## iter  40 value 0.000138
## iter  40 value 0.000061
## iter  40 value 0.000061
## final  value 0.000061
## converged
```

```r
nn_pred <- predict(nn_seeds, seeds_test,
                   type="class")

tab_seeds <- table(slice(
  seeds,
  -seeds_train_index) %>% pull(Class),
  nn_pred)

print(1-sum(diag(tab_seeds))/sum(tab_seeds))
```

```
## [1] 0.1111111
```

```r
library(nnet)
library(MASS)
```

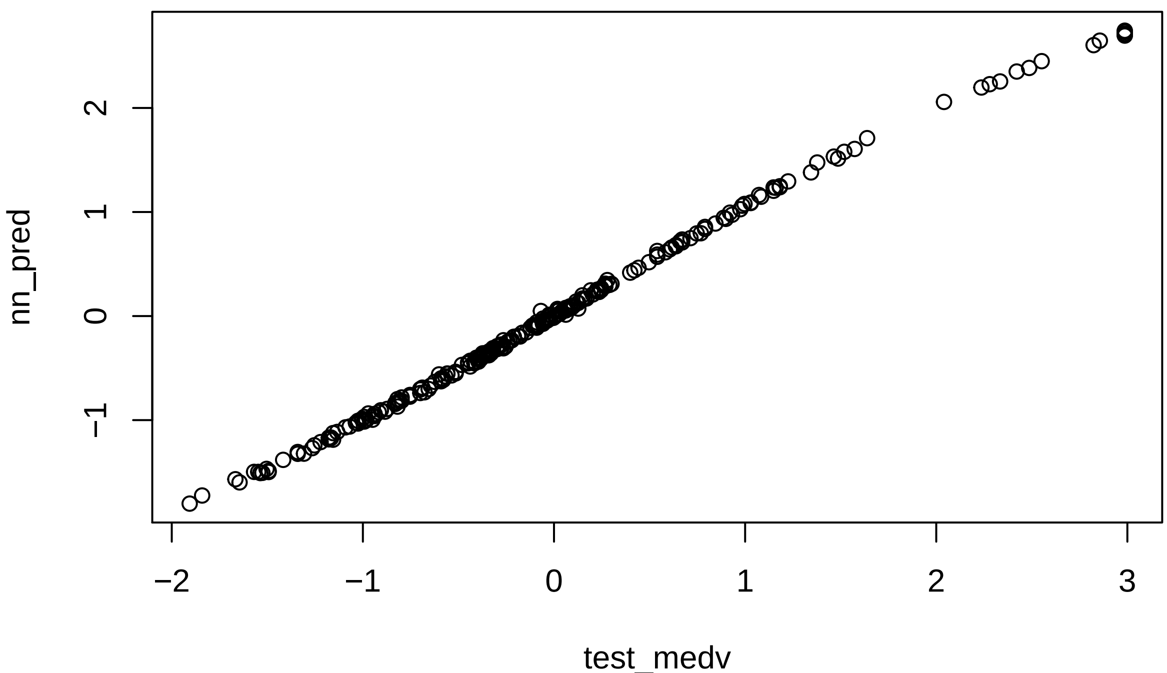
```
##
## Attaching package: 'MASS'

## The following object is masked from 'package:dplyr':
##
##     select
```

```r
train_Boston <- sample(
  1:nrow(Boston),
  nrow(Boston)/2
  )

x <- scale(Boston)

Boston_train <- x[train_Boston, ]
train_medv <- x[train_Boston, "medv"]
Boston_test <- x[-train_Boston, ]
test_medv <- x[-train_Boston, "medv"]

nn_Boston <- nnet(
  Boston_train,
  train_medv,
  size=10,
  decay=1,
  softmax=FALSE,
  maxit=1000,
  linout=TRUE
  )
```

```
## # weights:  161
## initial  value 469.211580
## iter  10 value 39.116735
## iter  20 value 22.164051
## iter  30 value 17.626264
## iter  40 value 14.619830
```

```
## iter  50 value 12.655570
## iter  60 value 11.292161
## iter  70 value 10.583592
## iter  80 value 10.254760
## iter  90 value 10.097962
## iter 100 value 10.015590
## iter 110 value 9.948224
## iter 120 value 9.917840
## iter 130 value 9.905889
## iter 140 value 9.901823
## iter 150 value 9.900874
## iter 160 value 9.900509
## iter 170 value 9.900410
## iter 180 value 9.900337
## iter 190 value 9.900141
## iter 200 value 9.900086
## iter 210 value 9.900065
## final  value 9.900062
## converged
```

```
nn_pred <- predict(
  nn_Boston,
  Boston_test,
  type="raw"
  )

plot(test_medv, nn_pred)
```




```
mean((test_medv - nn_pred)^2)
```

```
## [1] 0.003687532
```

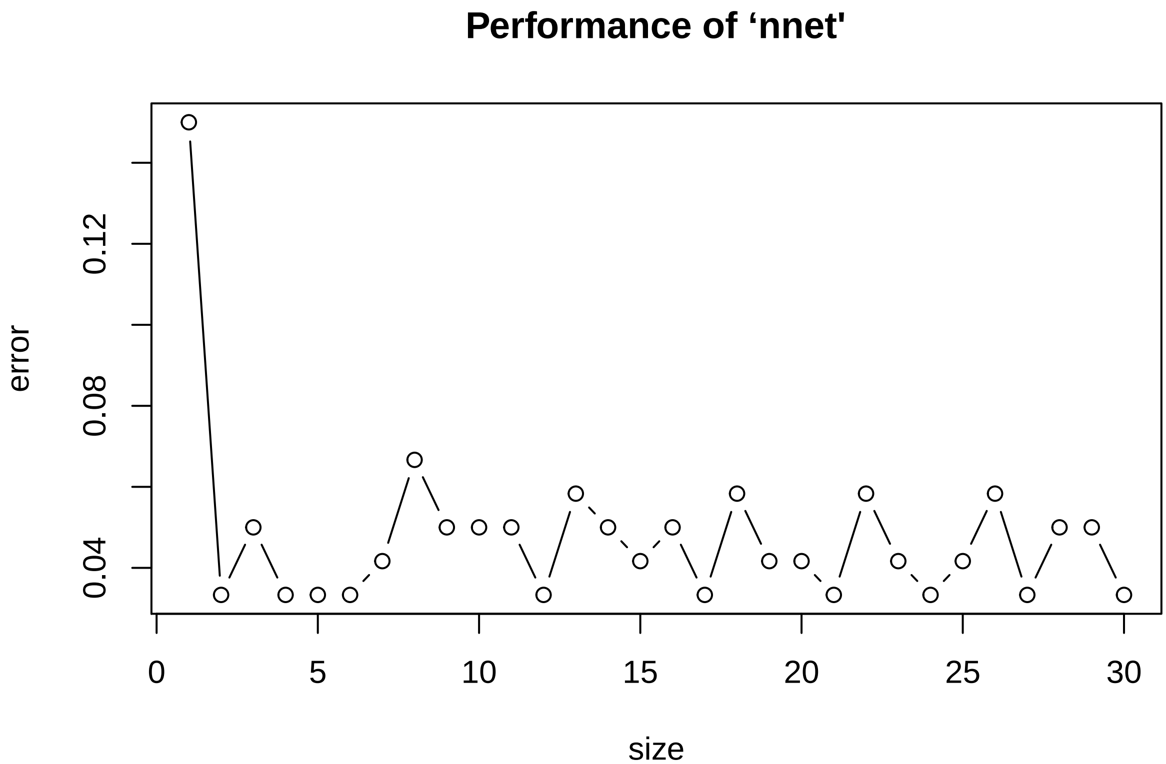
```
library(e1071)
library(cluster)
```

```r
library(dplyr)
library(nnet)
set.seed(1)

data("iris")

Species <- pull(iris, Species)

xy <- dplyr::select(iris, -Species) %>%
  scale() %>%
  data.frame() %>%
  mutate(Species = Species) # scale predictors

iris_train_index <- iris %>%
  mutate(ind = 1:nrow(iris)) %>%
  group_by(Species) %>%
  mutate(n = n()) %>%
  sample_frac(size = .8, weight = n) %>%
  ungroup() %>%
  pull(ind)

iris_train <- slice(xy, iris_train_index)
iris_test <- slice(xy, -iris_train_index)
class_labels <- pull(xy, Species) %>%
  class.ind()

iris_nnet1 <- tune.nnet(
  Species~.,
  data = iris_train,
  size = 1:30,
  tunecontrol = tune.control(sampling = "cross",cross=5)
  )

head(summary(iris_nnet1))
```

```
## $best.parameters
##   size
## 2    2
##
## $best.performance
## [1] 0.03333333
##
## $method
## [1] "nnet"
##
## $nparcomb
## [1] 30
##
## $train.ind
## $train.ind$`(0.881,24.8]`
##  [1]  40  83  90  35 111 112 120  78  22  70  28  37  61  46  67  71 116  44  49
## [20] 117  56  89  50   7  20 100  80  99  16   2 118  65  79 101  41  77 107  13
## [39] 109 114  82  19  17  57  11  31 115  74  95  55  45  52  68 119   9  97  81
## [58] 113 108  85  32  87  94  12  30  14  62   6  72  64  38 102  91   3 104  69
```

```
## [77]  54   5  88  33  84  47   8   4  98  18  27  36  63 110  25  21  66  73  23
## [96]  75
##
## $train.ind$`(24.8,48.6]`
##  [1] 106  96 103  60  51  93  34  10   1  43  59  26  15  58  29  24  42  48  76
## [20]  39 105  53  92  86  20 100  80  99  16   2 118  65  79 101  41  77 107  13
## [39] 109 114  82  19  17  57  11  31 115  74  95  55  45  52  68 119   9  97  81
## [58] 113 108  85  32  87  94  12  30  14  62   6  72  64  38 102  91   3 104  69
## [77]  54   5  88  33  84  47   8   4  98  18  27  36  63 110  25  21  66  73  23
## [96]  75
##
## $train.ind$`(48.6,72.4]`
##  [1] 106  96 103  60  51  93  34  10   1  43  59  26  15  58  29  24  42  48  76
## [20]  39 105  53  92  86  40  83  90  35 111 112 120  78  22  70  28  37  61  46
## [39]  67  71 116  44  49 117  56  89  50   7  95  55  45  52  68 119   9  97  81
## [58] 113 108  85  32  87  94  12  30  14  62   6  72  64  38 102  91   3 104  69
## [77]  54   5  88  33  84  47   8   4  98  18  27  36  63 110  25  21  66  73  23
## [96]  75
##
## $train.ind$`(72.4,96.2]`
##  [1] 106  96 103  60  51  93  34  10   1  43  59  26  15  58  29  24  42  48  76
## [20]  39 105  53  92  86  40  83  90  35 111 112 120  78  22  70  28  37  61  46
## [39]  67  71 116  44  49 117  56  89  50   7  20 100  80  99  16   2 118  65  79
## [58] 101  41  77 107  13 109 114  82  19  17  57  11  31 115  74  91   3 104  69
## [77]  54   5  88  33  84  47   8   4  98  18  27  36  63 110  25  21  66  73  23
## [96]  75
##
## $train.ind$`(96.2,120]`
##  [1] 106  96 103  60  51  93  34  10   1  43  59  26  15  58  29  24  42  48  76
## [20]  39 105  53  92  86  40  83  90  35 111 112 120  78  22  70  28  37  61  46
## [39]  67  71 116  44  49 117  56  89  50   7  20 100  80  99  16   2 118  65  79
## [58] 101  41  77 107  13 109 114  82  19  17  57  11  31 115  74  95  55  45  52
## [77]  68 119   9  97  81 113 108  85  32  87  94  12  30  14  62   6  72  64  38
## [96] 102
##
##
## $sampling
## [1] "5-fold cross validation"
```

```r
plot(iris_nnet1)
```




```
library(nnet)
nn_iris <- nnet(
  x = dplyr::select(iris_train, -Species),
  y = class_labels[iris_train_index, ],
  size = iris_nnet1$best.parameters[1,1],
  decay = 0,
  softmax = TRUE
  )
```

```
## # weights:  19
## initial  value 139.787195
## iter  10 value 51.659855
## iter  20 value 12.382653
## iter  30 value 2.538123
## iter  40 value 0.820028
## iter  50 value 0.000596
## iter  60 value 0.000139
## final  value 0.000086
## converged
```

```
nn_pred <- predict(
  nn_iris,
  dplyr::select(iris_test, -Species),
  type="class"
  )

tab <- table(pull(iris_test, Species),
  nn_pred
  )
```

```r
tab
```

```
##             nn_pred
##              setosa versicolor virginica
##   setosa         10          0         0
##   versicolor      0         10         0
##   virginica       0          2         8
```

```r
1- sum(diag(tab))/sum(tab)
```

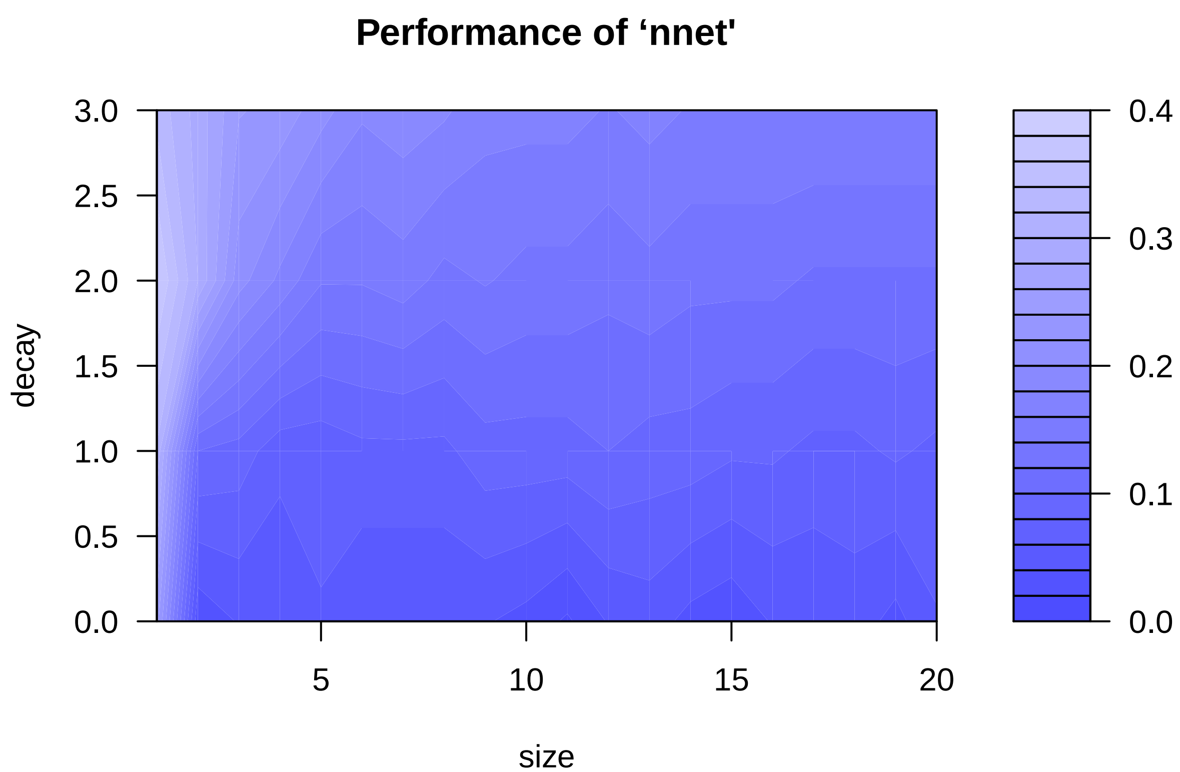
```
## [1] 0.06666667
```

```r
set.seed(1)

iris_nnet2 <- tune.nnet(
  Species~.,
  data = iris_train,
  size = 1:20,
  decay = 0:3,
  tunecontrol = tune.control(sampling = "cross",cross=5)
  )

head(summary(iris_nnet2))
```

```
## $best.parameters
##    size decay
## 11   11     0
##
## $best.performance
## [1] 0.01666667
##
## $method
## [1] "nnet"
##
## $nparcomb
## [1] 80
##
## $train.ind
## $train.ind$`(0.881,24.8]`
##  [1]  99  44 102  33  84  35  70 105  42  38  20  28  86  95  90  40  83  25 113
## [20] 119 111  88   6  24  32 114   2  45  18  22  65  13  81  94  48  63  23  46
## [39]  92  77  29  66  67  56 101  80  62  93  69 108  31 116  17   9  57  60  19
## [58]  26  30  72  53 110  10 118  11  27  75  15  50 103  91  16  47  12 104 112
## [77]   8  49   3  98  64  55  71  96  36   4 115   5  52  41  61 120  78  58 107
## [96]  76
##
## $train.ind$`(24.8,48.6]`
##  [1]  68  39   1  34  87  43  14  82  59  51  97  85  21 106  54  74   7  73  79
## [20] 109  37  89 100 117  32 114   2  45  18  22  65  13  81  94  48  63  23  46
## [39]  92  77  29  66  67  56 101  80  62  93  69 108  31 116  17   9  57  60  19
## [58]  26  30  72  53 110  10 118  11  27  75  15  50 103  91  16  47  12 104 112
## [77]   8  49   3  98  64  55  71  96  36   4 115   5  52  41  61 120  78  58 107
## [96]  76
##
## $train.ind$`(48.6,72.4]`
```

```
##  [1]  68  39   1  34  87  43  14  82  59  51  97  85  21 106  54  74   7  73  79
## [20] 109  37  89 100 117  99  44 102  33  84  35  70 105  42  38  20  28  86  95
## [39]  90  40  83  25 113 119 111  88   6  24  69 108  31 116  17   9  57  60  19
## [58]  26  30  72  53 110  10 118  11  27  75  15  50 103  91  16  47  12 104 112
## [77]   8  49   3  98  64  55  71  96  36   4 115   5  52  41  61 120  78  58 107
## [96]  76
##
## $train.ind$`(72.4,96.2]`
##  [1]  68  39   1  34  87  43  14  82  59  51  97  85  21 106  54  74   7  73  79
## [20] 109  37  89 100 117  99  44 102  33  84  35  70 105  42  38  20  28  86  95
## [39]  90  40  83  25 113 119 111  88   6  24  32 114   2  45  18  22  65  13  81
## [58]  94  48  63  23  46  92  77  29  66  67  56 101  80  62  93  47  12 104 112
## [77]   8  49   3  98  64  55  71  96  36   4 115   5  52  41  61 120  78  58 107
## [96]  76
##
## $train.ind$`(96.2,120]`
##  [1]  68  39   1  34  87  43  14  82  59  51  97  85  21 106  54  74   7  73  79
## [20] 109  37  89 100 117  99  44 102  33  84  35  70 105  42  38  20  28  86  95
## [39]  90  40  83  25 113 119 111  88   6  24  32 114   2  45  18  22  65  13  81
## [58]  94  48  63  23  46  92  77  29  66  67  56 101  80  62  93  69 108  31 116
## [77]  17   9  57  60  19  26  30  72  53 110  10 118  11  27  75  15  50 103  91
## [96]  16
##
##
## $sampling
## [1] "5-fold cross validation"
```

```
plot(iris_nnet2)
```



```r
nn_iris_d_s <- nnet(
  x = dplyr::select(iris_train, -Species),
  y = class_labels[iris_train_index, ],
  size = iris_nnet2$best.parameters[1,1],
  decay = iris_nnet2$best.parameters[1,2],
  softmax = TRUE
  )
```

```
## # weights:  91
## initial  value 164.446139
## iter  10 value 15.814895
## iter  20 value 1.891497
## iter  30 value 0.102615
## final  value 0.000056
## converged
```

```r
# Compute test error
nn_pred <- predict(
  nn_iris_d_s,
  dplyr::select(iris_test, -Species),
  type="class"
  )
```

```r
library(cluster)
library(factoextra) # PCA
```

```
## Welcome! Want to learn more? See two factoextra-related books at https://goo.gl/ve3WBa
```

```r
library(pgmm) # coffee data
data("coffee")
set.seed(1)
x <- dplyr::select(coffee, - Variety, - Country)
x_scaled <- scale(x)
kmeans_coffee <- kmeans(x_scaled, 2)
kmeans_coffee$tot.withinss
```

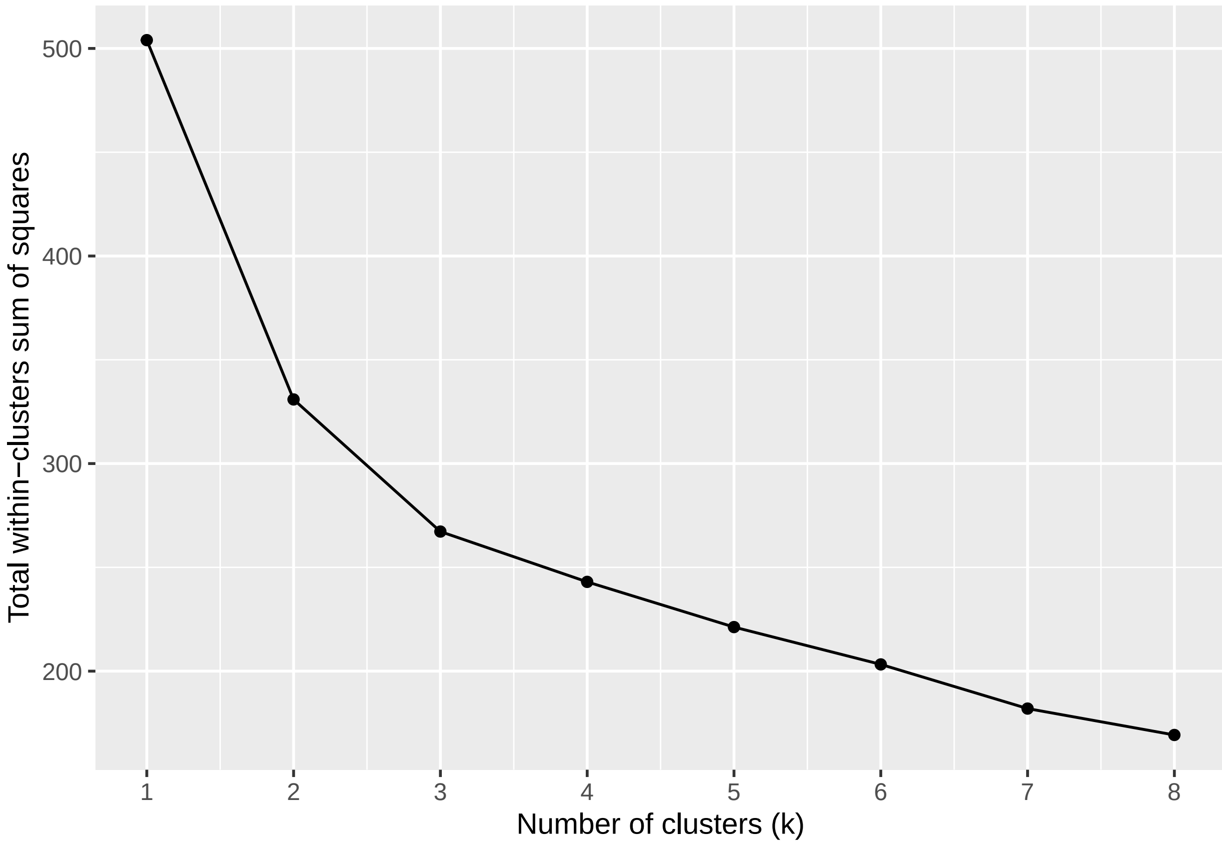
```
## [1] 330.8912
```

```r
kmeans_coffee <- kmeans(x_scaled, 3)
kmeans_coffee$tot.withinss
```

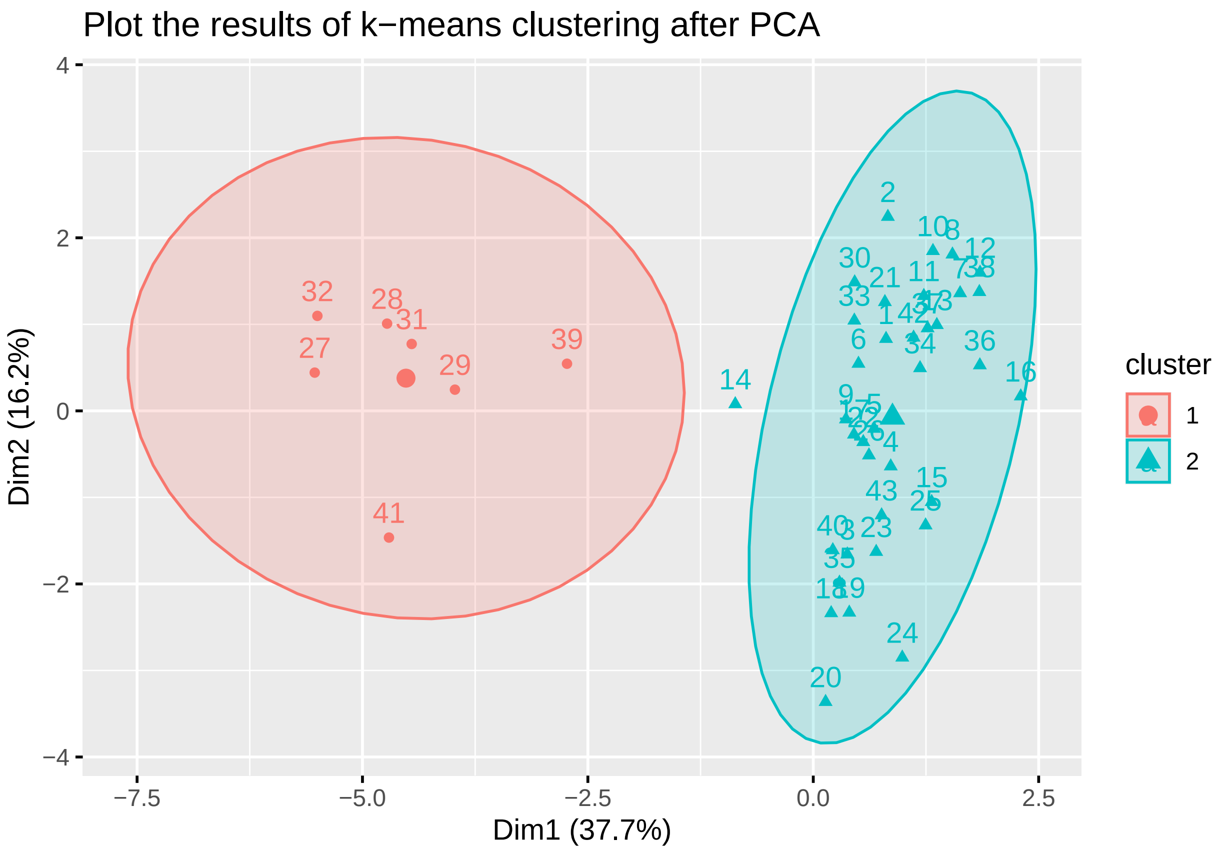
```
## [1] 267.2453
```

```r
# Let's select K using elbow method
withiclusterss <- function(K,x){
  kmeans(x, K)$tot.withinss
}

K <- 1:8

wcss <- lapply(as.list(K), function(k){
  withiclusterss(k, x_scaled)
}) %>% unlist()

ggplot(tibble(K = K, wcss = wcss), aes(x = K, y = wcss)) +
  geom_point() +
  geom_line() +
```

```
  xlab("Number of clusters (k)") +
  ylab("Total within-clusters sum of squares") +
  scale_x_continuous(breaks=c(seq(1,K[length(K)])))
```




```
kmeans_coffee <- kmeans(x_scaled, 2)
fvPCA <- fviz_cluster(kmeans_coffee,
                      x_scaled,
                      ellipse.type = "norm",
                      main = "Plot the results of k-means clustering after PCA")
fvPCA
```



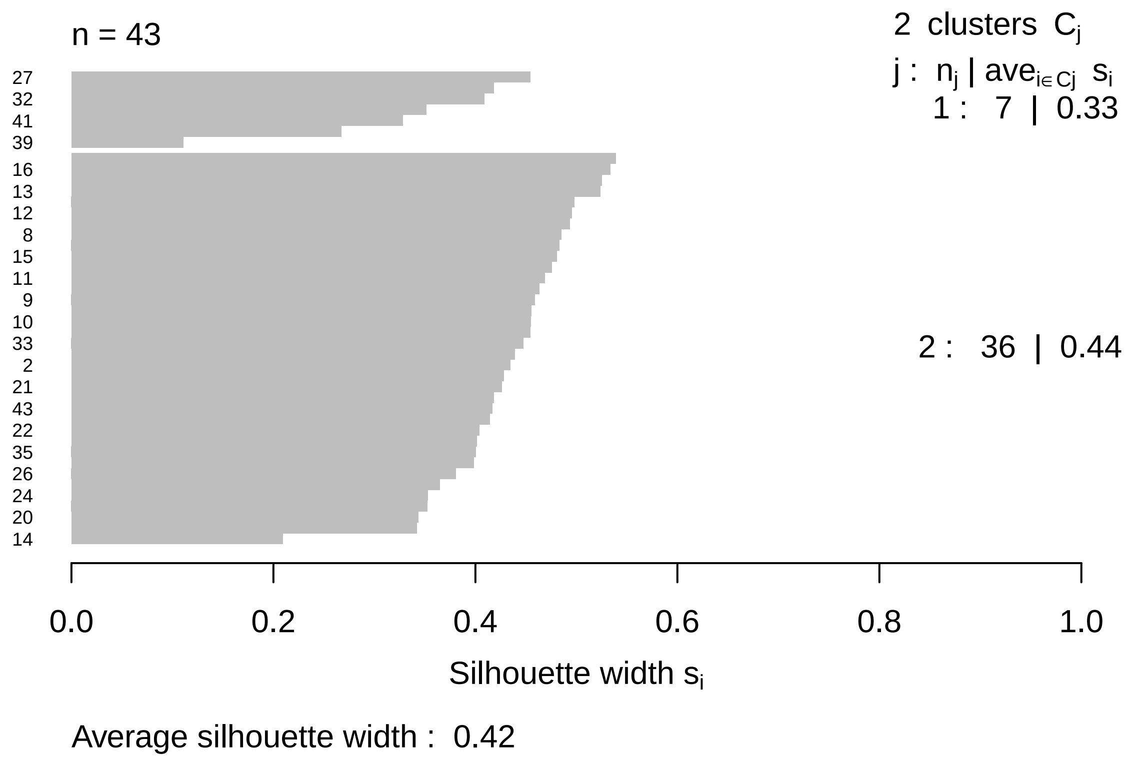

```
si <- silhouette(kmeans_coffee$cluster, dist(x_scaled))
head(si)
```

```
##      cluster neighbor sil_width
## [1,]       2        1 0.5252373
## [2,]       2        1 0.4346060
## [3,]       2        1 0.4143200
## [4,]       2        1 0.4932787
## [5,]       2        1 0.4632535
## [6,]       2        1 0.4832208
```

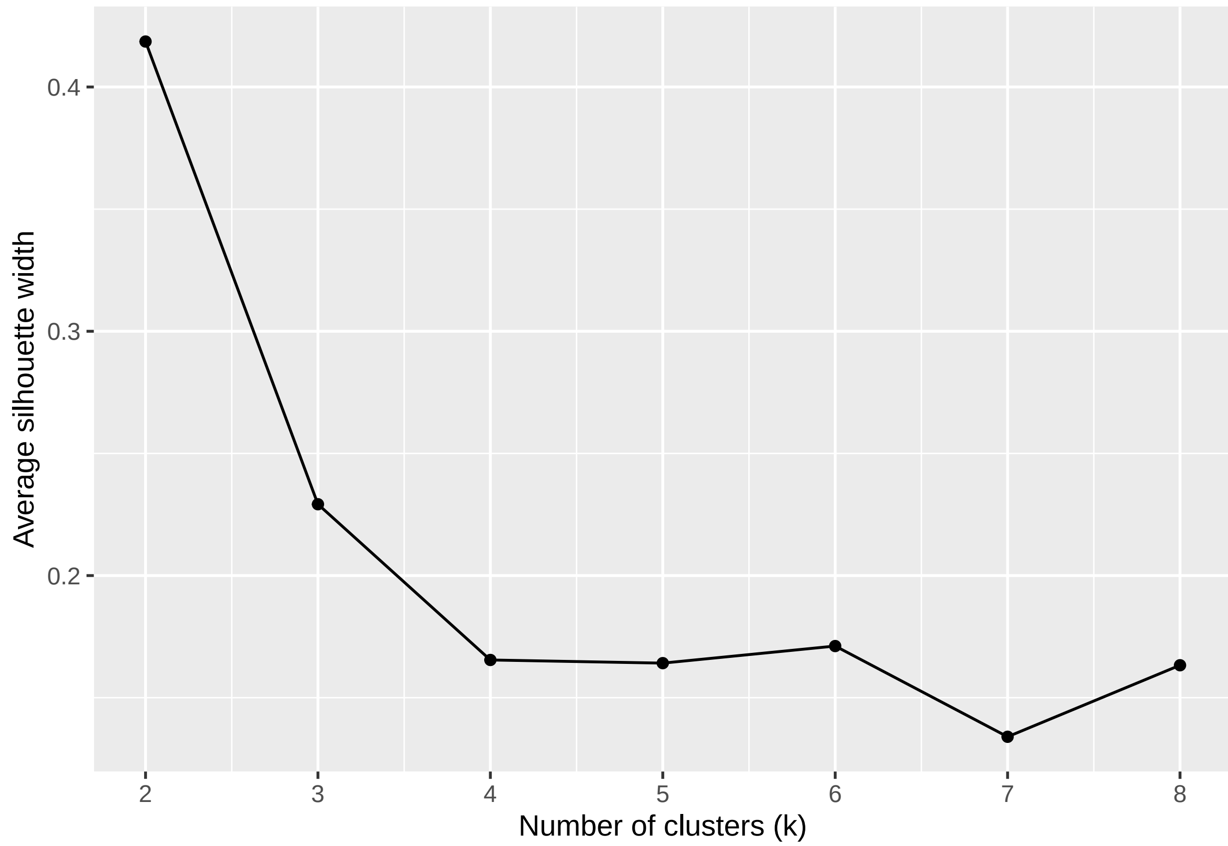
```
#average Silhouette width
mean(si[, 3])
```

```
## [1] 0.4186062
```

```
plot(si, nmax= 80, cex.names=0.6, main = "")
```



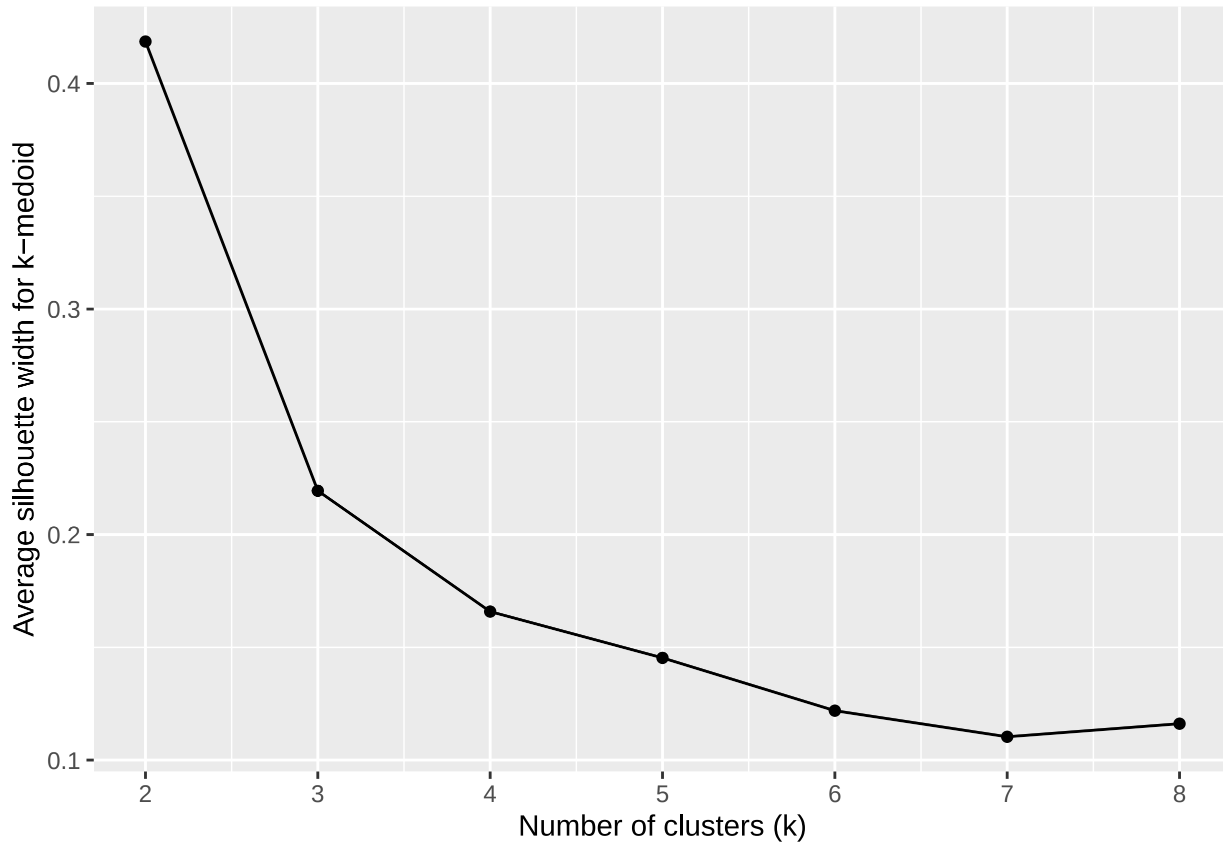

```r
# Let's select K using average Silhouette width
avgSilhouette <- function(K,x) {
  km_cl <- kmeans(x, K)
  sil <- silhouette(km_cl$cluster, dist(x))
  return(mean(sil[, 3]))
}

K <- 2:8

avgSil <- numeric()
for(i in K){
  avgSil[(i-1)] <- avgSilhouette(i, x_scaled)
}

ggplot(tibble(K = K, avgSil = avgSil), aes(x = K, y = avgSil)) +
  geom_point() +
  geom_line() +
  xlab("Number of clusters (k)") +
  ylab("Average silhouette width") +
  scale_x_continuous(breaks=c(seq(1,K[length(K)])))
```



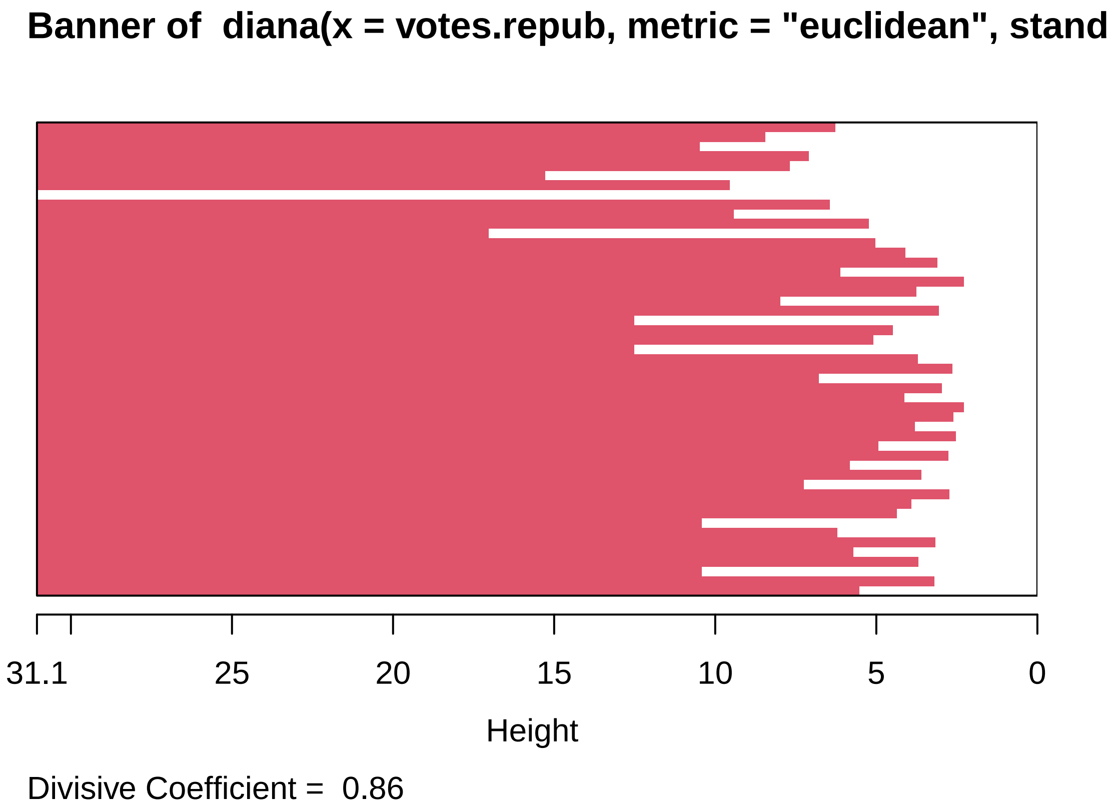

```
kmedoid_coffee <- pam(x_scaled, 2)
kmedoid_coffee$silinfo$avg.width
```

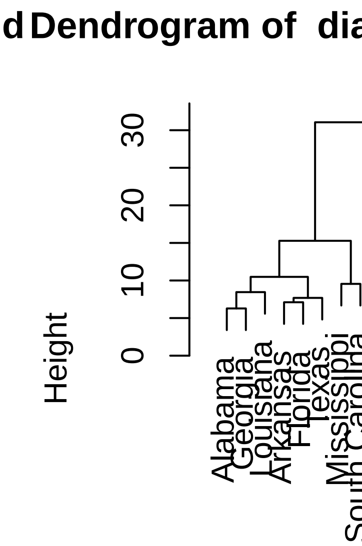
```
## [1] 0.4186062
```

```
avgSil <- lapply(as.list(2:8), function(k){
  kmedoid_coffee <- pam(x_scaled, k)
kmedoid_coffee$silinfo$avg.width
}) %>% unlist()

ggplot(tibble(K = 2:8, avgSil = avgSil), aes(x = K, y = avgSil)) +
  geom_point() +
  geom_line() +
  xlab("Number of clusters (k)") +
  ylab("Average silhouette width for k-medoid") +
  scale_x_continuous(breaks=c(seq(1,K[length(K)])))
```




```r
library(cluster)
library(factoextra)
divisive_votes <- diana(
  votes.repub,
  metric = "euclidean",
  stand = TRUE
  )

plot(divisive_votes)
```



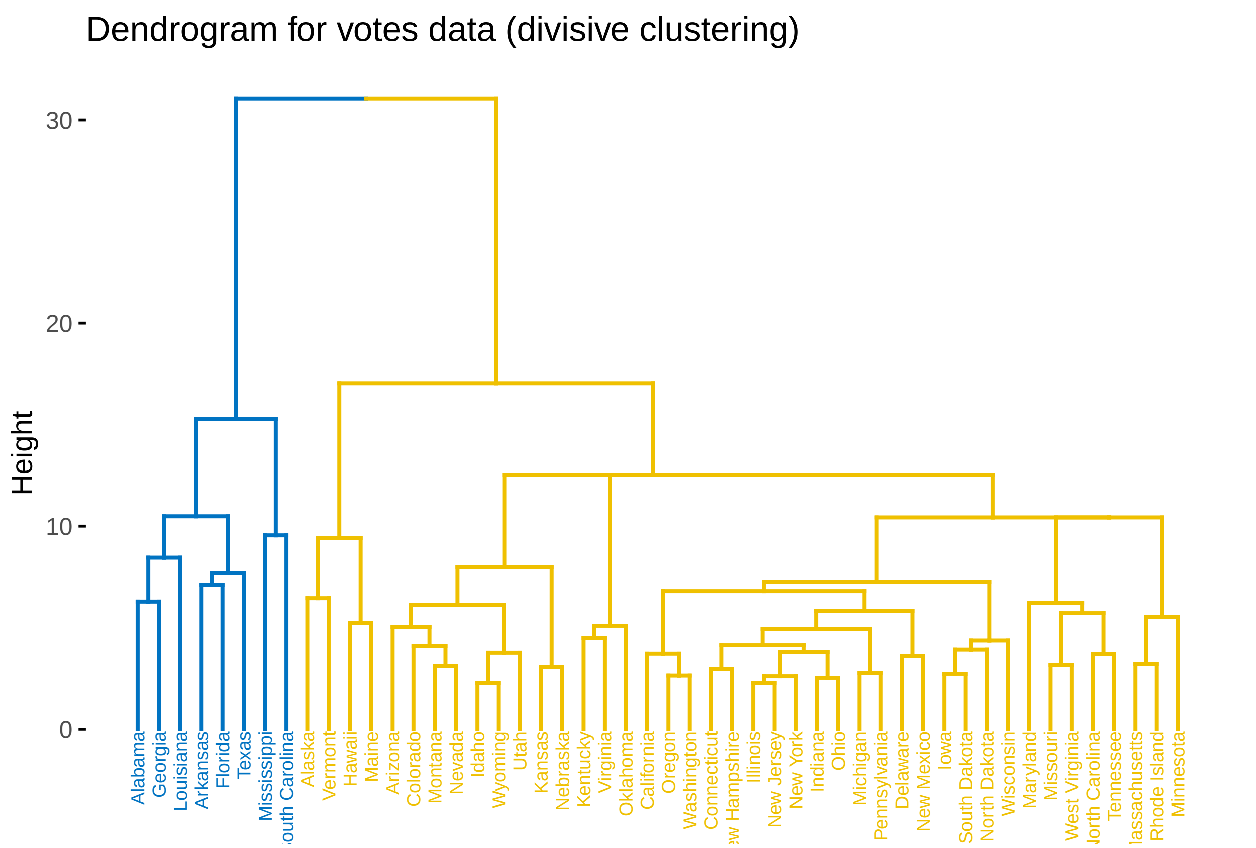

```r
cut_divisive_votes <- cutree(as.hclust(divisive_votes), k = 2)
table(cut_divisive_votes) # 8 and 42 group members
```

```
## cut_divisive_votes
##  1  2
##  8 42
```

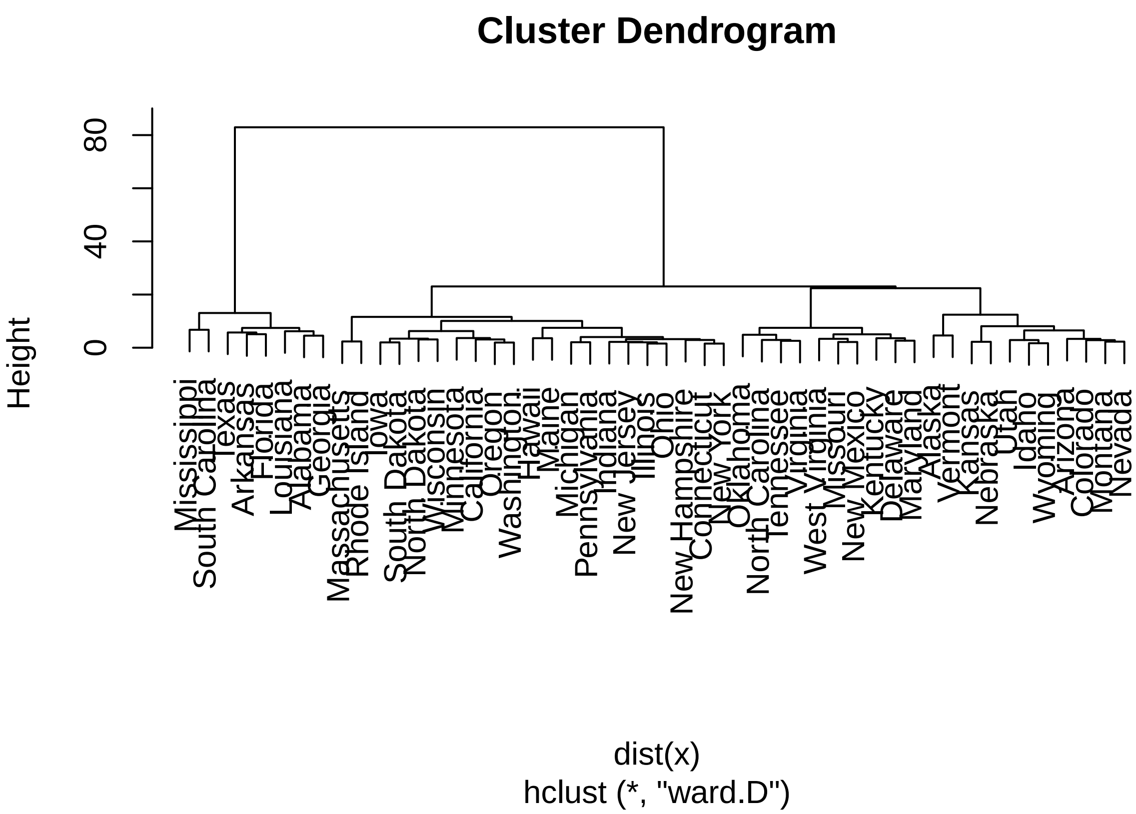
```r
rownames(votes.repub)[cut_divisive_votes == 1]
```

```
## [1] "Alabama"        "Arkansas"       "Florida"        "Georgia"
## [5] "Louisiana"      "Mississippi"    "South Carolina" "Texas"
```

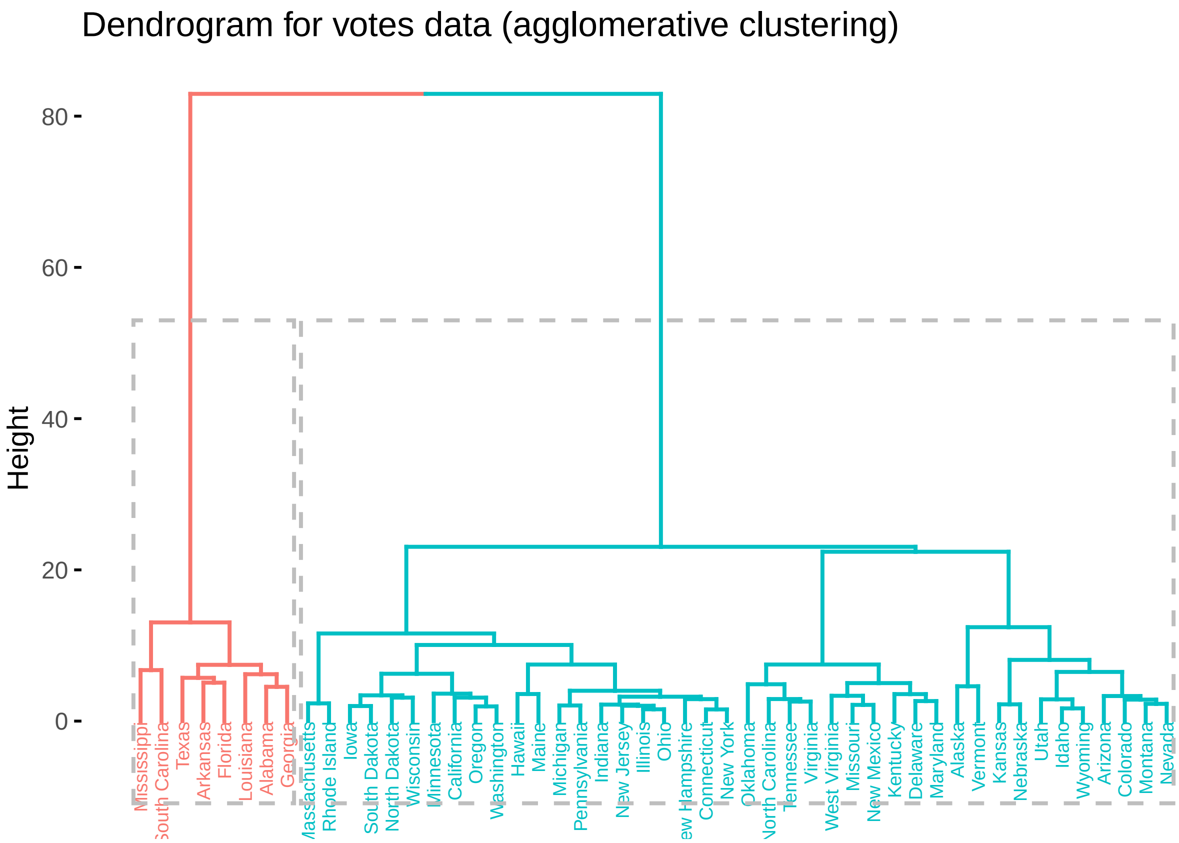
```r
# rownames(votes.repub)[cut_divisive_votes == 2]

#make a nice dendrogram
fviz_dend(
  divisive_votes,
  cex = 0.5,
  k = 2, # Cut in 2 groups
  palette = "jco", # Color palette
  main = "Dendrogram for votes data (divisive clustering)")
```




```
x <- votes.repub %>%
  scale()
hc_vote <- hclust(dist(x), "ward.D")
plot(hc_vote)
```




```r
#make a nice dendrogram
fviz_dend(
  hc_vote,
  k = 2, # Cut in 2 groups
  cex = 0.5,
  color_labels_by_k = TRUE,
  rect = TRUE,
  main = "Dendrogram for votes data (agglomerative clustering)"
  )
```


Dendrogram for votes data (agglomerative clustering)
Height
80
60
40
20
0
Mississippi
South Carolina
Texas
Arkansas
Florida
Louisiana
Alabama
Georgia
Massachusetts
Rhode Island
Iowa
South Dakota
North Dakota
Wisconsin
Minnesota
California
Oregon
Washington
Hawaii
Maine
Michigan
Pennsylvania
Indiana
New Jersey
Illinois
Ohio
New Hampshire
Connecticut
New York
Oklahoma
North Carolina
Tennessee
Virginia
West Virginia
Missouri
New Mexico
Kentucky
Delaware
Maryland
Alaska
Vermont
Kansas
Nebraska
Utah
Idaho
Wyoming
Arizona
Colorado
Montana
Nevada