Lab9

Lily Lau

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```
perimeter
                                                      length_of_kernel
##
         area
                                      compactness
           :10.59
                           :12.41
                                            :0.8081
                                                              :4.899
   \mathtt{Min}.
                    Min.
                                     Min.
                                                      Min.
   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
                                            :0.8710
                                                              :5.629
                                    Mean
                                                      Mean
##
  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.
                                                              1st Qu.:1
  1st Qu.:2.944
                    1st Qu.:2.5615
                                      1st Qu.:5.045
## Median :3.237
                    Median :3.5990
                                     Median :5.223
                                                              Median :2
## Mean
         :3.259
                    Mean
                           :3.7002
                                      Mean
                                             :5.408
                                                              Mean
##
   3rd Qu.:3.562
                                      3rd Qu.:5.877
                    3rd Qu.:4.7687
                                                              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
                                  0.9707706 -0.22957233
## area
                                                                      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
```

• Print tidy seeds data set.

```
dim(seeds)
```

[1] 210 8

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

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

• We scale the predictors.

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

• We split 75%/25% training/test set.

```
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)
```

• We create binary output units $y_k, k = 1, 2, 3$ using class.ind().

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

1	2	3
1	0	0
1	0	0
1	0	0
1	0	0
1	0	0
1	0	0

• Create predictor matrix for training/test set and output for training/test set.

```
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,]</pre>
```

- Let's look at the help page for nnet().
- Let's tune size = number of units in the hidden layer and decay = weight decay parameter.

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

```
## # weights: 47
## initial value 179.079752
## iter 10 value 10.357187
## iter 20 value 0.304073
## iter 30 value 0.002143
## iter 40 value 0.000061
## iter 40 value 0.000061
## final value 0.000061
## converged
```

• Compute test error for NN with size = 4 and decay = 0.

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

Neural networks (Boston data (quantitative response))

- Let's consider housing price data, Boston in MASS package.
- Response is quantitative.

```
library(nnet)
library(MASS)

##
## Attaching package: 'MASS'

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

• We scale predictors and response.
• We split training/test set.

train_Boston <- sample(
    1:nrow(Boston),
    nrow(Boston)/2
    )
x <- scale(Boston)</pre>
```

• Create predictor matrix for training/test set and output for training/test set.

```
Boston_train <- x[train_Boston, ]
train_medv <- x[train_Boston, "medv"]
Boston_test <- x[-train_Boston, ]
test_medv <- x[-train_Boston, "medv"]</pre>
```

• Let's tune size = number of units in the hidden layer and decay = weight decay parameter.

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

```
## # 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

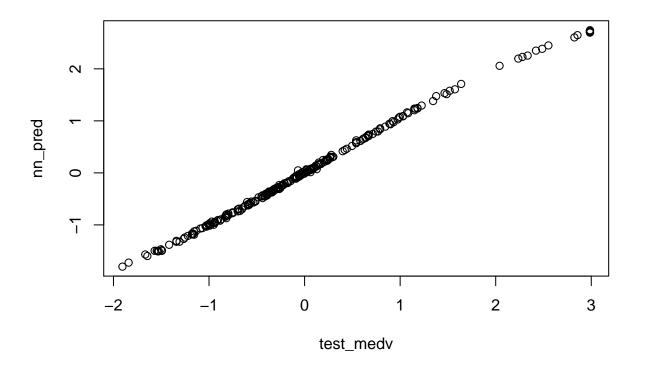
## iter 90 value 10.097962
```

```
## 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
```

Compute test error for the above model: NN with size = 10 and decay = 1.

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

```
plot(test_medv, nn_pred)
```



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

[1] 0.003687532

CV for NN - Iris data

• 80%/20% training/test set.

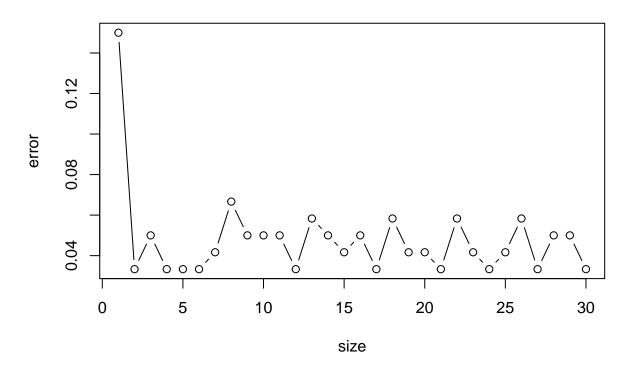
Let's vary the size of hidden layer- Iris data

```
library(e1071)
library(cluster)
set.seed(1)
data("iris")
Species <- pull(iris, Species)</pre>
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)</pre>
iris_test <- slice(xy, -iris_train_index)</pre>
class_labels <- pull(xy, Species) %>%
  class.ind()
iris_nnet1 <- tune.nnet(</pre>
  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
                                                     2 118
## [20] 117
                  89
                      50
                           7
                               20 100
                                           99
                                                             65
                                                                 79 101
                                                                              77 107
             56
                                       80
                                                16
                                                                          41
                                                                                       13
  [39] 109 114
                  82
                      19
                          17
                               57
                                   11
                                       31 115
                                                74
                                                    95
                                                        55
                                                             45
                                                                 52
                                                                     68 119
                                                                               9
                                                                                  97
                                                                                       81
                                                        72
                                                                 38 102
                                                                               3 104
## [58] 113 108
                  85
                      32
                          87
                               94
                                   12
                                       30
                                            14
                                                62
                                                     6
                                                             64
                                                                          91
                                                                                       69
## [77]
         54
              5
                  88
                      33
                          84
                               47
                                    8
                                        4
                                           98
                                                18
                                                    27
                                                        36
                                                             63 110
                                                                     25
                                                                          21
                                                                                 73
                                                                                       23
                                                                              66
         75
## [96]
##
## $train.ind$'(24.8,48.6]'
   [1] 106 96 103
                     60
                                                    59
                                                                     29
                                                                                       76
                          51
                               93
                                   34
                                       10
                                             1
                                                43
                                                        26
                                                             15
                                                                 58
                                                                          24
                                                                              42
                                                                                  48
## [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
                                                                                  97
                                                                                       81
  [58] 113 108
                  85
                      32
                          87
                               94
                                       30
                                            14
                                                     6
                                                        72
                                                             64
                                                                 38 102
                                                                               3 104
                                   12
                                                62
## [77]
                          84
         54
              5
                 88
                      33
                               47
                                    8
                                           98
                                                    27
                                                             63 110
                                                                     25
                                                                          21
                                        4
                                                18
                                                        36
                                                                              66
                                                                                 73
## [96]
         75
##
## $train.ind$'(48.6,72.4]'
    [1] 106 96 103
                      60
                          51
                               93
                                   34
                                       10
                                                    59
                                                        26
                                                             15
                                                                 58
                                                                     29
                                                                          24
                                                                              42
                                                                                  48
                                                                                       76
                                             1
                                                43
         39 105
                      92
                               40
                                   83
                                       90
                                            35 111 112 120
                                                             78
                                                                 22
                                                                     70
## [20]
                 53
                          86
                                                                          28
                                                                              37
                                                                                  61
                                                                                       46
## [39]
        67
             71 116
                          49 117
                                       89
                                                    95
                                                        55
                                                             45
                                                                 52
                                                                     68 119
                                                                                  97
                      44
                                   56
                                            50
                                                 7
                                                                               9
                                                                                       81
  [58] 113 108
                  85
                      32
                          87
                               94
                                   12
                                       30
                                            14
                                                62
                                                     6
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                                                             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
                                                                                       79
## [58] 101
             41
                 77 107
                          13 109 114
                                       82
                                            19
                                                17
                                                    57
                                                             31 115
                                                                     74
                                                                               3 104
                                                        11
                                                                          91
                                                                                       69
## [77]
         54
              5
                 88
                     33
                          84
                               47
                                    8
                                        4
                                           98
                                                18
                                                    27
                                                        36
                                                             63 110
                                                                     25
                                                                          21
                                                                              66
                                                                                 73
## [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
        39 105
                      92
                                            35 111 112 120
                                                             78
                                                                          28
  [20]
                 53
                          86
                               40
                                   83
                                       90
                                                                 22
                                                                     70
                                                                              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
                                            19
                                                17
                                                    57
                                                                     74
                                                                                       52
                                       82
                                                        11
                                                             31 115
                                                                          95
                                                                              55
                                                                                  45
                   9 97 81 113 108
   [77]
         68 119
                                       85
                                           32
                                                87
                                                    94
                                                        12
                                                             30
                                                                 14
                                                                     62
                                                                           6 72
##
  [96] 102
##
##
## $sampling
## [1] "5-fold cross validation"
```

Performance of `nnet'



Model selection - size = $iris_nnet1$ \$best.parameters[1,1] with relatively small CV error and dispersion of CV error.

Fit the model with $size = iris_nnet1\$best.parameters[1,1]$.

```
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
    )</pre>
```

```
## # 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
```

Compute test error for the selected model with size = iris_nnet1\$best.parameters[1,1]

```
nn_pred <- predict(</pre>
  nn_iris,
  dplyr::select(iris_test, -Species),
  type="class"
  )
tab <- table(pull(iris_test, Species),</pre>
  nn\_pred
  )
tab
##
                nn_pred
##
                 setosa versicolor virginica
##
     setosa
                     10
                                  0
##
                      0
                                             0
                                 10
     versicolor
     virginica
                      0
                                             8
1- sum(diag(tab))/sum(tab)
```

[1] 0.06666667

Let's tune decay and size - Iris data

```
set.seed(1)

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

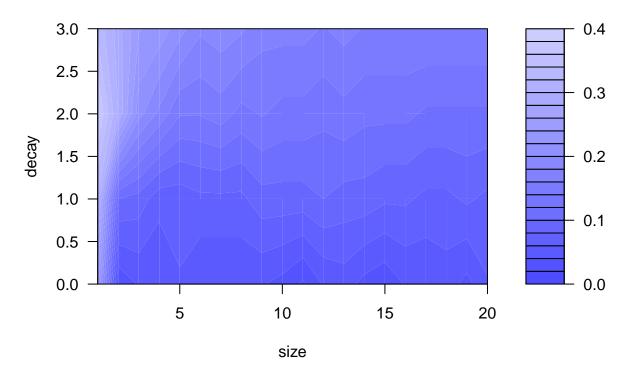
head(summary(iris_nnet2))</pre>
```

```
## $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]'
        99 44 102 33
    [1]
                          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
  [39]
         92
             77
                      66
                              56 101
                                      80
                                           62
                                               93
                                                    69 108
                                                                          9
##
                  29
                          67
                                                            31 116
                                                                     17
                                                                              57
                                                                                  60
                                                                                      19
             30
                      53 110
                                           27
                                                        50 103
   Г581
         26
                 72
                              10 118
                                       11
                                                75
                                                    15
                                                                 91
                                                                     16
                                                                         47
                                                                             12 104 112
             49
                                                                     61 120
## [77]
          8
                   3
                      98
                          64
                              55 71
                                       96
                                           36
                                                 4 115
                                                         5
                                                            52
                                                                41
                                                                             78
                                                                                  58 107
## [96]
         76
##
## $train.ind$'(24.8,48.6]'
                                                                                  73
##
        68
             39
                   1 34
                                       82
                                           59
                                               51
                                                    97
                                                        85
                                                            21 106
                                                                     54
                                                                         74
                                                                              7
                                                                                      79
   [1]
                          87
                              43 14
## [20] 109
             37
                 89 100 117
                              32 114
                                        2
                                           45
                                                18
                                                    22
                                                        65
                                                            13
                                                                 81
                                                                     94
                                                                         48
                                                                              63
                                                                                  23
                                                                                      46
             77
                                                    69 108
                                                            31 116
                                                                           9
## [39]
         92
                 29
                      66
                          67
                              56 101
                                       80
                                           62
                                                93
                                                                     17
                                                                              57
                                                                                  60
                                                                                      19
  [58]
         26
             30
                 72
                      53 110
                              10 118
                                           27
                                                75
                                                    15
                                                        50 103
                                                                         47
                                       11
                                                                 91
                                                                     16
                                                                             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
                 89 100 117
                                                                             28
             37
                              99
                                  44 102
                                           33
                                               84
                                                    35
                                                        70 105
                                                                 42
                                                                     38
                                                                         20
                                                                                  86
                                                                                      95
  [39]
             40
                  83
                      25 113 119 111
                                       88
                                            6
                                                24
                                                    69 108
                                                             31 116
                                                                     17
                                                                                  60
         26
             30
                 72
                      53 110
                              10 118
                                           27
                                                        50 103
                                                                         47
  [58]
                                       11
                                                75
                                                    15
                                                                 91
                                                                     16
                                                                             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]'
                                           59
                                               51
                                                    97
                                                        85
                                                            21 106
                                                                         74
                                                                              7
                                                                                  73
    [1]
        68
             39
                   1 34
                         87
                              43
                                  14
                                      82
                                                                     54
                                                                                      79
                                                                         20
                              99
                                                    35
                                                        70 105
                                                                     38
## [20] 109
             37
                 89 100 117
                                  44 102
                                           33
                                               84
                                                                 42
                                                                             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]'
##
        68
             39
                   1 34 87
                              43
                                  14 82 59
                                               51
                                                    97
                                                        85
                                                            21 106
                                                                         74
                                                                              7
                                                                                  73
                                                                                      79
   [1]
                                                                     54
## [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
                                                                         22
                                                                              65
                                                                                      81
                                                                     18
                                                                                  13
##
   [58]
         94
             48
                  63
                      23
                          46
                              92
                                   77
                                       29
                                           66
                                               67
                                                    56 101
                                                            80
                                                                 62
                                                                     93
                                                                         69 108
                                                                                  31 116
                                                                         15
## [77]
         17
              9
                 57
                      60
                          19
                              26
                                  30
                                       72
                                           53 110
                                                    10 118
                                                            11
                                                                 27
                                                                     75
                                                                             50 103
##
  [96]
         16
##
##
## $sampling
## [1] "5-fold cross validation"
```

plot(iris_nnet2)

Performance of `nnet'



We can choose size = iris_nnet2\$best.parameters[1,1] and decay iris_nnet2\$best.parameters[1,2]. Fit the model with size = iris_nnet2\$best.parameters[1,1] and decay = iris_nnet2\$best.parameters[1,2].

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

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

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

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

[1] 0.06666667

Clustering -coffee data

K-means clustering assignment depends on the initial cluster assignments. Thus, we need to run the clustering with different random assignment and select the best solution (the clustering with the minimum total within sum of squares).

Coffee - from the help page - data on the chemical composition of coffee samples collected from around the world, comprising 43 samples from 29 countries. We dropped the first two columns of the data.

k-means -coffee data

• Let's apply k-means for clustering.

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

## Warning: package 'factoextra' was built under R version 4.0.4

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

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

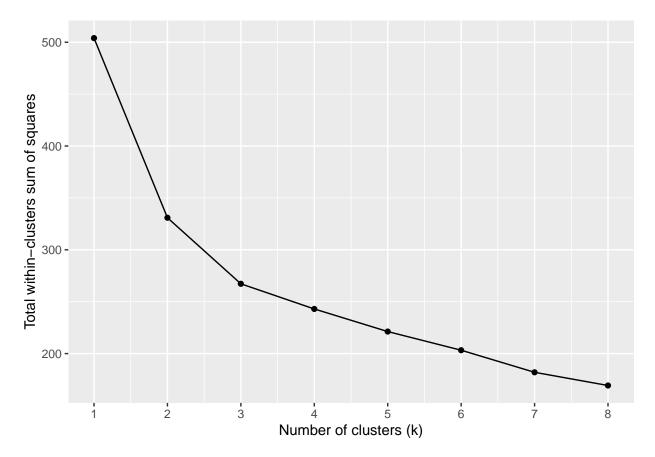
kmeans_coffee$tot.withinss</pre>
```

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

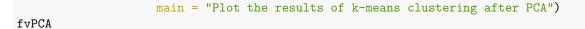
K <- 1:8

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

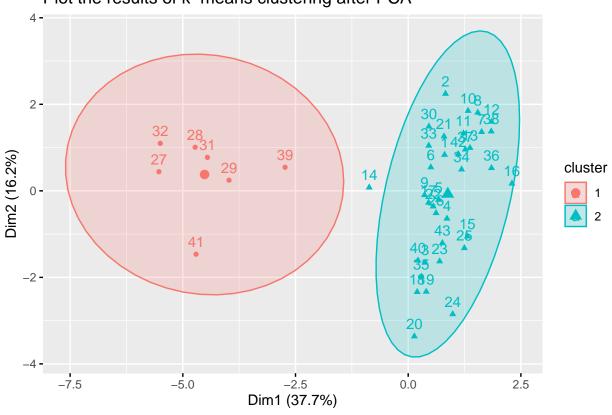
ggplot(tibble(K = K, wcss = wcss), aes(x = K, y = wcss)) +
   geom_point() +
   geom_line() +
   xlab("Number of clusters (k)") +
   ylab("Total within-clusters sum of squares") +
   scale_x_continuous(breaks=c(seq(1,K[length(K)])))
```



Based on the elbow method, we can use k = 2. There are $\dim(x_scaled)$ [2] variables. So we need to use dimensionality reduction technique and then plot the clusters in two-dimensions.



Plot the results of k-means clustering after PCA



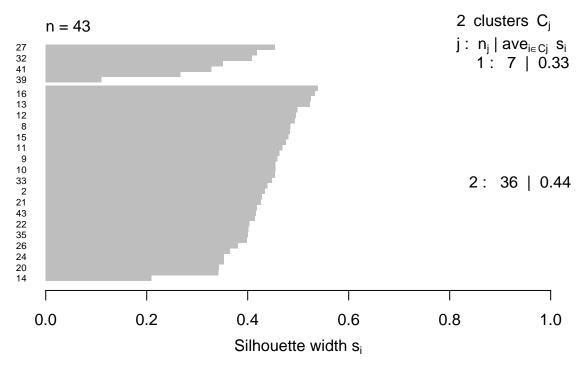
- Let's use silhouette plots to choose the best number of clusters.
 - Silhouette measures how similar observations are within clusters.
 - Large average silhouette width indicates an appropriate number of clusters.

si <- silhouette(kmeans_coffee\$cluster, dist(x_scaled)) head(si)</pre>

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

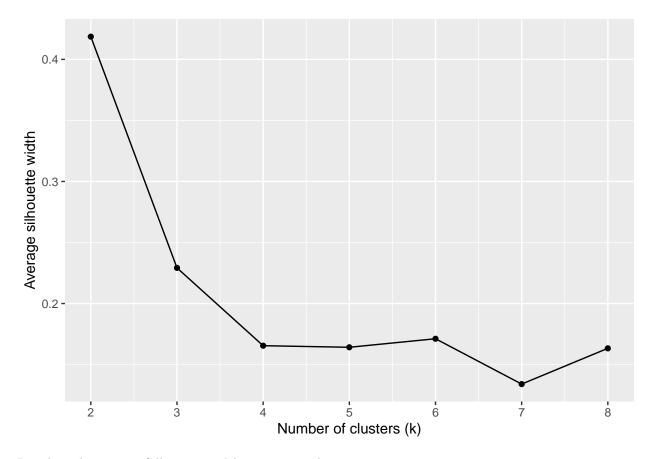
```
#average Silhouette width
mean(si[, 3])
```

[1] 0.4186062



Average silhouette width: 0.42

```
# Let's select K using average Silhouette width
avgSilhouette <- function(K,x) {</pre>
  km_cl <- kmeans(x, K)</pre>
  sil <- silhouette(km_cl$cluster, dist(x))</pre>
  return(mean(sil[, 3]))
}
K <- 2:8
avgSil <- numeric()</pre>
for(i in K){
  avgSil[(i-1)] \leftarrow 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)])))
```



Based on the average Silhouette width, we can use k=2.

k-medoid clustering

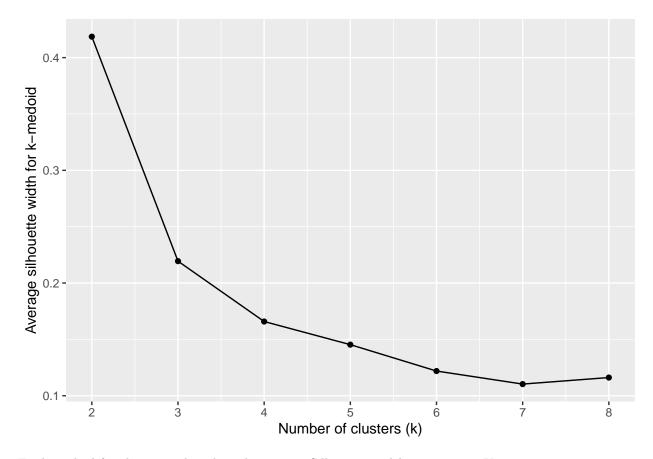
- Let's apply k-medoid clustering - coffee data

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

[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)])))
```



For k-medoid for clustering, based on the average Silhouette width, we can use K=2.

• We can also use Gap statistic to choose k - Reference Modern Statistics for Modern Biologists Chapter 5.7.1.

Clustering - votes data

- We will use *votes.repub* in the cluster package.
- Look at the help page for *votes.repub*

k-means

```
data(votes.repub) # from cluster package
votes.repub_scaled <- scale(votes.repub)
votes.repub_kmeans <- kmeans(votes.repub_scaled, 2)</pre>
```

Why kmean() doesn't work?

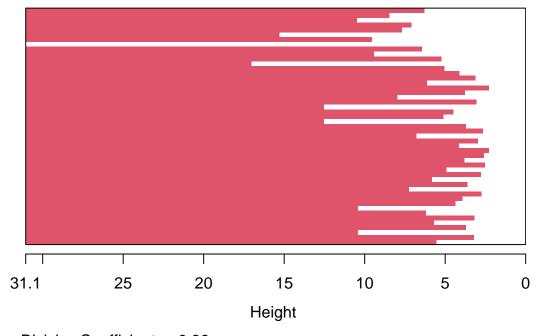
Hierarchical clustering - divisive clustering

• Apply divisive clustering

- To divide the selected cluster, the algorithm first looks for its most disparate observation (i.e., which has the largest average dissimilarity to the other observations of the selected cluster)
- This observation initiates the "splinter group".
- In subsequent steps, the algorithm reassigns observations that are closer to the "splinter group"

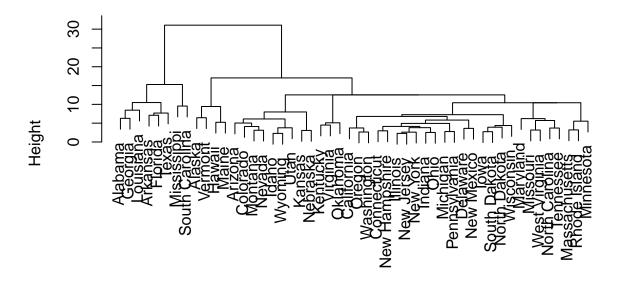
```
library(cluster)
library(factoextra)
divisive_votes <- diana(
  votes.repub,
  metric = "euclidean",
  stand = TRUE
  )
plot(divisive_votes)</pre>
```

Banner of diana(x = votes.repub, metric = "euclidean", stand



Divisive Coefficient = 0.86

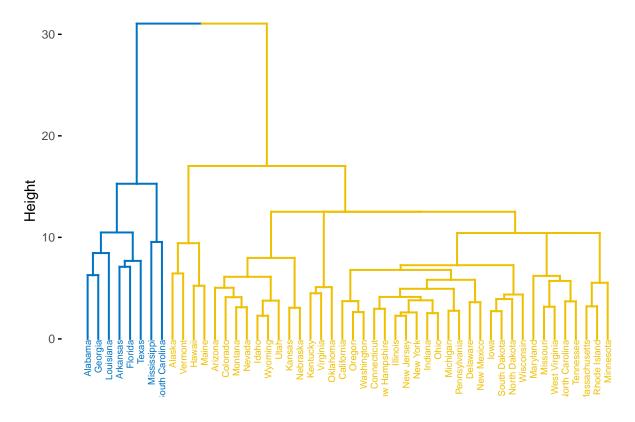
Dendrogram of diana(x = votes.repub, metric = "euclidean", stand = TF



votes.repub Divisive Coefficient = 0.86

```
cut_divisive_votes <- cutree(as.hclust(divisive_votes), k = 2)</pre>
table(cut_divisive_votes) # 8 and 42 group members
## cut_divisive_votes
## 1 2
   8 42
rownames(votes.repub)[cut_divisive_votes == 1]
## [1] "Alabama"
                        "Arkansas"
                                          "Florida"
                                                           "Georgia"
## [5] "Louisiana"
                        "Mississippi"
                                          "South Carolina" "Texas"
# 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)")
```

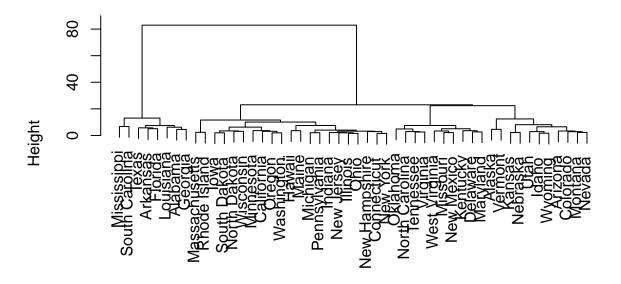
Dendrogram for votes data (divisive clustering)



Hierarchical clustering - agglomerative clustering

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

Cluster Dendrogram



dist(x) hclust (*, "ward.D")

```
#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)

