Intro to Computer Science Data Analysis

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Useful links

- Pseudocode for k-means: http://www.devmedia.com.br/data-mining-na-pratica-algoritmo-k-means/4584
- Similar algorithm: http://www.di.fc.ul.pt/~jpn/r/spectralclustering/spectralclustering.html (uses knn plus step one and do not executes the step five) Usa knn junto no passo 1 e nao executa passo 4 do algoritmo do artigo, meio diferente mas funciona

PETAL LENGTH/WIDTH DATA

Init

Get data from file and init vars

```
Dados <- read.csv("iris.data.csv", header=FALSE)
precision <- 5 # float precision
my.data <- as.matrix(Dados[,c(3,4)])

n <- nrow(my.data) # n = number of columns from dataset
S <- my.data # data to S
A <- matrix(rep(0,n^2) ,nrow = n ,ncol=n) # create empty matrix
# sigma2 <- sum ((S - mean(S))^2) / (n)  #var pop
sigma2 <- 3 # set a sigma (0 to 5 are good values)
D <- diag(n) # create a diagonal matrix
```

Spectral Clustering Algorithm

Step 1: Compute A Matrix (Affinity Matrix)___

```
for (i in 1:n){
  for(j in 1:n){
    if (i != j){
      # Euclidean distance
      A[i,j] <- exp( - sqrt(sum((S[i,]-S[j,])^2)) / 2*sigma2)
      #A[i,j] <- exp(- norm(as.matrix(S[i,]-S[j,]), type="F"))
    }
  }
}
```

```r
# set float precision (5)
round(A[1:8,1:8],precision)
```

```
##         [,1]    [,2]    [,3]    [,4]    [,5]    [,6]    [,7]    [,8]
## [1,] 0.00000 1.00000 0.86071 0.86071 1.00000 0.58226 0.86071 0.86071
## [2,] 1.00000 0.00000 0.86071 0.86071 1.00000 0.58226 0.86071 0.86071
## [3,] 0.86071 0.86071 0.00000 0.74082 0.86071 0.51129 0.80886 0.74082
## [4,] 0.86071 0.86071 0.74082 0.00000 0.86071 0.65425 0.80886 1.00000
## [5,] 1.00000 1.00000 0.86071 0.86071 0.00000 0.58226 0.86071 0.86071
## [6,] 0.58226 0.58226 0.51129 0.65425 0.58226 0.00000 0.62229 0.65425
## [7,] 0.86071 0.86071 0.80886 0.80886 0.86071 0.62229 0.00000 0.80886
## [8,] 0.86071 0.86071 0.74082 1.00000 0.86071 0.65425 0.80886 0.00000
```

Step 2: Compute D Matrix

2.1 Calcular matriz D

```r
for (i in 1:n){
  # sum of each row and insert into the diagonal matrix D
  D[i,i] <- sum (A[i,])
}
# set float precision (5)
round(D[1:8,1:8],precision)
```

```
##         [,1]    [,2]     [,3]     [,4]    [,5]     [,6]     [,7]     [,8]
## [1,] 39.1257  0.0000  0.00000  0.00000  0.0000  0.00000  0.00000  0.00000
## [2,]  0.0000 39.1257  0.00000  0.00000  0.0000  0.00000  0.00000  0.00000
## [3,]  0.0000  0.0000 36.39367  0.00000  0.0000  0.00000  0.00000  0.00000
## [4,]  0.0000  0.0000  0.00000 39.14224  0.0000  0.00000  0.00000  0.00000
## [5,]  0.0000  0.0000  0.00000  0.00000 39.1257  0.00000  0.00000  0.00000
## [6,]  0.0000  0.0000  0.00000  0.00000  0.0000 31.77652  0.00000  0.00000
## [7,]  0.0000  0.0000  0.00000  0.00000  0.0000  0.00000 37.99526  0.00000
## [8,]  0.0000  0.0000  0.00000  0.00000  0.0000  0.00000  0.00000 39.14224
```

Step 3: Compute L Matrix (using D)

```r
# get sqrt of each matrix element
raiz.D     <- sqrt (D)       #obs1 : raiz.D %*% raiz.D = D
                                  # raiz.D x raiz.D = D (mult matrix)
# solve() para pegar inversa
# solve() function to get inverse matrix
Inv.raiz.D <- solve(raiz.D)  #obs2 : compute inverse matrix = get sqrt from inverse matrix
                             # sqrt (solve (D)) = solve (sqrt (D))
# Compute L
L <- Inv.raiz.D %*% A %*% Inv.raiz.D

# Set float precision (5)
round(L[1:8,1:8],precision)
```

```
##         [,1]    [,2]    [,3]    [,4]    [,5]    [,6]    [,7]    [,8]
## [1,] 0.00000 0.02556 0.02281 0.02199 0.02556 0.01651 0.02232 0.02199
## [2,] 0.02556 0.00000 0.02281 0.02199 0.02556 0.01651 0.02232 0.02199
## [3,] 0.02281 0.02281 0.00000 0.01963 0.02281 0.01503 0.02175 0.01963
```

```
## [4,] 0.02199 0.02199 0.01963 0.00000 0.02199 0.01855 0.02097 0.02555
## [5,] 0.02556 0.02556 0.02281 0.02199 0.00000 0.01651 0.02232 0.02199
## [6,] 0.01651 0.01651 0.01503 0.01855 0.01651 0.00000 0.01791 0.01855
## [7,] 0.02232 0.02232 0.02175 0.02097 0.02232 0.01791 0.00000 0.02097
## [8,] 0.02199 0.02199 0.01963 0.02555 0.02199 0.01855 0.02097 0.00000
```

Step 4: Compute eigenvector and set matrix X with the k first eigenvectors from L

```
#get eigenvector
autovet <- eigen (L)$vectors
#autoval <- eigen (L)$values

# set the number of classes (k)
k <- 3

# get the 3 first eigenvectors (k first eigenvalues)
X <- autovet[,(1 : k)]
X
```

```
##              [,1]         [,2]          [,3]
##   [1,] 0.09071344 -0.117764013 -0.0075799337
##   [2,] 0.09071344 -0.117764013 -0.0075799337
##   [3,] 0.08748901 -0.113841916 -0.0076610337
##   [4,] 0.09073261 -0.117188034 -0.0068078243
##   [5,] 0.09071344 -0.117764013 -0.0075799337
##   [6,] 0.08175112 -0.102488451 -0.0024294243
##   [7,] 0.08939336 -0.115708328 -0.0070411595
##   [8,] 0.09073261 -0.117188034 -0.0068078243
##   [9,] 0.09071344 -0.117764013 -0.0075799337
##  [10,] 0.08786924 -0.113501100 -0.0066272665
##  [11,] 0.09073261 -0.117188034 -0.0068078243
##  [12,] 0.08819103 -0.112989140 -0.0054847214
##  [13,] 0.08734128 -0.113329680 -0.0072318283
##  [14,] 0.07607694 -0.099166977 -0.0068919918
##  [15,] 0.08271085 -0.107725846 -0.0073810220
##  [16,] 0.08638552 -0.110629953 -0.0053391753
##  [17,] 0.08333237 -0.107708733 -0.0064088126
##  [18,] 0.08939336 -0.115708328 -0.0070411595
##  [19,] 0.08366202 -0.105539709 -0.0032454314
##  [20,] 0.08944027 -0.115131015 -0.0062335893
##  [21,] 0.08376751 -0.106075137 -0.0037408987
##  [22,] 0.08638552 -0.110629953 -0.0053391753
##  [23,] 0.07215749 -0.094012043 -0.0064877975
##  [24,] 0.07853041 -0.097605882 -0.0013939651
##  [25,] 0.07447741 -0.091073467  0.0003416743
##  [26,] 0.08819103 -0.112989140 -0.0054847214
##  [27,] 0.08471351 -0.107524126 -0.0040694162
##  [28,] 0.09073261 -0.117188034 -0.0068078243
##  [29,] 0.09071344 -0.117764013 -0.0075799337
##  [30,] 0.08819103 -0.112989140 -0.0054847214
##  [31,] 0.08819103 -0.112989140 -0.0054847214
##  [32,] 0.08638552 -0.110629953 -0.0053391753
##  [33,] 0.08786924 -0.113501100 -0.0066272665
```

```
##  [34,] 0.09071344 -0.117764013 -0.0075799337
##  [35,] 0.08786924 -0.113501100 -0.0066272665
##  [36,] 0.08271085 -0.107725846 -0.0073810220
##  [37,] 0.08748901 -0.113841916 -0.0076610337
##  [38,] 0.08786924 -0.113501100 -0.0066272665
##  [39,] 0.08748901 -0.113841916 -0.0076610337
##  [40,] 0.09073261 -0.117188034 -0.0068078243
##  [41,] 0.08658263 -0.112392751 -0.0072447052
##  [42,] 0.08658263 -0.112392751 -0.0072447052
##  [43,] 0.08748901 -0.113841916 -0.0076610337
##  [44,] 0.07624159 -0.095087502 -0.0017926887
##  [45,] 0.07371805 -0.088862328  0.0018130972
##  [46,] 0.08939336 -0.115708328 -0.0070411595
##  [47,] 0.08819103 -0.112989140 -0.0054847214
##  [48,] 0.09071344 -0.117764013 -0.0075799337
##  [49,] 0.09073261 -0.117188034 -0.0068078243
##  [50,] 0.09071344 -0.117764013 -0.0075799337
##  [51,] 0.08866706  0.069178853  0.0564500310
##  [52,] 0.08999799  0.069114332  0.0775695766
##  [53,] 0.08752052  0.069854531  0.0184859771
##  [54,] 0.08093147  0.055643439  0.1248276779
##  [55,] 0.09006478  0.069939025  0.0641853011
##  [56,] 0.08749210  0.066315650  0.0870229569
##  [57,] 0.08940215  0.070461187  0.0405007538
##  [58,] 0.05977525  0.021396324  0.0998161680
##  [59,] 0.08713435  0.066847791  0.0742326416
##  [60,] 0.07681623  0.051719638  0.1168283648
##  [61,] 0.06442034  0.030957716  0.1116615439
##  [62,] 0.08365724  0.061245639  0.1008110244
##  [63,] 0.07490156  0.049358014  0.1192251908
##  [64,] 0.08866706  0.069178853  0.0564500310
##  [65,] 0.06773771  0.038889599  0.1120583944
##  [66,] 0.08851538  0.066643016  0.0944899740
##  [67,] 0.08999799  0.069114332  0.0775695766
##  [68,] 0.07609660  0.051711809  0.1153111767
##  [69,] 0.08999799  0.069114332  0.0775695766
##  [70,] 0.07574186  0.048978379  0.1250706352
##  [71,] 0.08773876  0.070415033  0.0053454640
##  [72,] 0.08093147  0.055643439  0.1248276779
##  [73,] 0.08752052  0.069854531  0.0184859771
##  [74,] 0.08278227  0.063730828  0.0621365538
##  [75,] 0.08643926  0.063562551  0.1083189175
##  [76,] 0.08851538  0.066643016  0.0944899740
##  [77,] 0.08720750  0.068655830  0.0410231563
##  [78,] 0.08770080  0.071173989 -0.0151872774
##  [79,] 0.08999799  0.069114332  0.0775695766
##  [80,] 0.06442034  0.030957716  0.1116615439
##  [81,] 0.07317926  0.045286194  0.1235948263
##  [82,] 0.06883456  0.039258843  0.1180821693
##  [83,] 0.07730259  0.050800767  0.1261136693
##  [84,] 0.08532541  0.069394184 -0.0206260865
##  [85,] 0.08999799  0.069114332  0.0775695766
##  [86,] 0.08835372  0.068157802  0.0670441706
##  [87,] 0.08965473  0.070323153  0.0495923362
```

```
##  [88,] 0.08724541  0.065209473  0.0984581523
##  [89,] 0.08321938  0.058723590  0.1216972690
##  [90,] 0.08093147  0.055643439  0.1248276779
##  [91,] 0.08459724  0.062697343  0.0987678615
##  [92,] 0.08932527  0.068979729  0.0706870305
##  [93,] 0.07991815  0.054295565  0.1260328156
##  [94,] 0.05977525  0.021396324  0.0998161680
##  [95,] 0.08506040  0.061368895  0.1161033253
##  [96,] 0.08326068  0.059490535  0.1166388437
##  [97,] 0.08506040  0.061368895  0.1161033253
##  [98,] 0.08643926  0.063562551  0.1083189175
##  [99,] 0.05319589  0.006702448  0.0757059456
## [100,] 0.08321938  0.058723590  0.1216972690
## [101,] 0.06309104  0.054321401 -0.1436183223
## [102,] 0.08629403  0.071040977 -0.0492991358
## [103,] 0.07193013  0.061597315 -0.1460390494
## [104,] 0.07785519  0.065533736 -0.1048212730
## [105,] 0.07372406  0.063070506 -0.1457280861
## [106,] 0.05275707  0.045803918 -0.1446435029
## [107,] 0.08602007  0.066635334  0.0557087870
## [108,] 0.05938471  0.051036456 -0.1343466965
## [109,] 0.07310239  0.061995413 -0.1206577574
## [110,] 0.06075797  0.052405997 -0.1435113449
## [111,] 0.08468410  0.069914962 -0.0570826067
## [112,] 0.08364387  0.069621528 -0.0773786834
## [113,] 0.07995226  0.067560335 -0.1174786575
## [114,] 0.08461954  0.069410372 -0.0423231265
## [115,] 0.07299475  0.060713968 -0.0739101167
## [116,] 0.07720033  0.064848560 -0.0988379576
## [117,] 0.08001359  0.067061511 -0.0945875179
## [118,] 0.04953223  0.043080762 -0.1401591995
## [119,] 0.04294485  0.037398954 -0.1242690690
## [120,] 0.08574524  0.068945152  0.0030428915
## [121,] 0.07406799  0.063254137 -0.1408019619
## [122,] 0.08385186  0.068276391 -0.0274909234
## [123,] 0.04976397  0.043205154 -0.1371696607
## [124,] 0.08805097  0.071243300 -0.0096883908
## [125,] 0.07670363  0.065311598 -0.1362697759
## [126,] 0.06786848  0.057912894 -0.1303887603
## [127,] 0.08773876  0.070415033  0.0053454640
## [128,] 0.08805097  0.071243300 -0.0096883908
## [129,] 0.07856415  0.066660527 -0.1281032360
## [130,] 0.06965593  0.058698969 -0.1008039138
## [131,] 0.06607377  0.056653191 -0.1402980714
## [132,] 0.05804394  0.050161858 -0.1454278390
## [133,] 0.07742465  0.065813683 -0.1319909565
## [134,] 0.08364646  0.067710781 -0.0117921874
## [135,] 0.06958982  0.057687364 -0.0641113612
## [136,] 0.06463070  0.055709444 -0.1506636491
## [137,] 0.07293261  0.062129078 -0.1317536015
## [138,] 0.08001359  0.067061511 -0.0945875179
## [139,] 0.08773876  0.070415033  0.0053454640
## [140,] 0.08096648  0.068102321 -0.1050871074
## [141,] 0.07293261  0.062129078 -0.1317536015
```

```
## [142,] 0.07652196  0.063573172 -0.0724524481
## [143,] 0.08629403  0.071040977 -0.0492991358
## [144,] 0.06988244  0.059996416 -0.1493266975
## [145,] 0.06838047  0.058440888 -0.1332987362
## [146,] 0.07710166  0.064427853 -0.0858867645
## [147,] 0.08662257  0.070846811 -0.0342376639
## [148,] 0.08406067  0.069800936 -0.0713677783
## [149,] 0.07692306  0.064924906 -0.1111551895
## [150,] 0.08665450  0.071074334 -0.0399197845
```

```
#dec.espec <- autovet %*% diag(autoval) %*% t(autovet) -> return to L matrix
```

Step 5: Compute Y Matrix using X Matrix: Normalize Y Matrix

```
# Create a matrix with n rows and k columns
Y <- matrix (0,nrow=n,ncol=k)

# For each element from X, div(elem)/sqrt(each element from row squared)
for(i in 1:n){
  for(j in 1:k){
    Y[i,j] <- X[i,j] / (sqrt (sum(X[i,j])^2))
  }
}
# Normalized Y matrix: only 1 and -1 values
Y
```

```
##        [,1] [,2] [,3]
##   [1,]    1   -1   -1
##   [2,]    1   -1   -1
##   [3,]    1   -1   -1
##   [4,]    1   -1   -1
##   [5,]    1   -1   -1
##   [6,]    1   -1   -1
##   [7,]    1   -1   -1
##   [8,]    1   -1   -1
##   [9,]    1   -1   -1
##  [10,]    1   -1   -1
##  [11,]    1   -1   -1
##  [12,]    1   -1   -1
##  [13,]    1   -1   -1
##  [14,]    1   -1   -1
##  [15,]    1   -1   -1
##  [16,]    1   -1   -1
##  [17,]    1   -1   -1
##  [18,]    1   -1   -1
##  [19,]    1   -1   -1
##  [20,]    1   -1   -1
##  [21,]    1   -1   -1
##  [22,]    1   -1   -1
##  [23,]    1   -1   -1
##  [24,]    1   -1   -1
##  [25,]    1   -1    1
##  [26,]    1   -1   -1
```

```
##  [27,]    1   -1   -1
##  [28,]    1   -1   -1
##  [29,]    1   -1   -1
##  [30,]    1   -1   -1
##  [31,]    1   -1   -1
##  [32,]    1   -1   -1
##  [33,]    1   -1   -1
##  [34,]    1   -1   -1
##  [35,]    1   -1   -1
##  [36,]    1   -1   -1
##  [37,]    1   -1   -1
##  [38,]    1   -1   -1
##  [39,]    1   -1   -1
##  [40,]    1   -1   -1
##  [41,]    1   -1   -1
##  [42,]    1   -1   -1
##  [43,]    1   -1   -1
##  [44,]    1   -1   -1
##  [45,]    1   -1    1
##  [46,]    1   -1   -1
##  [47,]    1   -1   -1
##  [48,]    1   -1   -1
##  [49,]    1   -1   -1
##  [50,]    1   -1   -1
##  [51,]    1    1    1
##  [52,]    1    1    1
##  [53,]    1    1    1
##  [54,]    1    1    1
##  [55,]    1    1    1
##  [56,]    1    1    1
##  [57,]    1    1    1
##  [58,]    1    1    1
##  [59,]    1    1    1
##  [60,]    1    1    1
##  [61,]    1    1    1
##  [62,]    1    1    1
##  [63,]    1    1    1
##  [64,]    1    1    1
##  [65,]    1    1    1
##  [66,]    1    1    1
##  [67,]    1    1    1
##  [68,]    1    1    1
##  [69,]    1    1    1
##  [70,]    1    1    1
##  [71,]    1    1    1
##  [72,]    1    1    1
##  [73,]    1    1    1
##  [74,]    1    1    1
##  [75,]    1    1    1
##  [76,]    1    1    1
##  [77,]    1    1    1
##  [78,]    1    1   -1
##  [79,]    1    1    1
##  [80,]    1    1    1
```

```
##  [81,]    1    1    1
##  [82,]    1    1    1
##  [83,]    1    1    1
##  [84,]    1    1   -1
##  [85,]    1    1    1
##  [86,]    1    1    1
##  [87,]    1    1    1
##  [88,]    1    1    1
##  [89,]    1    1    1
##  [90,]    1    1    1
##  [91,]    1    1    1
##  [92,]    1    1    1
##  [93,]    1    1    1
##  [94,]    1    1    1
##  [95,]    1    1    1
##  [96,]    1    1    1
##  [97,]    1    1    1
##  [98,]    1    1    1
##  [99,]    1    1    1
## [100,]    1    1    1
## [101,]    1    1   -1
## [102,]    1    1   -1
## [103,]    1    1   -1
## [104,]    1    1   -1
## [105,]    1    1   -1
## [106,]    1    1   -1
## [107,]    1    1    1
## [108,]    1    1   -1
## [109,]    1    1   -1
## [110,]    1    1   -1
## [111,]    1    1   -1
## [112,]    1    1   -1
## [113,]    1    1   -1
## [114,]    1    1   -1
## [115,]    1    1   -1
## [116,]    1    1   -1
## [117,]    1    1   -1
## [118,]    1    1   -1
## [119,]    1    1   -1
## [120,]    1    1    1
## [121,]    1    1   -1
## [122,]    1    1   -1
## [123,]    1    1   -1
## [124,]    1    1   -1
## [125,]    1    1   -1
## [126,]    1    1   -1
## [127,]    1    1    1
## [128,]    1    1   -1
## [129,]    1    1   -1
## [130,]    1    1   -1
## [131,]    1    1   -1
## [132,]    1    1   -1
## [133,]    1    1   -1
## [134,]    1    1   -1
```

```
## [135,]    1    1   -1
## [136,]    1    1   -1
## [137,]    1    1   -1
## [138,]    1    1   -1
## [139,]    1    1    1
## [140,]    1    1   -1
## [141,]    1    1   -1
## [142,]    1    1   -1
## [143,]    1    1   -1
## [144,]    1    1   -1
## [145,]    1    1   -1
## [146,]    1    1   -1
## [147,]    1    1   -1
## [148,]    1    1   -1
## [149,]    1    1   -1
## [150,]    1    1   -1
```

K-Means (Step 6)

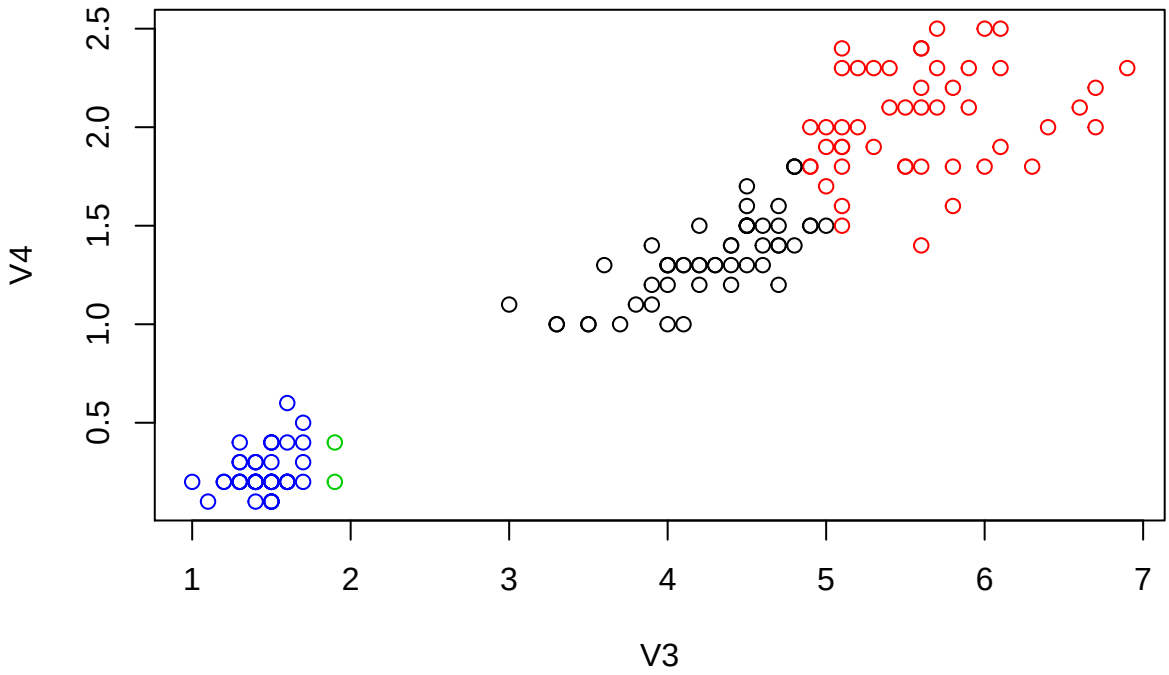
Step 6.1: Set vars and set centroids

```
xnew <- Y
obs <- as.numeric()

# seta centroides iniciais (criando combinacao de -1 e 1) -> RUIM
#center1<- sample(seq(-1,1,by=0.1),3,replace=T)
#center2<- sample(seq(-1,1,by=0.1),3,replace=T)
#center3<- sample(seq(-1,1,by=0.1),3,replace=T)

# seta centroides iniciais com heuristica (sabendo que esses 3 pontos sao disitntos)
#center1 <- xnew[1,]
#center2 <- xnew[70,]
#center3 <- xnew[149,]

# trocar -1 por 0 para ficar tudo com valores 0 ou 1
#for(n in 1:150){
#  for(m in 1:3){
#    if (xnew[n,m] == -1){
#      xnew[n,m] = 0
#    }
#  }
#}

# get different centroids
flag <- TRUE
while(flag){
  center1 <- xnew[sample(1:150,1),]
  center2 <- xnew[sample(1:150,1),]
  center3 <- xnew[sample(1:150,1),]
  if (!(all(center1 == center2) || all(center1 == center3) || all(center2 == center3)) ){
    icenter1 <- center1
    icenter2 <- center2
    icenter3 <- center3
```

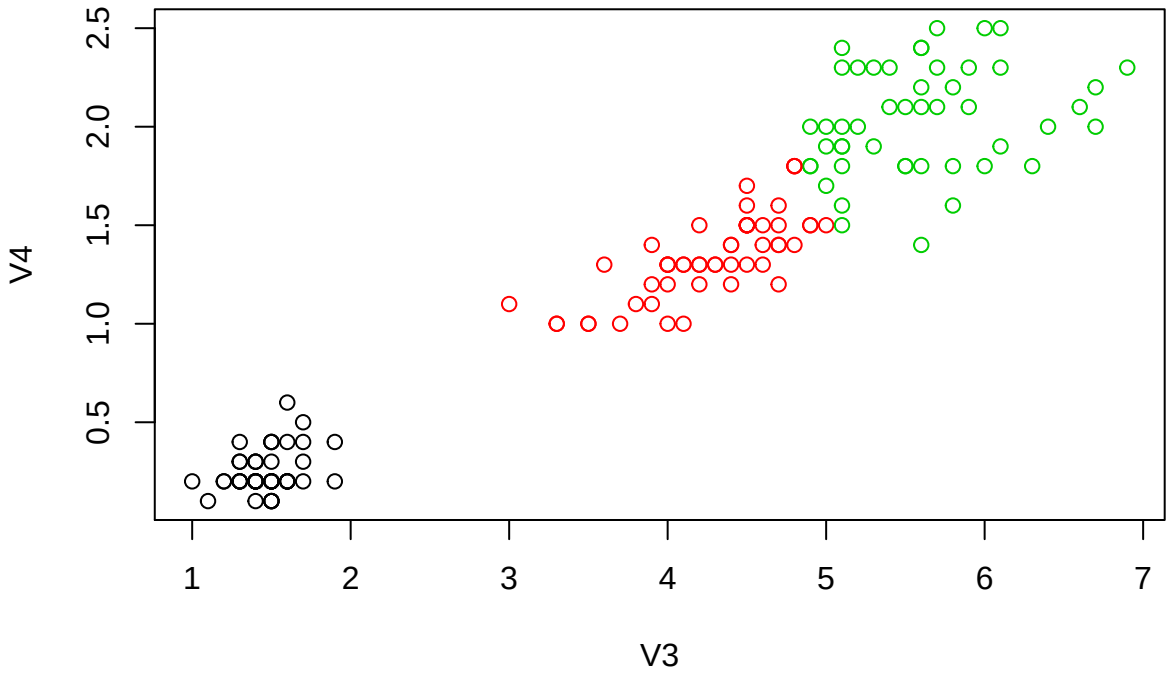
```
    flag <- FALSE
  }
}
```

Step 6.2: K-Means Algorithm and Plot Graphs

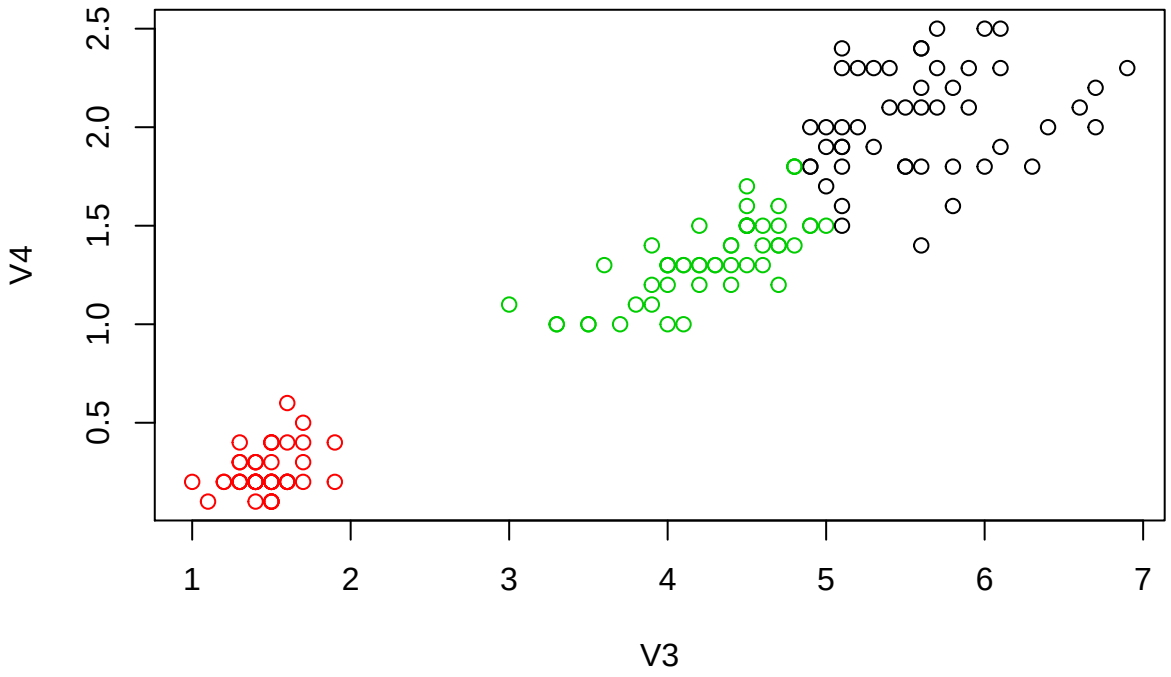
```
for(n in 1:40000){ # upgrade centroids
  for(i in 1:150){ # 150 instances
    dist1<- sum((xnew[i,]-center1)^2)
    dist2<- sum((xnew[i,]-center2)^2)
    dist3<- sum((xnew[i,]-center3)^2)

    if(dist1<=dist2 && dist1<=dist3){
      obs[i]<-1
    }
    else if(dist2<=dist1 && dist2<=dist3){
      obs[i]<-2
    }
    else{
      obs[i]<-3
    }
  }

  grupo1<-xnew[(obs == 1),]
  grupo2<-xnew[(obs == 2),]
  grupo3<-xnew[(obs == 3),]

  d1 <- dim(grupo1)[1]
  d2 <- dim(grupo2)[1]
  d3 <- dim(grupo3)[1]

  # Check if different class
  if (d1 != 0){
    center1<-c(mean(grupo1[,1]),mean(grupo1[,2]),mean(grupo1[,3]))
  }

  if (d2 != 0){
    center2<-c(mean(grupo2[,1]),mean(grupo2[,2]),mean(grupo2[,3]))
  }

  if (d3 != 0){
    center3<-c(mean(grupo3[,1]),mean(grupo3[,2]),mean(grupo3[,3]))
  }

}
# R kmeans
km <- kmeans (Y,4,nstart=20)
#km <- kmeans (X,3,nstart=20)
plot(S, col=km$cluster)
```




```
km <- kmeans (Y,3,nstart=20)
#km <- kmeans (X,3,nstart=20)

# Plot
plot(S, col=km$cluster)
```




```
plot(S, col=obs)
```



Compare centroinds values (initial and final values)

```
center1
```

```
## [1]  1  1 -1
```

```
center2
```

```
## [1]  1.00 -1.00 -0.92
```

```
center3
```

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

```
icenter1
```

```
## [1]  1  1 -1
```

```
icenter2
```

```
## [1]  1 -1 -1
```

```
icenter3
```

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