

Homewok5

Jun Rao

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```
library(stats)
library(ggplot2)
library(data.table)
library(kernlab)

# use data.table::fread to read the compressed CSV data file into R as a data
# table.
dt<- fread("zip.test.gz")

#To exclude the Label column (that is the first column)
df<-as.matrix(dt[, -1])
```

Spectral clustering involves computing an $N \times N$ affinity/kernel matrix (quadratic time/space in N), then an eigen-decomposition (cubic time in N), which results in a matrix of eigenvectors, which are new features/column that can be clustered with a standard algorithm like kmeans. Spectral clustering is useful for detecting clusters that are non-linear/non-spherical in shape.

1. Use kernlab::specc in R to compute a spectral clustering on the first 300 rows of the zip.test data, from 1 to 20 clusters. Compute ARI of each clustering and plot y=ARI as a function of x=number of clusters using default parameters of specc. What number of clusters is the most accurate?

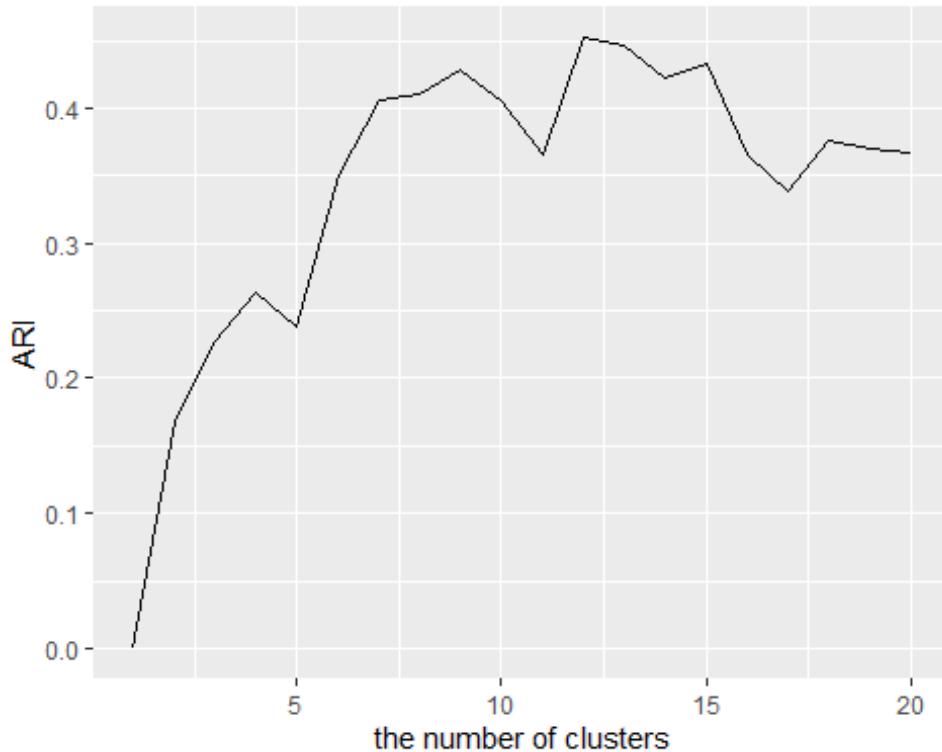
```
metrics.dt.list <- list()

for(n.clusters in 1: 20){
  if(n.clusters == 1){
    result = data.table(n.clusters,ARI=0)
  }
  else{
    fit <- specc(df[1:300,],n.clusters)
    result <- data.table(n.clusters,ARI=pdfCluster::adj.rand.index(fit@.Data, dt[1:300,][["V1"]]))}

  metrics.dt.list[[paste(n.clusters)]] <- result

}
metrics.dt <- do.call(rbind, metrics.dt.list)
```

```
ggplot() + geom_line(aes(n.clusters, ARI), data=metrics.dt) + xlab("the number of clusters") + ylab("ARI")
```



From the picture, we can find that when the cluster is 12, it is the accurate.

2. Again compute spectral clusterings but using a polynomial kernel (kernlab:polydot) instead of the default RBF kernel. Compute clusterings using three different polynomial degree values (2, 4, 6) and 1 to 20 clusters. Compute ARI of each clustering and plot y=ARI as a function of x=number of clusters, using different colors for the different polynomial degrees. What number of clusters and polynomial degree is most accurate? accurate?

```
dt <- data.table(matrix(numeric(), 60, 3))
index = 1
for(n.clusters in 1: 20){
  for (degree in seq(2,6,2)) {
    if(n.clusters == 1){
      temp <- c(n.clusters,degree,0)
      dt[index,names(dt) := as.list(temp)]
    }
    else{
      fit <- specc(df[1:300,],n.clusters,polydot(degree=degree))
      ARI = pdfCluster::adj.rand.index(fit@.Data, dt[1:300,][["V1"]])
      temp <- c(n.clusters,degree,ARI)
      dt[index,names(dt) := as.list(temp)]
    }
  }
}
```

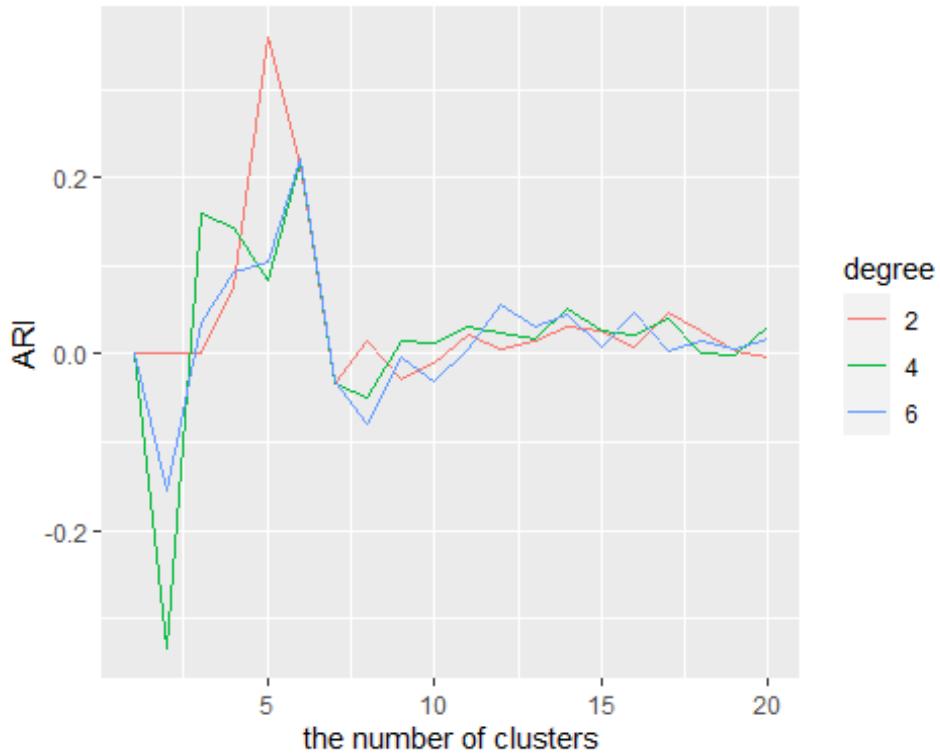
```

        index = index + 1
    }

}

# g <- ggplot() + geom_line(aes(V1, V3), data=dt) + xLab("the number of clusters")
# + yLab("ARI")
#
# g + facet_grid(rows = vars(V2))
ggplot( aes(x=V1, y=V3, group=V2, color=factor(V2)), data=dt) +
  geom_line() +
  labs(x = "the number of clusters", y="ARI", color = "degree")

```



From the picture, we can find that the most accurate at

when degree = 2 and cluster = 5

when degree = 4 and cluster = 6

when degree = 6 and cluster = 6

3. Use microbenchmark to compute timings of kmeans, hclust, and specc for several subset sizes N. Plot y=time in seconds versus x=subset size, with each algorithm in a different color. Use log/log scales so that different time complexity classes appear as lines with

different slopes. Use a large enough range of N so that the complexity class of each algorithm is clear (kmeans linear, hclust quadratic, specc cubic).

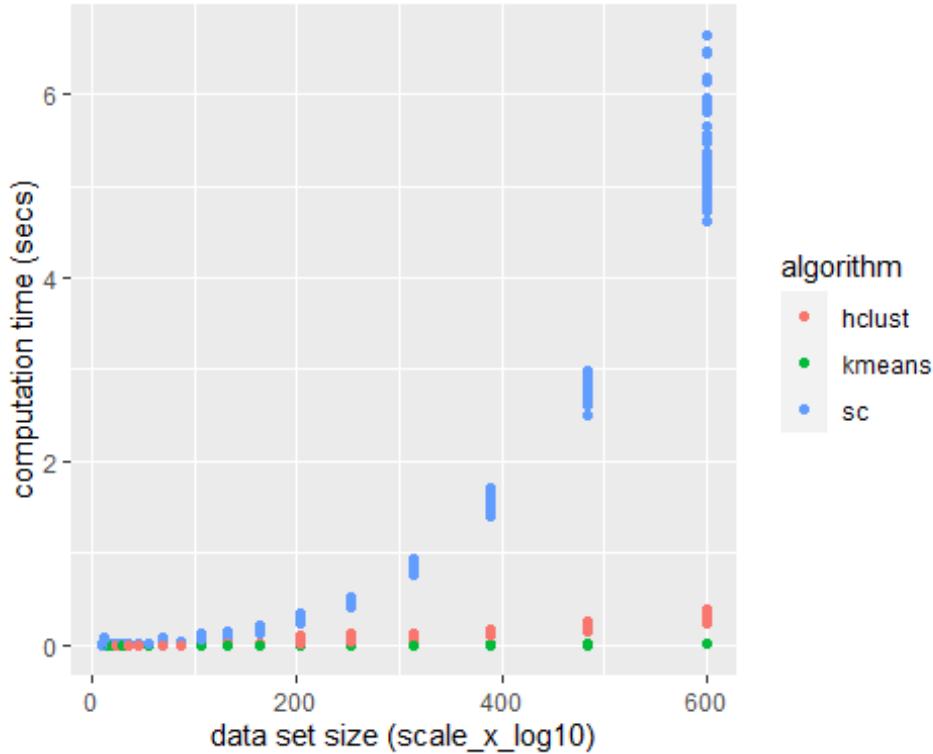
```
Myplot <- function(data.set){
  time.dt.list <- list()
  (log.scale.seq <- as.integer(c(10^seq(1, log10(600), l=20))))
  # seq(10, 1000, by =100)
  for (N in log.scale.seq) {
    X <- data.set[1:N,]
    timing.df <- microbenchmark::microbenchmark(hclust={
      d.mat <- stats::dist(X, method="manhattan")
      as.matrix(d.mat)
      cl.tree <- stats::hclust(d.mat, method="single")
      stats::cutree(cl.tree, k=3)
    },
    kmeans={
      stats::kmeans(X, 3)
    },
    sc ={
      specc(X,3)
    })
    time.dt.list[[paste(N)]] <- data.table(N, timing.df)
  }
  time.dt <- do.call(rbind, time.dt.list)
  time.dt[, data.size := N]
  time.dt[, time.seconds := time/1e9]
  time.dt[, algorithm := expr]

  g<-ggplot()+
    geom_point(aes(x=data.size,y=time.seconds,color=algorithm),data=time.dt
)+  

    xlab("data set size (scale_x_log10)") + ylab("computation time (secs)")

  return(g)
}

Myplot(df[1:1000,])
```



Code a simple spectral clustering algorithm from scratch (without using any special packages like kernlab), using the descriptions in the textbooks. Compute a kernel/similarity matrix, then either the un-normalized or normalized graph Laplacian, then compute its eigenvalues/vectors, then consider the eigenvectors corresponding to the smallest eigenvalues, then run stats::kmeans. Run the algorithm on the halfcircle/moons data we saw in class, and draw the two different clusters in different colors.

```
# spectral clustering
SPC <- function(data.matrix, K){

  #we total have two parameters in the function
  if(is.na(data.matrix) || is.na(K)){
    stop("You need to input valid parameters!!")
  }

  nodes <- dim(data.matrix)[1]

  #initialize Similarity matrix or adjacency matrix
  similarity.matrix <- matrix(NA, nrow = nodes, ncol=nodes)

  # Using Gaussian kernel (sigma = 0.09) to cluster the data
  #if two points have the small similarity value,
  #these two points will have a stronger link

  sigma <- 0.09
```

```

for (i in 1:nodes){
  for (j in 1: nodes){
    similarity.matrix[i,j] <- exp(-sum((data.matrix[i,] - data.matrix[j,
    ,])^2)/(2*sigma^2))
  }
}

#calculate the degree matrix
#it means how many connection between
#the first data point to the rest N-1 data points
S_degree <- rowSums(similarity.matrix)

#calculate Laplacian
Laplacian <- diag(S_degree) - similarity.matrix
normalize.Laplacian <- diag(S_degree^(-1/2)) %*% similarity.matrix %*% diag(S_degree^(-1/2))

#error = sum()
# ev <- eigen(Laplacian)
#
# e <- kmeans(ev$vectors[,which.min(ev$values)], K, iter.max=50)$cluster

ev <-eigen(normalize.Laplacian)
ev.vector <- ev$vectors[,1:K]

for (index in 1:nodes) {
  ev.vector[index,] <- ev.vector[i,] / sqrt(sum(ev.vector[index,]^2))
}

e <- kmeans(ev.vector, K, iter.max=50)$cluster

return(e)
}

set.seed(1)
halfcircle <- function(r, center = c(0, 0), class, sign, N=150, noise=0.5) {
  angle <- runif(N, 0, pi)
  rad <- rnorm(N, r, noise)
  data.table(
    V1 = rad * cos(angle) + center[1],
    V2 = sign * rad * sin(angle) + center[2],
    class = factor(class))
}

X.dt <- rbind(

```

```

halfcircle(4, c(0, 0), 1, 1),
halfcircle(4, c(4, 2), 2, -1))

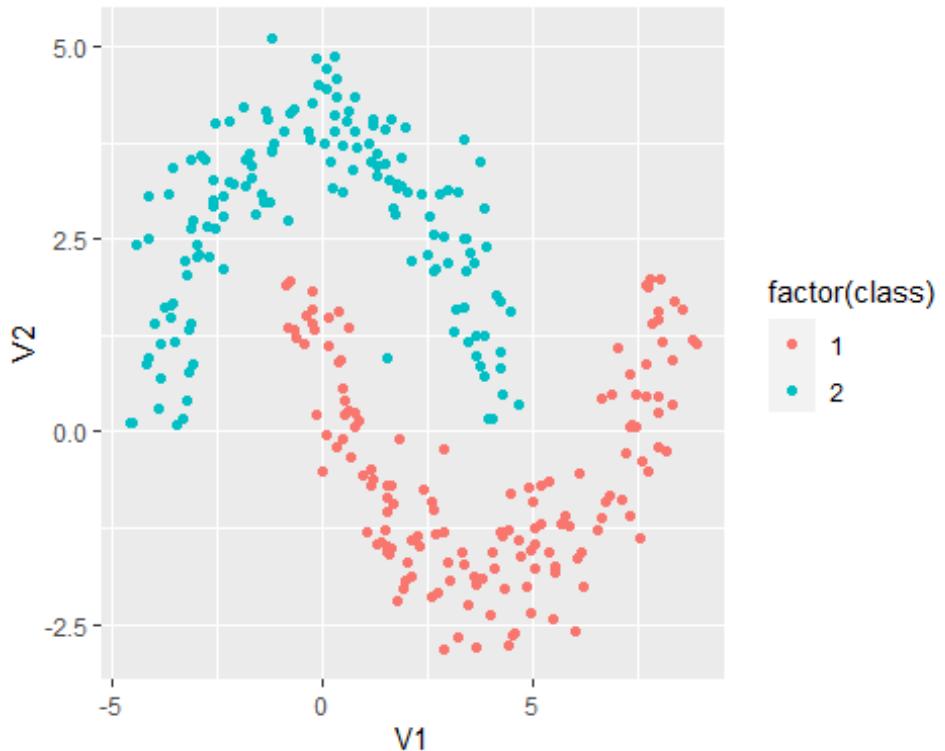
X.mat <- as.matrix(X.dt[, 1:2])

K <- 2
class = SPC(X.mat,K)

DF <- as.data.frame(cbind(X.mat,class))

ggplot()+
  geom_point(aes(
    V1, V2, color=factor(class)),
    data=DF)

```



I code my own function by using Gaussian kernel ($\sigma = 0.09$) to build similarity matrix. I find something very interesting, when $\sigma = 0.09$, the answer is most accurate.