BIRCH

Introduction

BIRCH(Balanced Iterative Reducing and Clustering using Hierarchies), proposed by Zhang et al., is an incremental clustering algorithm, which mainly targets at large-scale data sets, has fast running speed, can effectively deal with noise. The algorithm complexity can reach $O(N)$.

Features

- Each cluster contains a triple tuple: $CF = (N, LS, SS)$. Where, N is the sample size in the cluster; LS is a vector, representing the linear sum of points in each dimension within the cluster ($\sum_{i=1}^{N} \vec{X}$); SS is a scalar, representing the sum of squares of all sample points in the cluster($\sum_{i=1}^{N} \vec{X}^2$)
- CF tree is a highly balanced tree, containing three parameters: the maximum CF number of leaf nodes L (leaf), the maximum CF number of internal node (non-leaf node) B(branch), and the cluster radius threshold T(threshold).

Algorithm Flow

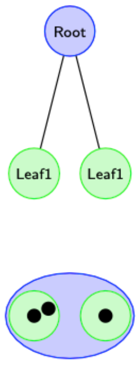
1. Construct a CF tree
2. (optional) Build a smaller tree(cut off outlier nodes, combining similar nodes etc.)
3. Global Clustering(use K-Means to cluster the leaf nodes)
4. (optional) Cluster Refining(relabel the points based on previous clustering centroids)

Example

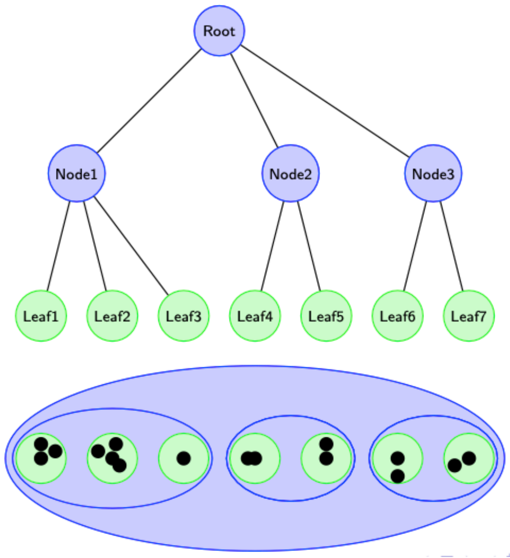
1. Let $B = L = 3, T = 0.1$: Insert the first point, construct a new node.

2. Add in a new point, according to T and the distance between the node and the new point, judge whether could be added in the same node(here the answer is yes).

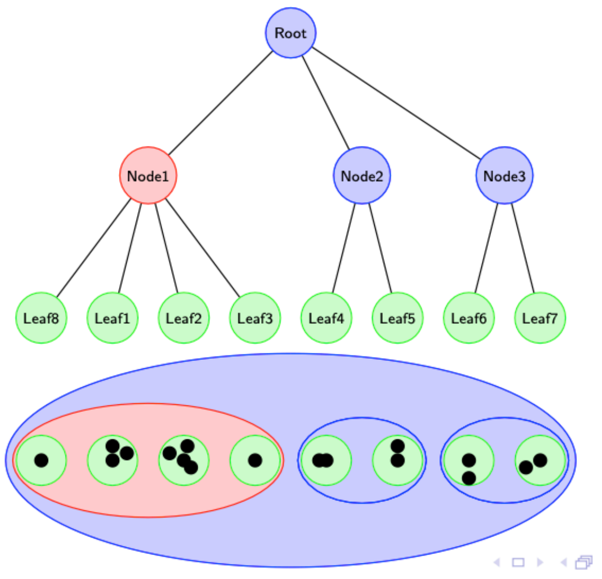
3. Repeat 2, construct a new node and a root node to connect the 2 nodes together.



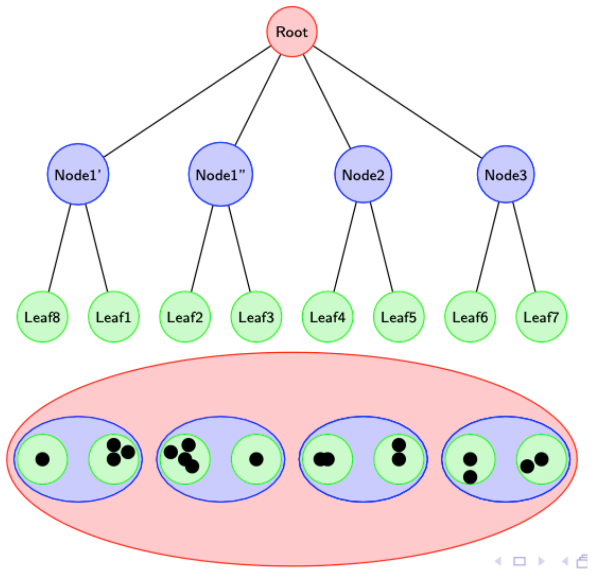
4. Keep repeating step 2(3).



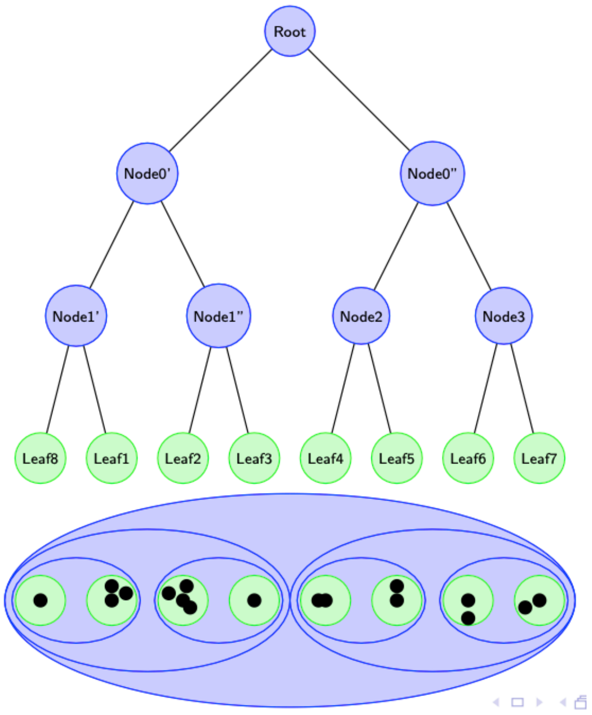
5. Add in a new point. The pink Node1 contains 4 leaves, which is larger than L.



6. Split Node1 into Node1' and Node1'' according to the distances between the clusters(nodes). The Root node contains 4 internal nodes, which is larger than B.



7. Split Root node into Node0' and Node0'', and increase the tree height(construct a new root node).



Codes in R

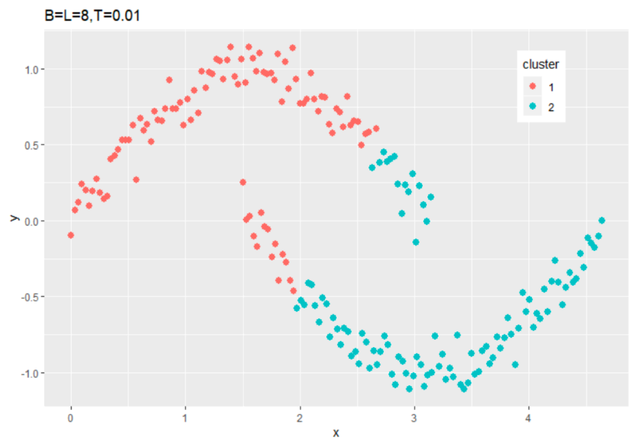
```
library(dplyr)
BIRCH<-function(dataset, B, L, Thre, dist){
  dataset<-as.data.frame(dataset)
  CFtree<<-list()
  for(i in 1:nrow(dataset)){
    Generate_CFtree(newpoint=dataset[i,]%>%as.numeric(), B, L, Thre, i, dist)
    print(i)
  }
}
#=============MAIN FUNCTION==============
Generate_CFtree<-function(newpoint, B=3, L=3, Thre=0.3, i, dist){
  depth<-length(CFtree)
  if(depth==0){ #when tree is empty, build a 2 layer CF tree directly
    Generate_nullnode(newpoint, 0, 1, 1, 1)
  }
  else{
    index<-Find_nearCF(newpoint, depth, CI=CFtree[[depth]][[1]]$CI)
    depth<-2
    cf_leaf<-CFtree[[1]][[index]]
    PN<-cf_leaf$PI
    cf0<-CFtree[[2]][[PN]]
    #whether within the radius of T
    if(distance(newpoint, CFtree[[1]][[index]]$LS/CFtree[[1]][[index]]$N)<=Thre){
      #update the new added leaf node
      CFtree[[1]][[index]]<<-list(N=cf_leaf$N+1, LS=cf_leaf$LS+newpoint, 
SS=cf_leaf$SS+sum(newpoint^2), 
                                PI=cf_leaf$PI, CI=append(cf_leaf$CI,i), 
index=cf_leaf$index)
    }
    else{ #without the radius, create the new leaf node CF and update root node
      cf_new<-Generate_nullnode(newpoint, 1, i, PN, NULL)
      #update root node, triple group already updated in 'Find_nearCF'
      CFtree[[2]][[PN]]$CI<<-append(cf0$CI, cf_new$index)
      #whether need to split node
      Split_node(B, L, 1, CI=CFtree[[2]][[PN]]$CI, i, dist)
      }
    }
  }
#=======CREATE NEW NODE======
Generate_nullnode<-function(newpoint, depth=1, i, PI=0, CI){
  if(depth==0){ #empty tree
    temp<-list(N=1, LS=newpoint, SS=sum(newpoint^2), PI=1, CI=1, index=1)
    CFtree[[paste0('height_',depth+1)]]<<-list(temp)
    temp<-list(N=1, LS=newpoint, SS=sum(newpoint^2), PI=0, CI=1, index=1)
    CFtree[[paste0('height_',depth+2)]]<<-list(temp)
  }
  else if(depth==1){ #if leaf node, requires PI
    temp<-list(N=1, LS=newpoint, SS=sum(newpoint^2), PI=PI, CI=i, 
index=length(CFtree[[1]])+1)
    CFtree[[paste0('height_',depth)]][[temp$index]]<<-temp
  }
  else{ #not leaf node, requires PI, CI
    if(is.null(CFtree[[paste0('height_',depth)]])==T){#create root node
      temp<-list(N=i, LS=newpoint, SS=Extract(depth-1, 1)$SS%>%unlist%>%as.numeric(), 
PI=PI, CI=CI, index=1)
      CFtree[[paste0('height_',depth)]]<<-list(temp)
    }
    else{#create split node, N is the sample size of every CI
      #a<-sapply(Extract(depth-1, CI)$CI,'[',i = 1:max(sapply(Extract(depth-1, CI)$CI, 
length)))%>%t()%>%as.data.frame()%>%is.na()
      temp<-list(N=Extract(depth-1, CI)$N%>%as.data.frame()%>%sum(), LS=newpoint, 
SS=sapply(Extract(depth-1, CI)$SS,'[',i = 1)%>%unlist%>%sum(), PI=PI, CI=CI, 
index=length(CFtree[[depth]])+1)
      CFtree[[paste0('height_',depth)]][[temp$index]]<<-temp
    }
  }
}
#===========DISTANCE FUNCTION=========
distance=function(point_1, point_2){
  return(sqrt(sum((point_1-point_2)^2)))
```

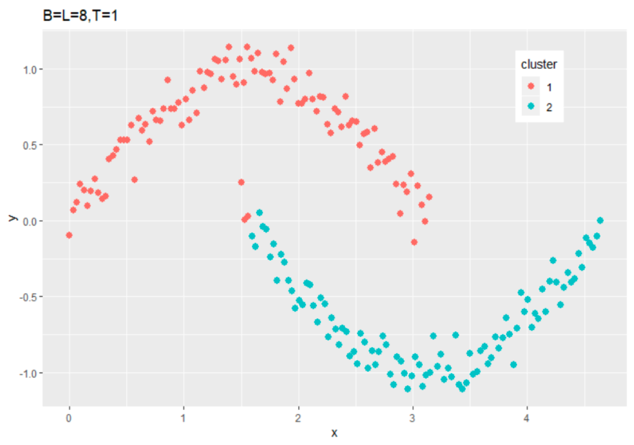
```
}
distance_CF = function(CF_1, CF_2, dist='intercluster' ){
  if (dist == 'Euclidean'){
    temp = distance(CF_1$LS/CF_1$N, CF_2$LS/CF_2$N)
  }
  else if (dist == 'Manhattan'){
    temp = abs(CF_1$LS/CF_1$N-CF_2$LS/CF_2$N)
  }
  else if (dist == 'intercluster'){
    temp = sqrt(CF_1$SS/CF_1$N-2*sum(CF_1$LS*CF_2$LS)/(CF_1$N*CF_2$N)+CF_2$SS/CF_2$N)
  }
  else{
    stop('The distance method doesn\'t exist.')
  }
  return(temp)
}
#=======AMONG NODE where DEPTH=depth-1, FIND NEAREST NODE to 'newpoint'===
#=======UPDATE ROOT NODE AFTER INSERT=====================================
Find_nearCF<-function(newpoint, depth, CI){
  PN<-CFtree[[depth-1]][[CI[1]]]$PI
  cf0<-CFtree[[depth]][[PN]]
  CFtree[[depth]][[PN]]<<-list(N=cf0$N+1, LS=cf0$LS+newpoint,
                               SS=cf0$SS+sum(newpoint^2),
                               PI=cf0$PI, CI=cf0$CI, index=cf0$index)
  mindist<-Inf
  for(cf in CFtree[[depth-1]][CI]){
    temp<-distance(newpoint, cf$LS/cf$N)
    if(temp<mindist){
      mindist<-temp
      near<-cf$index
      CN<-cf$CI
    }
  }
  if(depth==2)
    return(near)
  else
    return(Find_nearCF(newpoint, depth-1, CN))
}
#===========SPLIT NODE===========
Split_node<-function(B, L, depth, CI, i, dist){
  BL<-ifelse(depth==1, L, B)
  if(length(CI)>BL){
    PPI<-Find_farCF(depth, CI, i, dist)
    depth<-depth+1
    if(depth<length(CFtree))
      return(Split_node(B, L, depth, CI=CFtree[[depth+1]][[PPI]]$CI, i, dist))
```

```r
  }
  return(1)
}

#===========FIND FARTHEST 2 CF============
Find_farCF<-function(depth, CI=1:length(CFtree[[1]]), i, dist){
  #compute distance of every 2 CF
  comb<-combn(CI,2)
  maxdist<--Inf
  for(k in 1:ncol(comb)){
    temp<-distance_CF(CFtree[[depth]][[comb[1,k]]], CFtree[[depth]][[comb[2,k]]], dist)
    if(temp>maxdist){
      maxdist<-temp
      far<-comb[,k]
    }
  }
  #find where CF belong except the farthest 2
  which_cf<-c()
  for(cf in CFtree[[depth]][CI[!CI%in%far]]){
    temp<-c(distance_CF(cf, CFtree[[depth]][[far[1]]], dist), distance_CF(cf,
CFtree[[depth]][[far[2]]], dist))%>%which.min()
    which_cf<-c(which_cf,temp)
  }
  #judge whether need to increase the layer of the tree, build 2 root nodes and reallocate
the child nodes
  tag<-0
  if(length(CFtree[[depth+1]])==1){#if the number of nodes that needs to split is 1
                                    #then need to increase the layer
    Generate_nullnode(CFtree[[depth+1]][[1]]$LS, depth+2, i, PI=0, CI=1:2)
    tag<-1
  }
  PN<-CFtree[[depth]][[CI[1]]]$PI
  CN<-c(far[1],CI[!CI%in%far][which(which_cf==1)])
  PPI<-ifelse(tag==1, 1, CFtree[[depth+1]][[PN]]$PI)
  #build the first node
  cf_new<-Generate_nullnode(newpoint=apply(Extract(depth, CN)[,2]%>%as.data.frame,1,sum),
depth+1, i, PI=PPI, CI=CN)
  CN1<-CI[!CI%in%CN]
  ls<-apply(Extract(depth, CN1)[,2]%>%as.data.frame,1,sum)
  #build the second node
  CFtree[[depth+1]][[PN]]<<-list(N=Extract(depth, CN1)$N%>%as.data.frame()%>%sum, LS=ls,
SS=Extract(depth, CN1)[,3]%>%as.data.frame%>%sum, PI=PPI, CI=CN1, index=PN)
  #if tree layer doesn't increase, then need to update the CI of the root node
  if(tag==0)
    CFtree[[depth+2]][[PPI]]$CI<<-append(CFtree[[depth+2]][[PPI]]$CI, cf_new$index)
  #update the parent node of the child node
  for(j in 1:length(CI)){
    CFtree[[depth]][[CI[j]]]$PI<<-ifelse(CI[j]%in%CN, cf_new$index, PN)
  }
  return(PPI)
}

Extract<-function(depth, CI=1:length(CFtree[[depth]])){
  CFdf<-as.data.frame(t(sapply(CFtree[[depth]][CI], "[", i = 1:max(sapply(CFtree[[1]],
length)))))
  return(CFdf)
}
```

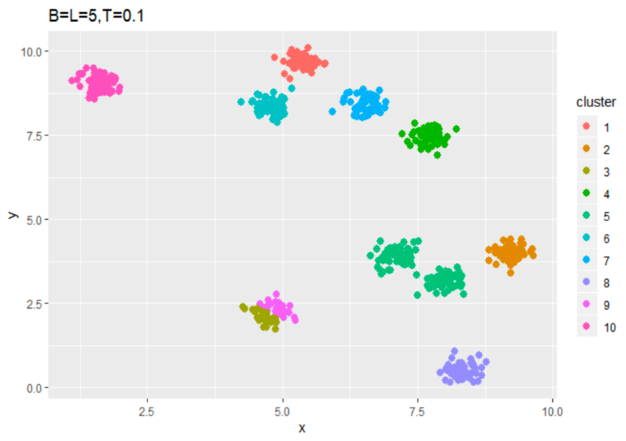
Visualization

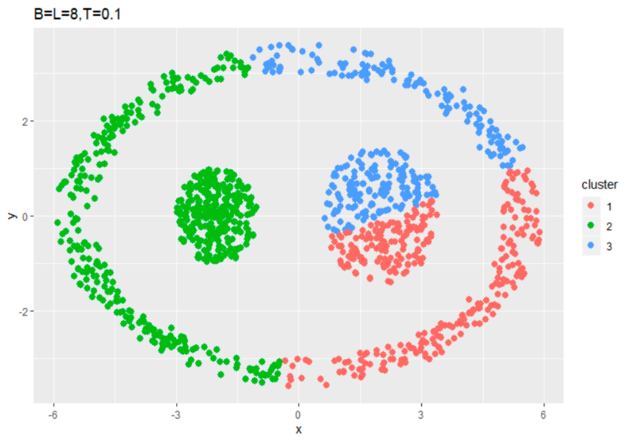
- Sensitive to T Parameter





- Show ineffective results when facing with nonspherical clusters





ROCK

Introduction

ROCK(RObust Clustering using linKs) , proposed by Guha et al. is used to classify discrete and Boolean type data, mianly based on calculating "Goodness" function to quantify the connectivity between point sets.

Algorithm Flow

1. Sampling
2. ROCK clustering
3. Label data

Definition

- Sampling size: $s \geq fN + \frac{N}{|u|}\log\left(\frac{1}{\delta}\right) + \frac{N}{|u|}\sqrt{\log\left(\frac{1}{\delta}\right)^2 + 2f|u|\log\left(\frac{1}{\delta}\right)}$, where $|u|$ represents the cluster point numbers, f, δ are decimals between 0 and 1, N means data set size.
- Similarity Function: $sim(p_i, p_j) = \frac{|p_i \bigcap p_j|}{|p_i \bigcup p_j|}$, where $|p_i|$ means the items within p_i
- Neighbor: if $sim(p_i, p_j) \geq \theta$, where $0 \leq \theta \leq 1$
- Link Function: Number of the common Neighbors between p_i, p_j
- Goodness Function: $g(C_i, C_j) = \frac{\text{link}(C_i, C_j)}{(n_i+n_j)^{1+2f(\theta)} - n_i^{1+2f(\theta)} - n_j^{1+2f(\theta)}}$, where C_i means clusters, n_i means sample size within C_i, $f(\theta) = \frac{1-\theta}{1+\theta}$

Innovation

Revise the Similarity Function into Euclidean Distance Function, and the Link Function into $sim(p_i, p_j) \leq \theta$, which makes it applicable into continuous data sets.

Codes in R

```
rm(list=ls())
library(dplyr)
#===========phase1 SAMPLE============
sampleROCK<-function(dataset,f,delta,umin){
  N<-nrow(dataset)
  #minimum sample size
  s<-
min(ceiling(f*N+N/umin*log(1/delta)+N/umin*sqrt((log(1/delta))^2+2*f*umin*log(1/delta))),N
)
  #sampling the serial number
  sample_id<<-sample(1:N,s,replace = F)
  left_id<<-setdiff(1:N,sample_id)
  dat<-dataset[sample_id,]
  #if no difference in sample size before and after sampling,
  #then return original sample(or not consistent on labeling)
  if(nrow(dat)==nrow(dataset)){
    warning('equal sample size as original data, return with original data')
    return(dataset)
  }
  else return(dat)
}
#=============phase2 ROCK CLUSTERING=============
avesamp<-function(samp){
  n <- nrow(samp)
  comb<-combn(n,2,simplify=T)
  averdis <- 0
  for(i in 1:ncol(comb)){
    averdis <- averdis + sqrt(sum(samp[comb[1,i],]-samp[comb[2,i],])^2)
  }
  averdis <<- averdis/(ncol(comb))
}


Similarity<-function(p1, p2, funct='Jaccard'){
  if(funct=='Jaccard'){
    s1<-sum(p1|p2)
    if(s1==0) s1<-1
    return(sum(p1&p2)/s1)
  }
  if(funct=='cosine'){
    return(sum(p1*p2)/sqrt(sum(p1^2)*sum(p2^2)))
  }
  if(funct=='L2'){
    return(sqrt(sum((p1-p2)^2))/averdis)
  }
}

Goodness<-function(theta, n1, n2, link){
  return(link/((n1+n2)^(1+2*f(theta))-n1^(1+2*f(theta))-n2^(1+2*f(theta))))
}

f<-function(theta){
  return((1-theta)/(1+theta))
}

Compute_link<-function(dataset, theta, funct, type){
  n<-nrow(dataset)
  link<-nbr<-matrix(rep(0,n*n), nrow=n)
  for(i in 1:(n-1))
    for(j in (i+1):n)
      nbr[j,i]<-nbr[i,j]<-Similarity(dataset[i,],dataset[j,],funct)
  nbr[type==1]<-nbr<=theta
  nbr[type!=1]<-nbr>=theta

  #nbr%*%nbr, diagnal=0
```

```r
  #nbr%*%nbr, diagnal=0
  for(i in 1:n){
    if(which(nbr[i,]==T)%>%length>1){
    comb<-combn(which(nbr[i,]==T),2)
      for(j in 1:ncol(comb)){
        link[comb[1,j],comb[2,j]]<-link[comb[1,j],comb[2,j]]+1
        link[comb[2,j],comb[1,j]]<-link[comb[2,j],comb[1,j]]+1
      }
    }
  }
  return(link)
}

#============MAIN FUNCTION=============
Build_localheap<-function(dataset, link, theta){
  localheap<-list()
  for(i in 1:nrow(dataset)){
    goodness<-data.frame(goodness=NA, j=NA)
    count<-1
    for(j in which(link[i,]!=0)){
      goodness[count,1]<-Goodness(theta, 1, 1, link[i,j])
      goodness[count,2]<-j
      count<-count+1
    }
    localheap[[i]]<-list(gninf=goodness, index=i)
  }
  return(localheap)
}

Build_globalheap<-function(localheap){
  globalheap<-data.frame(max_goodness=NA, max_i=NA, max_j=NA)
  count<-1
  for(i in 1:length(localheap)){
    c_i<-localheap[[i]]
    if(is.na(c_i$gninf[1,1])) next
    else{
      globalheap[count,]<-c(c_i$gninf[,1]%>%max,
                            i,
                            c_i$gninf[,2][c_i$gninf[,1]%>%which.max])
      count<-count+1
    }
  }
  return(globalheap)
}



ROCK<-function(dataset, theta, k, funct, type){
```

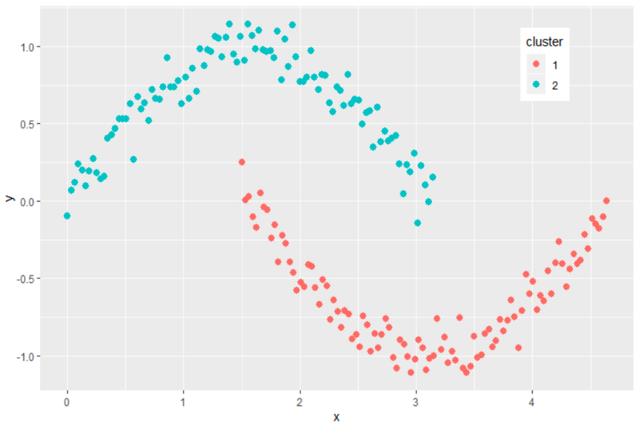
```
Rock<-function(dataset, theta, k, funct, type){
  if(funct=='L2') avesamp(dataset)
  link<-Compute_link(dataset, theta,funct,type)
  localheap<-Build_localheap(dataset, link, theta)
  globalheap<-Build_globalheap(localheap)
  while(nrow(globalheap)>k){
    u<-globalheap[which.max(globalheap$max_goodness),3]
    v<-globalheap[which.max(globalheap$max_goodness),2]
    globalheap<-globalheap[-which(globalheap[,2]==u|globalheap[,2]==v),]
    w<-length(localheap)+1
    localheap[[w]]<-list(gninf=data.frame(goodness=NA, j=NA),
index=c(localheap[[u]]$index, localheap[[v]]$index)%>%sort)
    inter<-c(localheap[[u]]$gninf[,2],localheap[[v]]$gninf[,2])%>%base::unique()
    inter<-inter[-which(inter==v|inter==u)]
    link<-link%>%cbind(rep(0,nrow(link)))%>%rbind(rep(0,ncol(link)+1))
    if(length(inter)!=0){
      for(x in inter){
        link[w,x]<-link[x,w]<-link[x,u]+link[x,v]#no need to judge x,u(write into
symmetric matrix)
        #delete u,v in 'localheap[[x]]'
        localheap[[x]]$gninf<-localheap[[x]]$gninf[-
which(localheap[[x]]$gninf[,2]==u|localheap[[x]]$gninf[,2]==v),]
        gn_wx<-
Goodness(theta,length(localheap[[w]]$index),length(localheap[[x]]$index),link[w,x])
        #update 'localheap[[x]]' and add 'localheap[[w]]'
        localheap[[x]]$gninf<-rbind(localheap[[x]]$gninf,c(gn_wx,w))
        localheap[[w]]$gninf<-rbind(localheap[[w]]$gninf,c(gn_wx,x))
        #update the max goodness in 'globalheap' (might change)
        c_x<-localheap[[x]]
        globalheap[which(globalheap$max_i==x),]<-c(c_x$gninf[,1]%>%max, x,
                            c_x$gninf[,2][c_x$gninf[,1]%>%which.max])
      }
    localheap[[w]]$gninf<-localheap[[w]]$gninf[-1,]
    }
    globalheap<-rbind(globalheap, c(localheap[[w]]$gninf[,1]%>%max, w,
                                    localheap[[w]]$gninf[,2]
[localheap[[w]]$gninf[,1]%>%which.max]))
    localheap[[u]]<-w
    localheap[[v]]<-w
    print(nrow(globalheap))
  }
  globalheap<<-globalheap;localheap<<-localheap
  link<<-link
  return(1)
}


#===============phase3 LABEL DATA============
label<-function(dataset,u,newpoint,theta,k,funct,type){
  criteria<-c()
  for(i in 1:length(u)){
    d<-dataset[clu[which(clu[,2]==i),][,1],]
    sim<-c()
    for(j in 1:nrow(d)) sim<-c(sim,Similarity(newpoint,d[j,],funct = funct))
    ni<-ifelse(type==1,sum((sim<=theta)+0),sum((sim>=theta)+0))
    criteria<-c(criteria,ni/(1+nrow(d))^f(theta))
  }
  clu[nrow(clu)+1,]<<-c(index=left_id[k],cluster=which.max(criteria))
}
#main function

LableonDisk<-function(dataset,samp,theta,funct,type){
  u<-globalheap$max_i
  sequ<-seq(1,length(u),1)
  index_sample<-c()
  cl<-c()
  for(i in 1:length(u)){
    l<-localheap[[u[i]]]$index
    index_sample<-c(index_sample,l)
    cl<-c(cl,rep(sequ[i],length(l)))
  }
  #resort the serial no and the belonging cluster after sampling
  clu<<-data.frame(index=index_sample,cluster=cl)
  if(nrow(dataset)==nrow(samp)) return(clu)
  clu$index<<-sample_id[clu$index]
  if(length(left_id)!=1)  for(k in 1:length(left_id)) {
    label(dataset,u,dataset[left_id,][k,],theta,k,funct,type)
    print(k)
  }
  else  label(dataset,u,dataset[left_id,],theta,1,funct)
  return(clu)
}
```

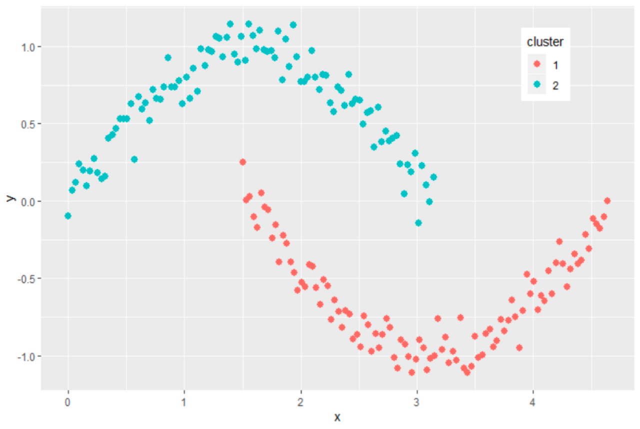
Visualization

- Not sensitive to θ parameter

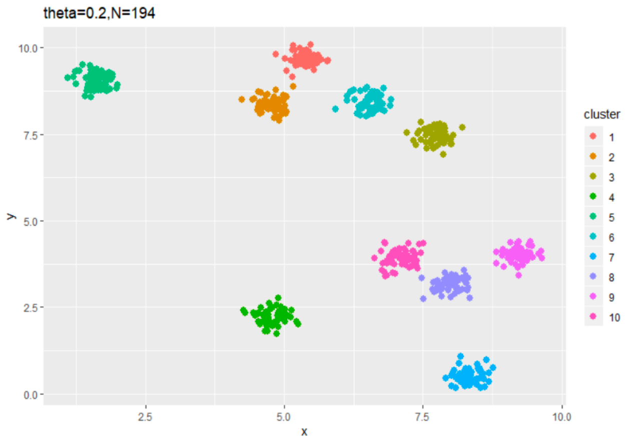
theta=0.5,N=89

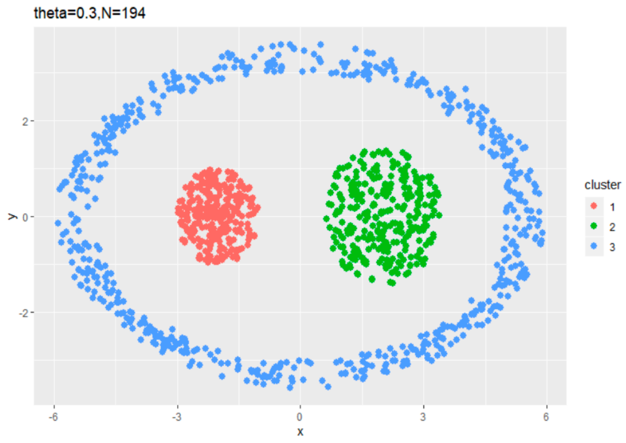
theta=0.8,N=89





- Perform well for continuous data





- Perform well on simulated descrete data set

	1	2	3	4	5	6	7	8	9	10	real cluster	ROCK cluster
1	1	1	1	1	1	0	0	0	0	0	a	a
2	1	1	1	0	1	0	0	0	0	0	a	a
3	0	1	0	1	1	0	0	0	0	0	a	a
4	0	1	1	0	0	0	0	0	0	0	a	a
5	0	0	1	1	1	0	0	0	0	0	a	a
6	0	0	0	0	0	1	0	1	0	1	b	b
7	0	1	0	1	0	0	1	0	0	0	b	b
8	0	0	0	0	0	1	1	1	1	1	b	b
9	0	0	0	0	0	1	1	0	1	1	b	b
10	0	0	0	0	0	0	1	1	1	1	b	b
11	0	0	0	0	0	1	0	0	0	0	b	b
12	0	0	0	0	0	1	0	0	1	1	b	b
13	1	0	0	0	0	1	0	0	1	0	b	b
14	0	0	0	0	0	0	0	1	0	1	b	b