RAProject

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```
sce0 <- readRDS('toyTCRdata.rds')
sce <- clonoStats(sce0, method = 'EM')

#A<-sce0$contigs[sce0$contigs[, 'chain'] %in% c('TRA','TRB')]
# for (i in 1:length(sce0$contigs)){
#   #sce0$contigs[[i]]  "DFrame"  "S4Vectors"
#   #sce0$contigs[[i]]<-sce0$contigs[[i]] %>% filter(chain %in% c("TRA","TRB"))
#   #sce0$contigs[[i]]<-sce0$contigs[[i]][filter(sce0$contigs[[i]]$chain %in% c("TRA","TRB")),]
#   sce0$contigs[[i]]<-sce0$contigs[[i]][order(sce0$contigs[[i]]$chain),]
#
# }
```

Generate sample pool

```
poolSize=2000
SampleSize=5000
AmiNoAcids=c('A','R','N','D','C','Q','E','G','H','I','L','K','M','F','P','S','T','W','Y','V')
getCDR3 <- function(x){

  cdr3=sample(AmiNoAcids,15, replace=T)
  return(paste(cdr3,collapse = ''))
}

TemplateClonotype=sce0$contigs[[4]][c(2,1),]
getClonotypeForPool<-function(clonotype_index, CDRAlpha, CDRBeta){
    result=TemplateClonotype
    result$cdr3[1]=CDRAlpha
    result$cdr3[2]=CDRBeta
    return(result)
}
getSamplePool <- function(poolSize){
    Alpha_pool=sapply(1:poolSize,getCDR3,simplify = TRUE)
    Beta_pool=sapply(1:poolSize,getCDR3,simplify = TRUE)

    CDR_Alpha=sample(Alpha_pool,poolSize, replace=T)
    CDR_Beta=sample(Beta_pool,poolSize, replace=T)


    barcode <- paste('cell', 1:poolSize)
```

```r
    samplePool <- lapply(1:poolSize, function(clonotype_index){
        getClonotypeForPool(clonotype_index, CDR_Alpha[clonotype_index], CDR_Beta[clonotype_index])
    })
    samplePool <- SplitDataFrameList(samplePool)
    samplePool[,'barcode'] <- barcode
    samplePool[,'sample'] <- 'sim'
    names(samplePool) <- barcode

    # sample1<-as(sample,'SplitDFrameList')
    return(samplePool)

}
samplePool=getSamplePool(poolSize)
```

Functions for generate a sample

```r
getClonotype<-function(clonotype_index, numberA, numberB, errorProb = .01){
    result=DataFrame()
    indexInPool=sample.int(poolSize, 3, replace=FALSE)
    setAlpha <- hashset()
    setBeta <- hashset()

    if (numberA>=1){
        if(runif(1) < errorProb){
          result=rbind(result,samplePool[[indexInPool[2]]][1,])
          insert(setAlpha,indexInPool[2])
        }else{
          result=rbind(result,samplePool[[indexInPool[1]]][1,])
          insert(setAlpha,indexInPool[1])
        }
        numberA=numberA-1
    }
    if (numberB>=1){
        if(runif(1) < errorProb){
          result=rbind(result,samplePool[[indexInPool[3]]][2,])
          insert(setBeta,indexInPool[3])
        }else{
          result=rbind(result,samplePool[[indexInPool[1]]][2,])
          insert(setBeta,indexInPool[1])
        }

        numberB=numberB-1
    }
    while(numberA>0){
        indexInPool=sample.int(poolSize, 1, replace=TRUE)
        while(setAlpha[indexInPool]==TRUE){
          indexInPool=sample.int(poolSize, 1, replace=TRUE)
        }
        insert(setAlpha,indexInPool)
        result=rbind(result,samplePool[[indexInPool]][1,])
        numberA=numberA-1


    }
    while(numberB>0){
        indexInPool=sample.int(poolSize, 1, replace=TRUE)
        while(setBeta[indexInPool]==TRUE){
          indexInPool=sample.int(poolSize, 1, replace=TRUE)
        }
        insert(setBeta,indexInPool)
        result=rbind(result,samplePool[[indexInPool]][2,])
        numberB=numberB-1


    }
    return(result)

}
```

Use the functions to generate a sample with size 50

However, function 'clonoStats' is not compatible with SimpleDFrameList, how to transform SimpleDFrameList to CompressedSplitDFrameList

```
getSample <- function(samplesize){
    sample=DataFrame()
    DistributeTRA=sum(sce0$contigs[,'chain']=='TRA')
    DistributeTRB=sum(sce0$contigs[,'chain']=='TRB')
    # table(DistributeTRA,DistributeTRB)
    IndexnAnBMap=cbind(DistributeTRA,DistributeTRB)
    RandomIntegers <- sample(1:(length(IndexnAnBMap)/2), samplesize, replace=T)

    barcode <- paste('cell', 1:samplesize)


    sample <- lapply(1:samplesize, function(clonotype_index){
        getClonotype(clonotype_index, IndexnAnBMap[RandomIntegers[clonotype_index],1], IndexnAnBMap[Ran
    })
    sample <- SplitDataFrameList(sample)
    sample[,'barcode'] <- barcode
    sample[,'sample'] <- 'sim'
    names(sample) <- barcode

    # sample1<-as(sample,'SplitDFrameList')
    return(sample)

}
# samplelist=getSample(SampleSize)
# EMpredicted <- clonoStats(samplelist, method = 'EM')
# UNpredicted <- clonoStats(samplelist, method = 'unique')
```

Generate hashmap. Key is clonotype in Truth(sample pool), Value is percentage of the clonotype in Truth

```r
TruthPercentageMap=hashmap()

for(i in 1:poolSize){

  key=paste(samplePool[[i]]$cdr3[1],samplePool[[i]]$cdr3[2],sep=' ')

  if(is.null(TruthPercentageMap[[key]])){
    TruthPercentageMap[[key]]<-1/poolSize
  }
  else{
    TruthPercentageMap[[key]]<-TruthPercentageMap[[key]]+1/poolSize
  }

}
```

Get Variation Distance

```r
getDistance<-function(predicted){

  clonotypes=clonoNames(predicted)
  abundance=clonoAbundance(predicted)
  SumAbundance=sum(abundance)
  distance=0
  seen <- hashmap()
  for(i in 1:length(abundance)){
    if(is.null(TruthPercentageMap[[clonotypes[i]]])){
      distance=distance+abundance[i]/SumAbundance
    }
    else{
      seen[[clonotypes[i]]]<-TruthPercentageMap[[clonotypes[i]]]
      distance=distance+abs(abundance[i]/SumAbundance-TruthPercentageMap[[clonotypes[i]]])
    }
  }

  distance=distance+Reduce("+", values(TruthPercentageMap)) -Reduce("+", values(seen))
  return(distance)
}
```

Test

```r
time0=Sys.time()
samplelist=getSample(5000)
time1=Sys.time()
```

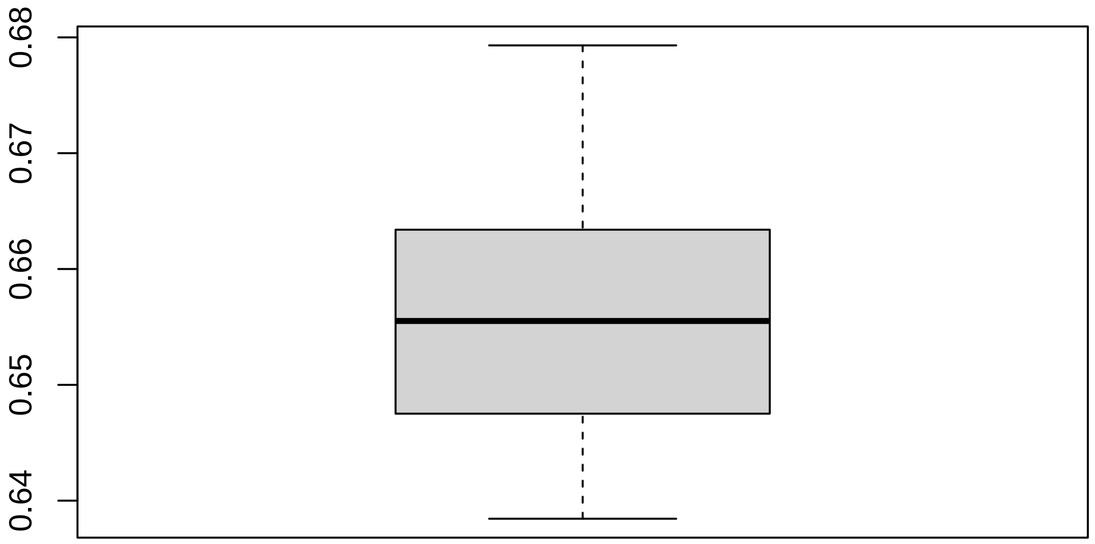
```
print(time1-time0)
EMpredicted <- clonoStats(samplelist, method = 'EM')
time2=Sys.time()
print(time2-time1)
distance1=getDistance(EMpredicted)
time3=Sys.time()
print(time3-time2)
UNpredicted <- clonoStats(samplelist, method = 'unique')
time4=Sys.time()
print(time4-time3)
distance2=getDistance(UNpredicted)
time5=Sys.time()
print(time5-time4)
```

Calculate distances for samples

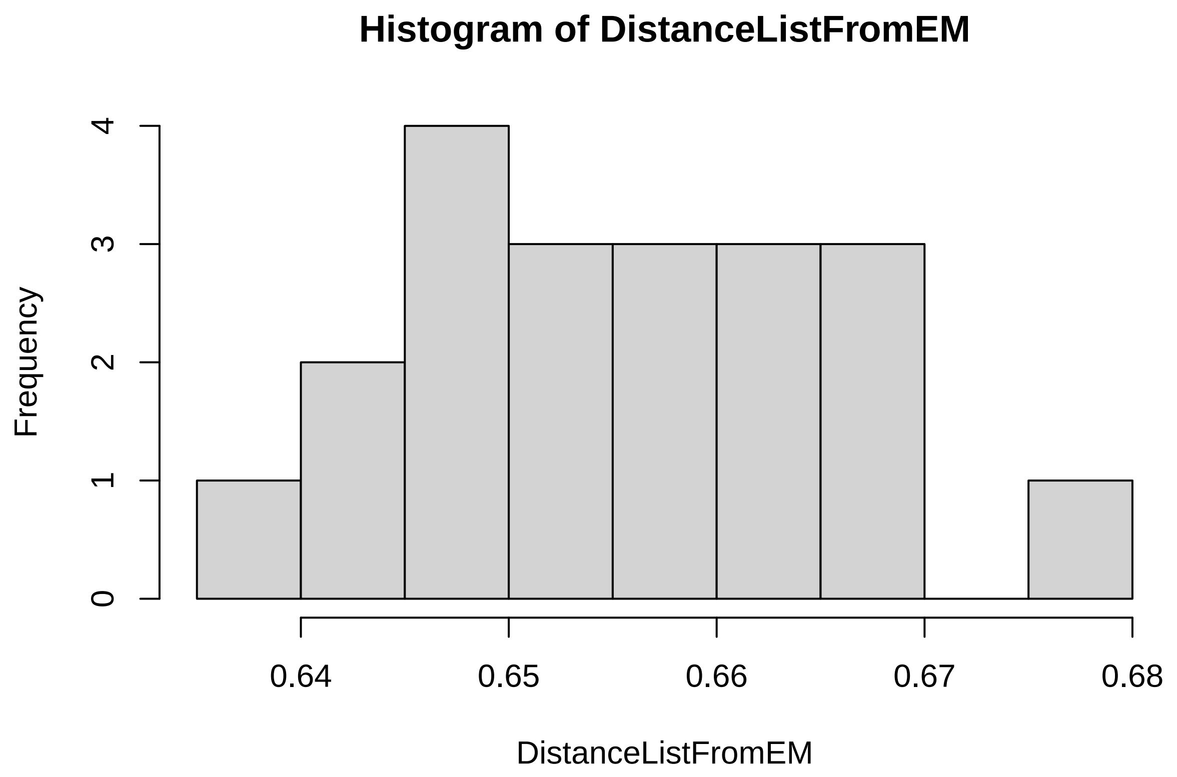
```
DistanceListFromEM=c()
DistanceListFromUN=c()
for(i in 1:20){
  samplelist=getSample(SampleSize)
  EMpredicted <- clonoStats(samplelist, method = 'EM')
  distance1=getDistance(EMpredicted)
  DistanceListFromEM[i]=distance1
  UNpredicted <- clonoStats(samplelist, method = 'unique')
  distance2=getDistance(UNpredicted)
  DistanceListFromUN[i]=distance2
}
```

Visualize

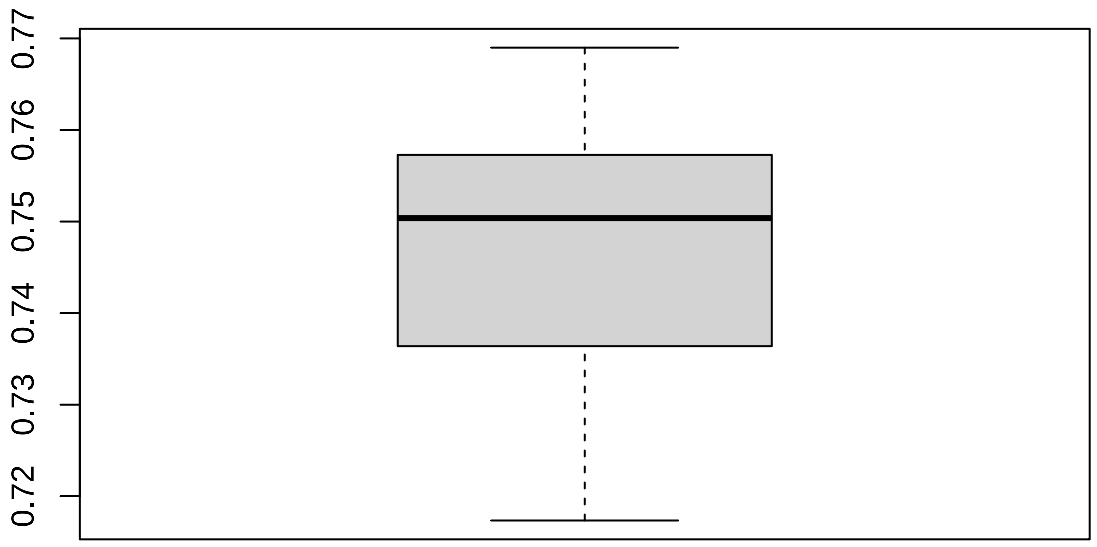
```
boxplot(DistanceListFromEM)
```



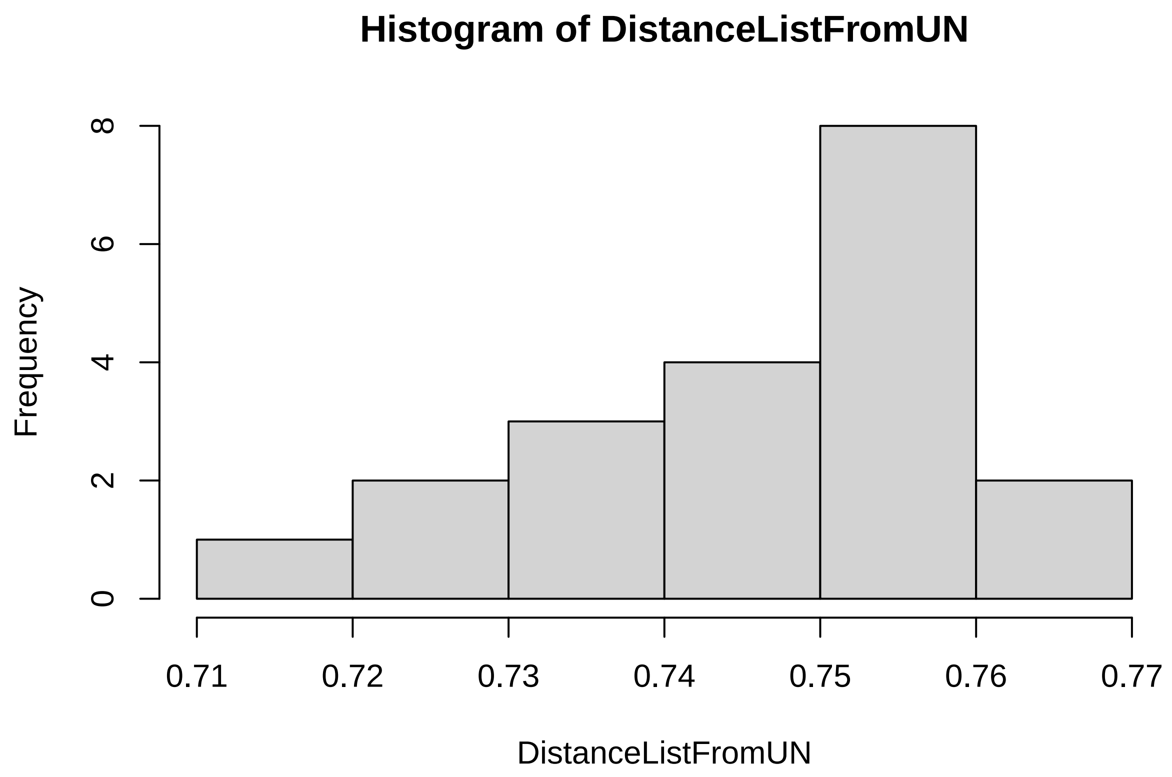
```
hist(DistanceListFromEM)
```



```
boxplot(DistanceListFromUN)
```



```
hist(DistanceListFromUN)
```



```
print(median(DistanceListFromEM))
```

```
## [1] 0.6555145
```

```
print(median(DistanceListFromUN))
```

```
## [1] 0.7503566
```

```
print(mean(DistanceListFromEM))
```

```
## [1] 0.6552086
```

```
print(mean(DistanceListFromUN))
```

```
## [1] 0.7464658
```