SSD

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2022-08-30

Introduction

SSD can obtain an estimator based on small-size pilot data which could be used to generate different sizes of training data and test data. Then it will calculate the corresponding classification error/ARI/AMI and draw the plot which has the same trend as the true data. People can determine the sample size according the plot we draw.

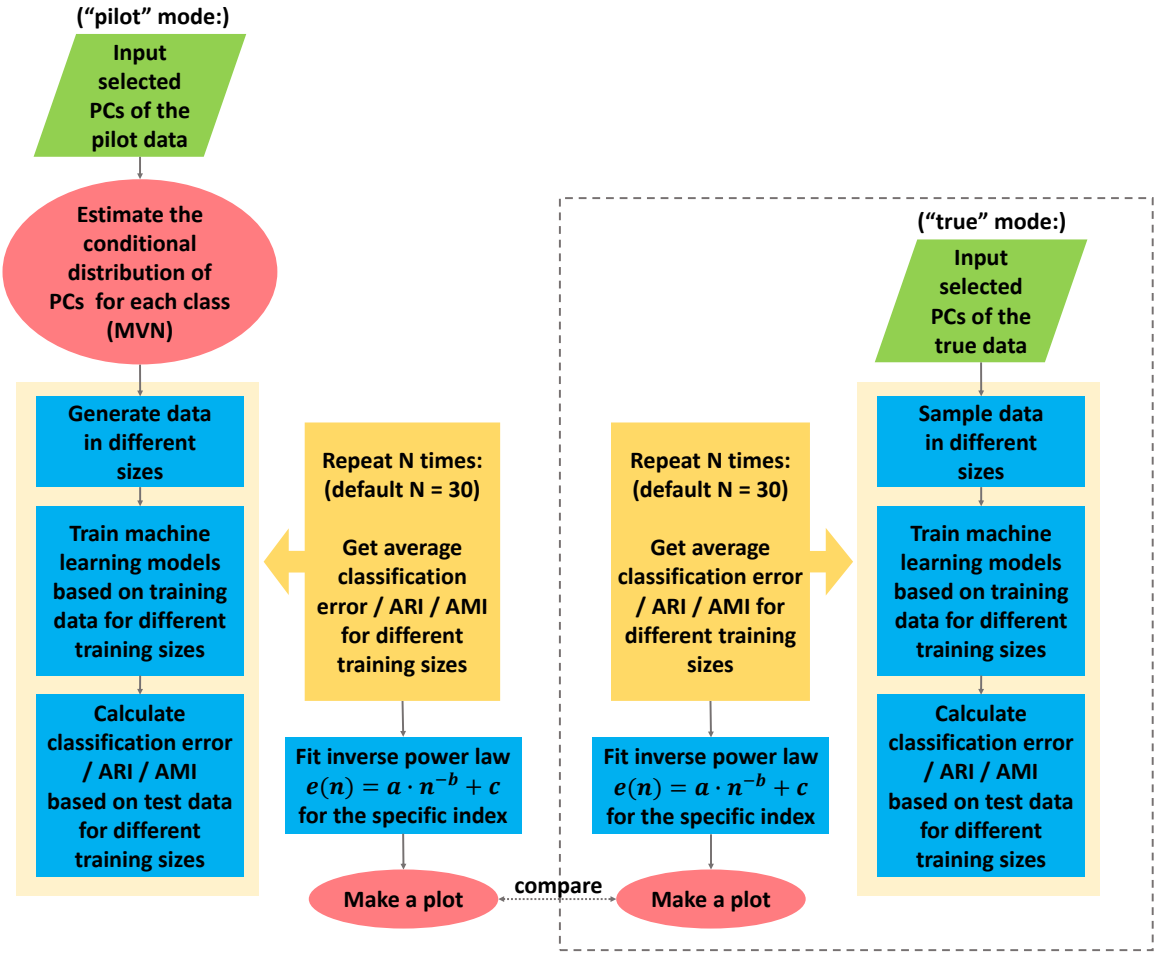


Figure 1: Workflow of the SSD package

Preparations

Before we dive into the main task, we need to load the package and an example dataset for our task. The dataset we use is the **pbmc_68k** dataset from 10x Genomics.

We pre-processed the dataset: In this dataset, *phenoid* is the y label which has 10 classes. We sampled 15 observations from the original dataset for each class and assemble them as the pilot data. we normalize and scale the pilot data at first and then run principal component analysis (PCA) and keep 18 PCs according to *JackStrawPlot* and *ElbowPlot* mentioned in Seurat - Guided Clustering Tutorial. The *JackStrawPlot* and *ElbowPlot* are shown below:

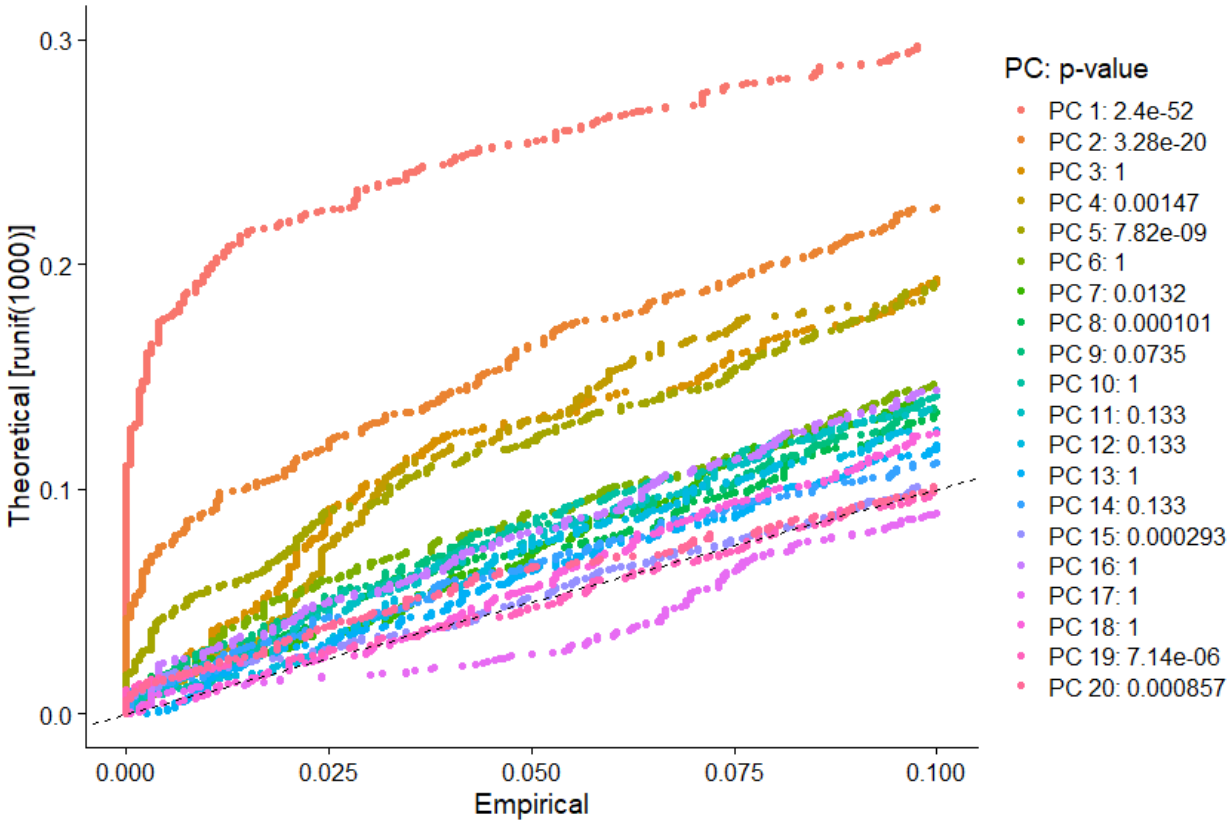


Figure 2: JackStrawPlot of the pilot data

For the whole dataset, we pre-processed it using the same stratigies and keep 24 PCs according to *JackStrawPlot* and *ElbowPlot*.

We put the pro-processed data into our package and we can load them directly.

```
library(SSD)

# load data ------------------------------------------------------------------------
pilot_data <- read.csv(system.file("extdata", "data_pbmc_pilot_18pc.csv", package = "SSD"),row.names=1)
true_data <- read.csv(system.file("extdata", "data_pbmc_24pc.csv", package = "SSD"),row.names=1)

print(table(pilot_data$phenoid))
#>
#>              CD14+_Monocyte                    CD19+_B
#>                          15                         15
```

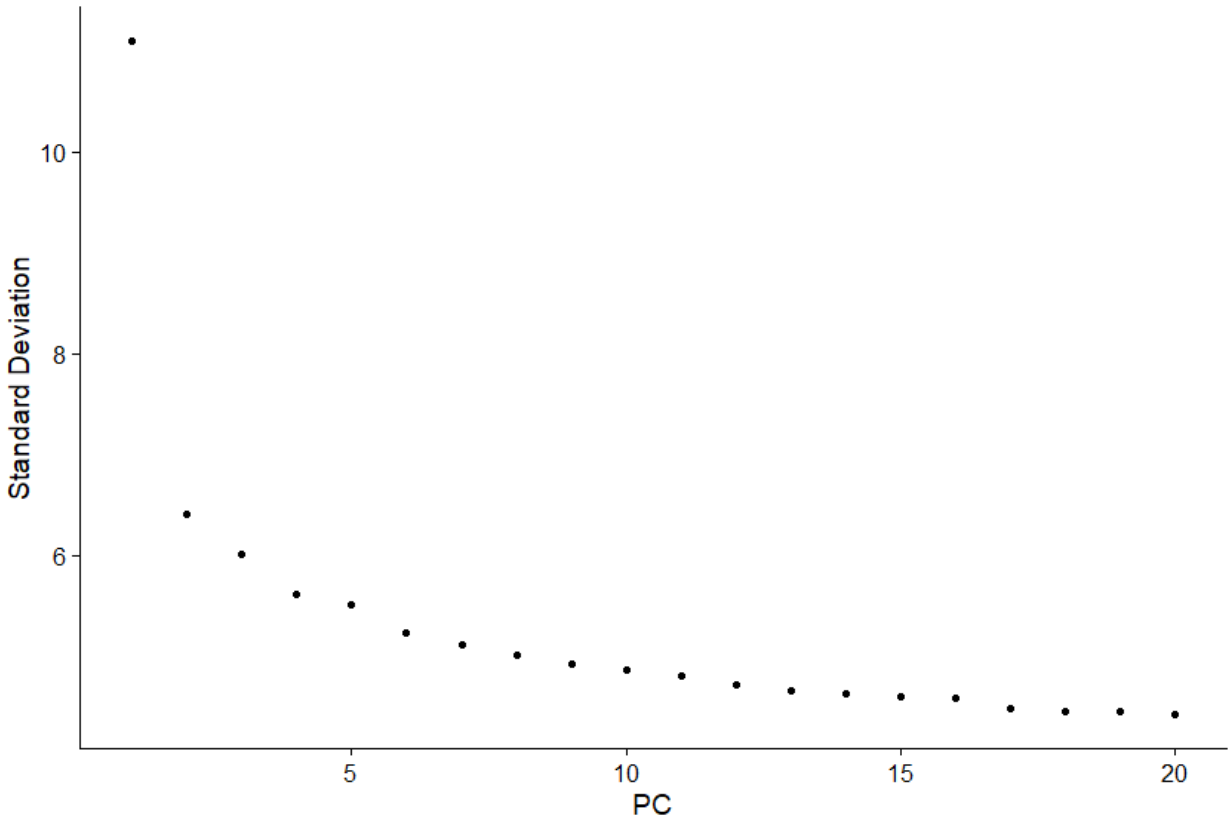


Figure 3: ElbowPlot of the pilot data

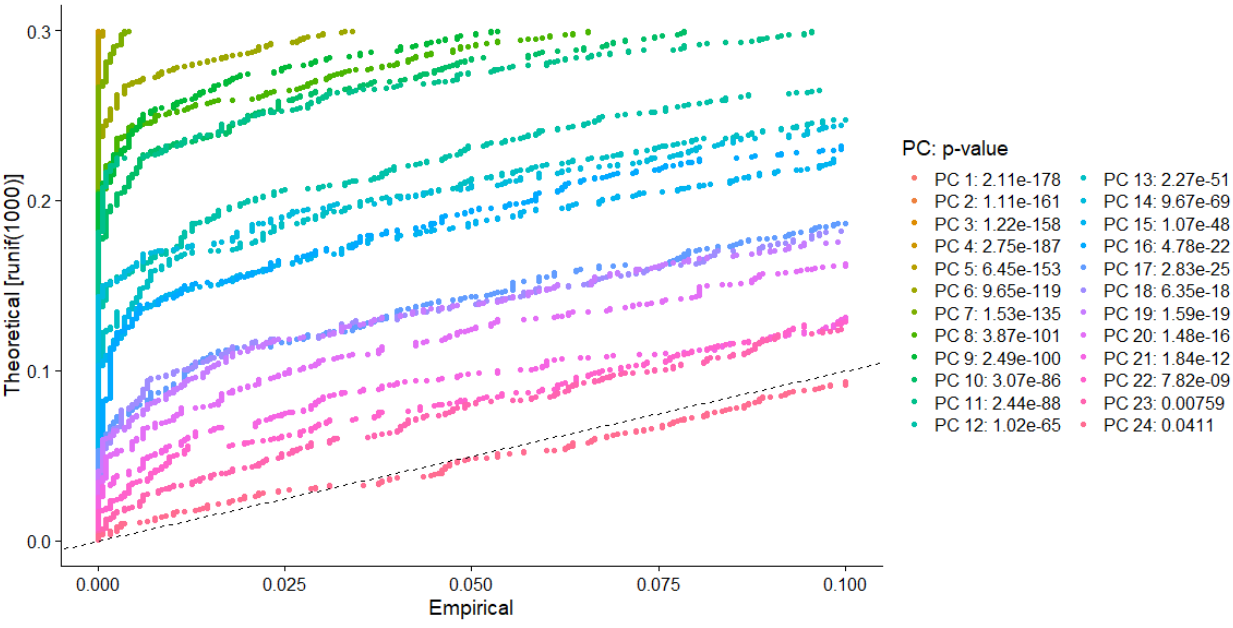


Figure 4: JackStrawPlot of the whole dataset

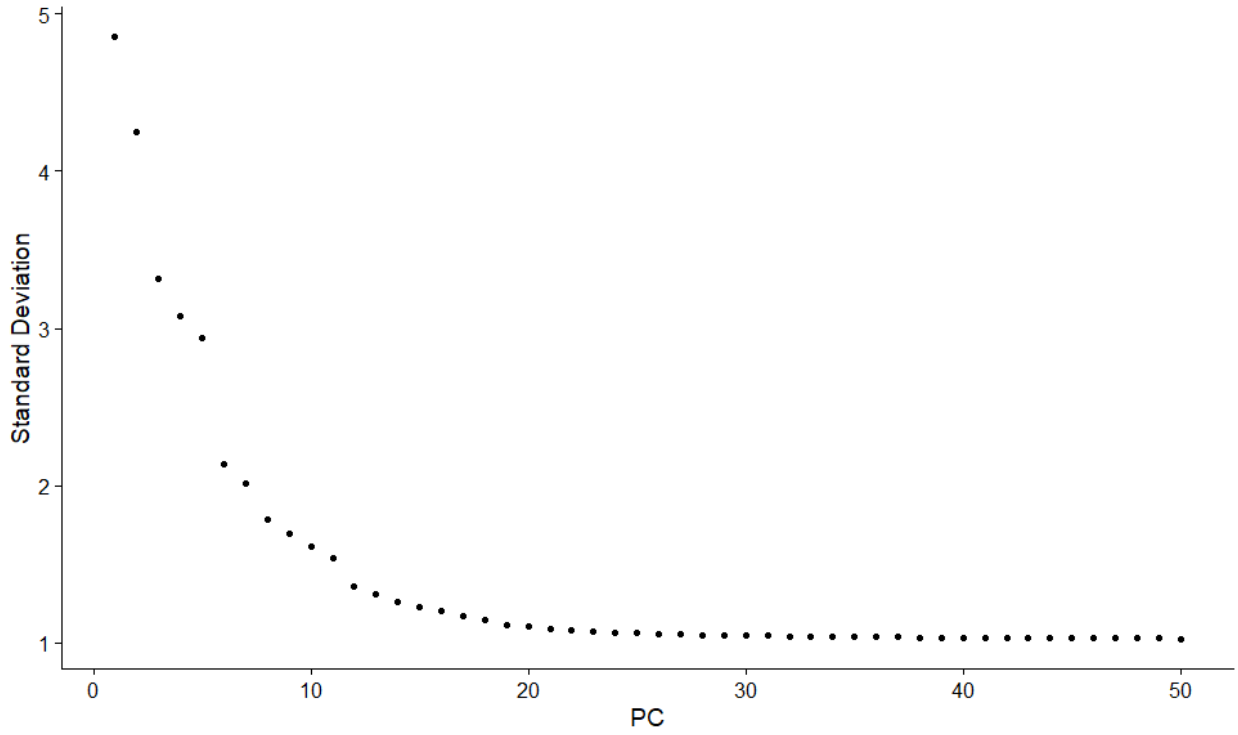


Figure 5: ElbowPlot of the whole dataset

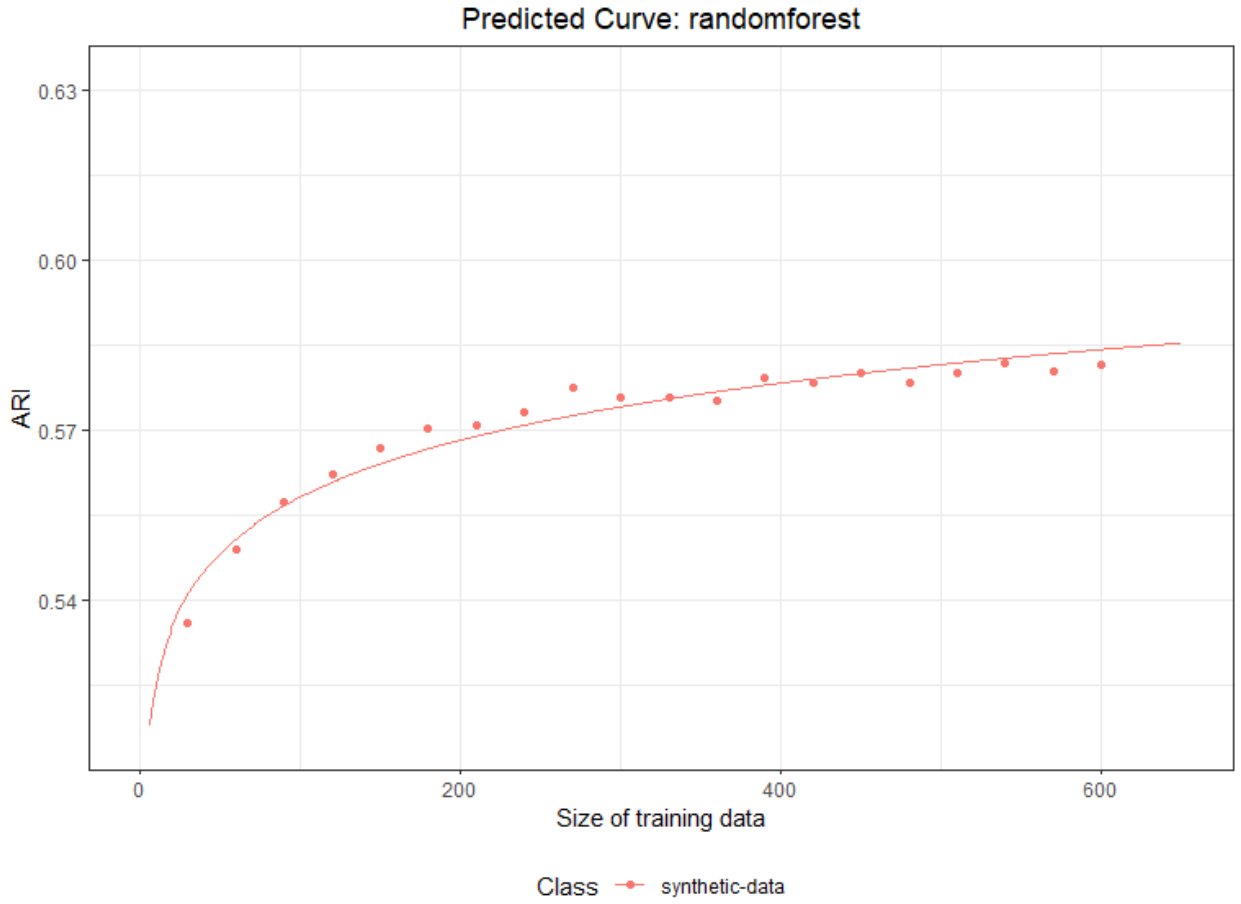
```
#>              CD4+/CD25_T_Reg   CD4+/CD45RA+/CD25-_Naive_T
#>                           15                           15
#>         CD4+/CD45RO+_Memory              CD4+_T_Helper2
#>                           15                           15
#>                     CD56+_NK CD8+/CD45RA+_Naive_Cytotoxic
#>                           15                           15
#>            CD8+_Cytotoxic_T                   Dendritic
#>                           15                           15
print(table(true_data$phenoid))
#>
#>               CD14+_Monocyte                       CD19+_B
#>                         3817                          3306
#>              CD4+/CD25_T_Reg   CD4+/CD45RA+/CD25-_Naive_T
#>                         2812                          3126
#>         CD4+/CD45RO+_Memory              CD4+_T_Helper2
#>                         5859                         11445
#>                     CD56+_NK CD8+/CD45RA+_Naive_Cytotoxic
#>                        14112                         21975
#>            CD8+_Cytotoxic_T                   Dendritic
#>                         1865                           262
```

Task

With pilot data, draw the plot and determine sample size using the built-in model

In the default setting, we use the built-in *random forest* to train the model. The `index` we use is Adjusted Rand Index (ARI). By default, the size of training data for each class is (30, 60, 90, 120, ... , 540, 570, 600) and the size of test data for each class is 300.

```
x_pilot = pilot_data[,-length(pilot_data)]
y_pilot = pilot_data[,length(pilot_data)]

result_pilot = ssd(x_pilot, y_pilot)
```



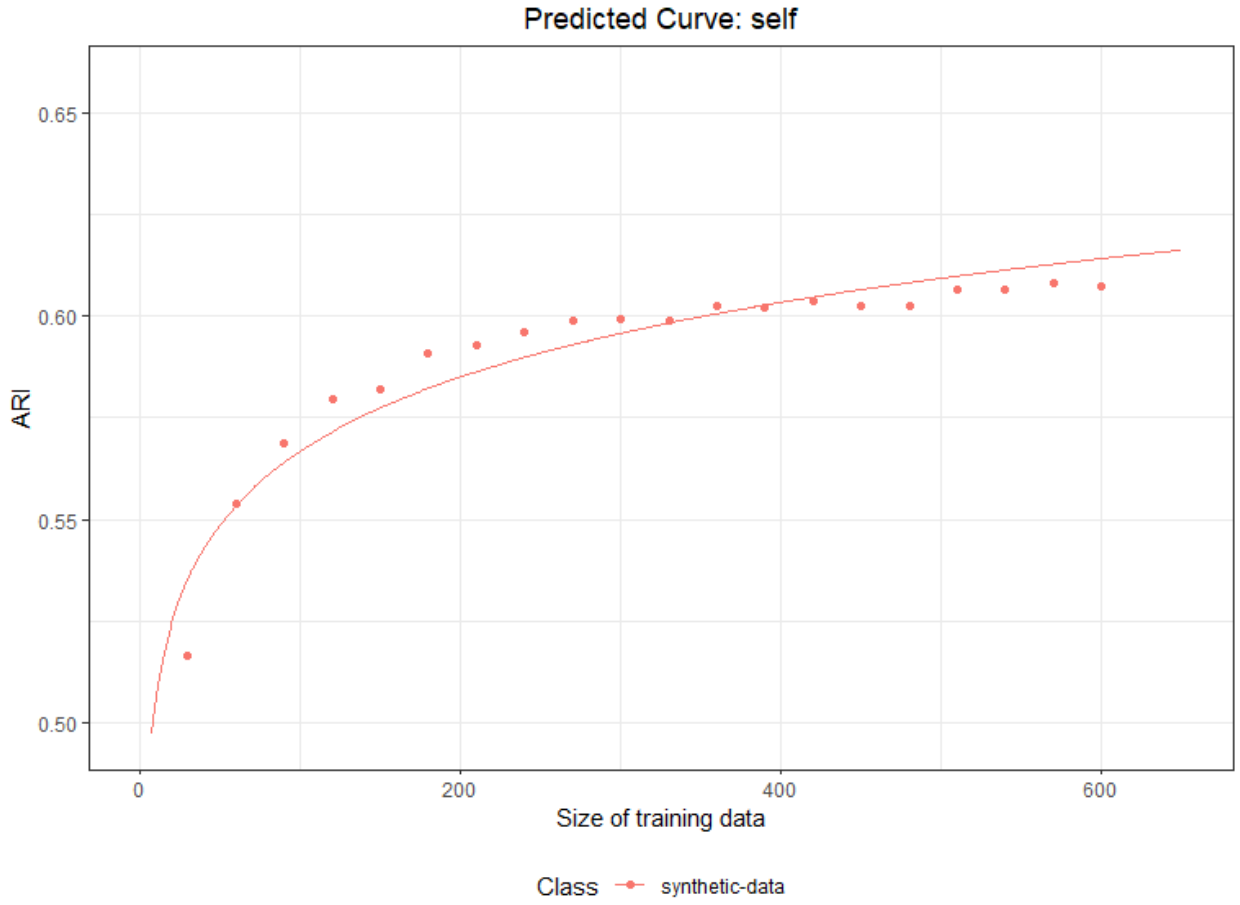
The plot is drawn only based on the pilot data and we could use the plot to determine the sample size if we don't have large enough true. We should focus on the trends of the plots because the results produced by synthetic data are usually better than true data, but the trends are pretty similar.

With pilot data, draw the plot and determine sample size using the self-defined model

If you want to use the model defined by yourself. Then you need to write a "predict_model" function including your model. The function should take *train_data_x* and *train_data_y* as the first two inputs to train the model and then take *test_data_x* as the third input and return the predicted result of *test_data_x*. Then you could set `model` to *self* and set `func` to *predict_model*, and run the model using your self-defined function.

```
library(e1071)

predict_model <- function(train_data_x, train_data_y, test_data_x){
    train_data = data.frame(train_data_x, as.factor(train_data_y))
    names(train_data)[length(train_data)] = "class"
    fit_svm<-svm(class~.,data=train_data,probability=TRUE)
    pred <- predict(fit_svm, test_data_x)
    return(pred)
}
```

```
result_pilot_self = ssd(x_pilot, y_pilot, model="self", func=predict_model)
```



You could use the following code to check the function you defined. The result has to be the predicted value of *test_data_x*.

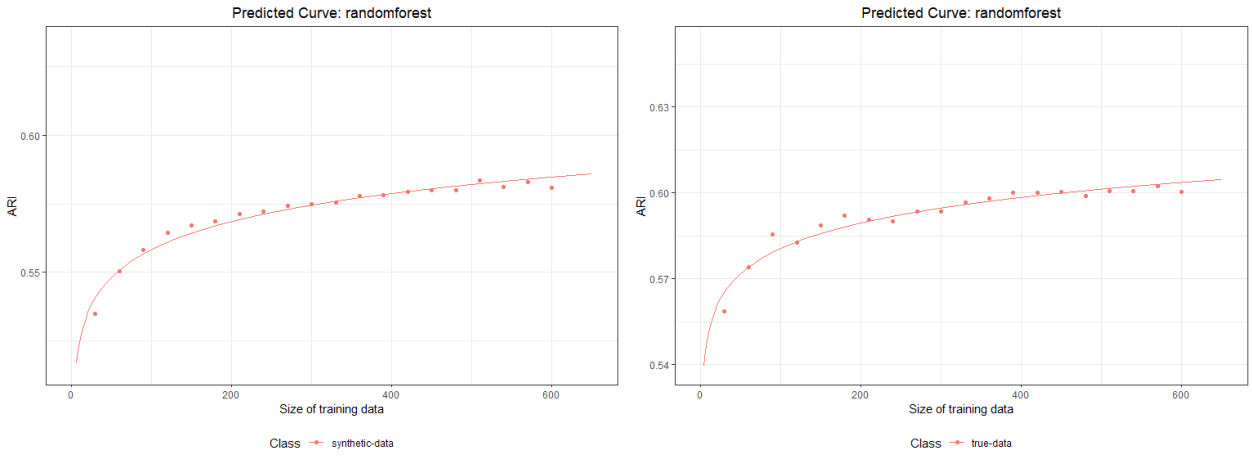
```
num_class=10
n_train=60
n_test=200

for(i in 1:num_class){
  class_i_ids = which(true_data$phenoid == names(table(true_data$phenoid))[i])

  train_test_i_ids = sample(class_i_ids, (n_train+n_test))
  train_i_data = true_data[train_test_i_ids[1:n_train],]
  test_i_data = true_data[train_test_i_ids[(n_train+1):(n_train+n_test)],]
```

```
  if(i == 1){
    train_data = train_i_data
    test_data = test_i_data
  }else{
    train_data = rbind(train_data, train_i_data)
    test_data = rbind(test_data, test_i_data)
  }
}

train_data_x = train_data[,-length(test_data)]
train_data_y = train_data$phenoid
test_data_x = test_data[,-length(test_data)]

result = predict_model(train_data_x, train_data_y, test_data_x)
```

With pilot data and large true data, draw the plot and compare the result

If we have large enough true data and try to compare the plot drawn based on pilot data and the plot drawn based on true data, we could change `mode` to *true* and compare the results.

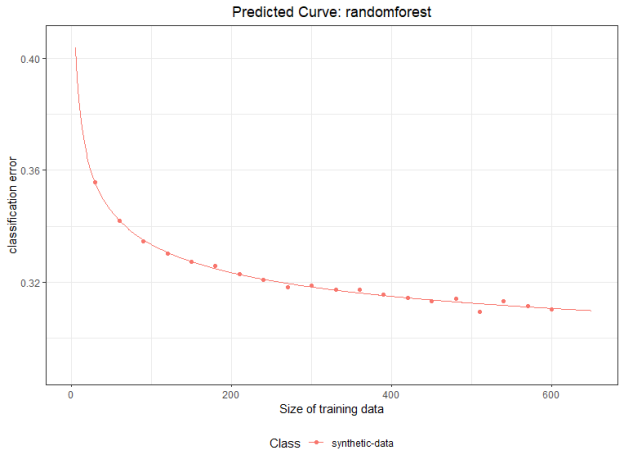
```
# prepare large true data
x_true = data[,-length(data)]
y_true = data[,length(data)]

# run the model using the previous pilot data, index using 'ARI'
result_pilot_11 = ssd(x_pilot, y_pilot,model = "randomforest",index = "ARI",n_train_list=seq(from=30, to
# run the model using the true data, index using 'ARI'
result_true_11 = ssd(x_true , y_true ,model = "randomforest",index = "ARI",n_train_list=seq(from=30, to=
```

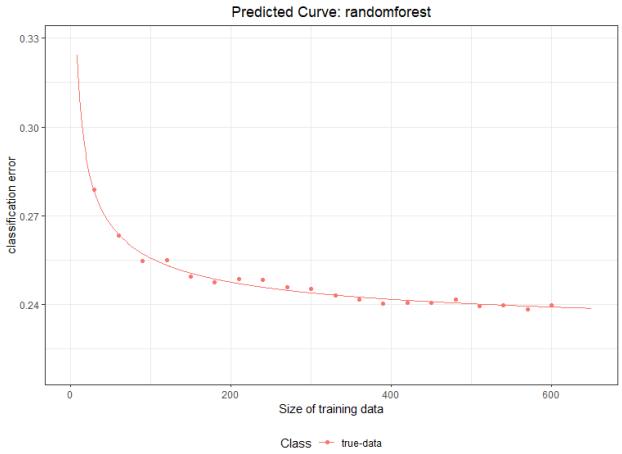


From the results above,even though the values of ARI are different, we can see that the two plots have almost the same trend, which could help us determine the sample size.

We could also try when `index` is *classification error* or *AMI* for this dataset.

```
# run the model using the previous pilot data, index using 'classification error'
result_pilot_12 = ssd(x_pilot, y_pilot,model = "randomforest",index = "classification error",n_train_lis
# run the model using the true data, index using 'classification error'
result_true_12 = ssd(x_true , y_true ,model = "randomforest",index = "classification error",n_train_list
```






```
# prepare large true data
x_true = data[,-length(data)]
y_true = data[,length(data)]

# run the model using the previous pilot data, index using 'AMI'
result_pilot_13 = ssd(x_pilot, y_pilot,model = "randomforest",index = "AMI",n_train_list=seq(from=30, t
# run the model using the true data, index using 'AMI'
result_true_13 = ssd(x_true , y_true ,model = "randomforest",index = "AMI",n_train_list=seq(from=30, to
```