## SSD

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### 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.

## **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 **pmbc\_68k** dataset from 10x Genomics, which consists of >68,000 single cells. With all 32,738 genes.

```
library(SSD)
# load data ------
data_pmbc <- read.csv(system.file("extdata", "data_pmbc_24pc.csv", package = "SSD"),row.names=1)
data = data_pmbc</pre>
```

We pre-processed the dataset: we normalize and scale the date at first and then run principal component analysis (PCA) and keep 24 PCs according to JackStrawPlot and ElbowPlot mentioned in Seurat - Guided Clustering Tutorial. The JackStrawPlot and ElbowPlot are shown below:

### Task

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

The selected PCs of the pilot data is extract from the dataset imported before:

```
### use pilot data:
p = 15
num_class = length(table(data$phenoid))
num_PC = length(colnames(data))-1
for(i in 1:num_class){
    class_i_ids = which(data$phenoid == names(table(data$phenoid))[i])
    pilot_i_ids = sample(class_i_ids, p)
    pilot_i_data = data[pilot_i_ids,]
    if(i == 1){
        pilot_data = pilot_i_data
    }else{
        pilot_data = rbind(pilot_data, pilot_i_data)
```

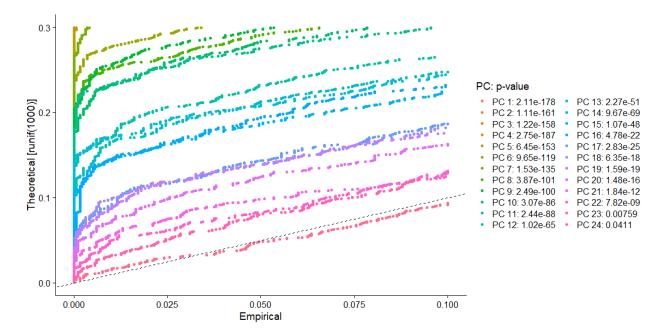


Figure 1: JackStrawPlot

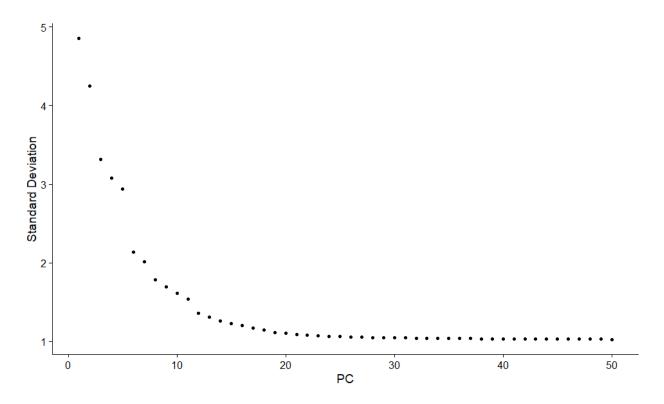
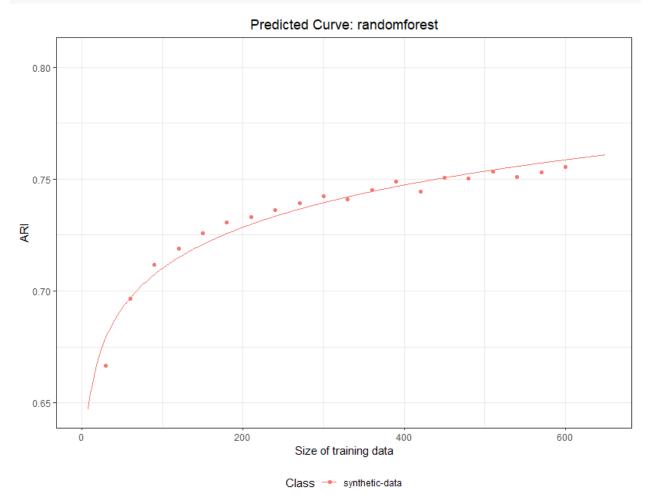


Figure 2: ElbowPlot

```
}
}
x_pilot = pilot_data[,-length(pilot_data)]
y_pilot = pilot_data[,length(pilot_data)]
print(table(pilot_data$phenoid))
#>
#>
                  CD14+_Monocyte
                                                         CD19+_B
#>
                               15
                                                              15
#>
                 CD4+/CD25_T_Reg
                                    CD4+/CD45RA+/CD25-Naive_T
#>
#>
             CD4+/CD45RO+_Memory
                                                 CD4+_T_Helper2
#>
#>
                        CD56+_NK CD8+/CD45RA+_Naive_Cytotoxic
#>
                                                              15
#>
                \mathit{CD8+\_Cytotoxic\_T}
                                                      Dendritic
```

In this dataset, *phenoid* is the y label which has 10 classes. In the selected PCs of the pilot data, each class has 15 observations. In the default setting, we use the built-in *random forest* to train the model. The **index** we use is Adjusted Rand Index (ARI).

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.

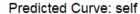
# With selected PCs of the pilot data, draw the plot and determine sample size using the self-defined model

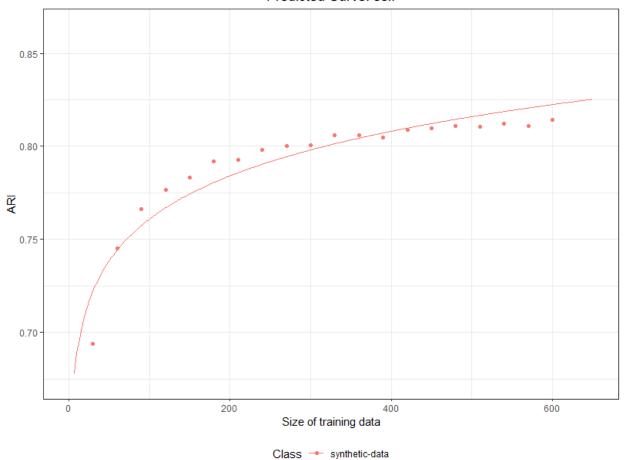
If you want to use the model defined by yourself. Then you need to write a "predict\_model" function including your model. The function should take  $train\_data\_x$  and  $train\_data\_y$  as the first two inputs to train the model and then take  $test\_data\_x$  as the third input and return the predicted 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)</pre>
```





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(data$phenoid == names(table(data$phenoid))[i])

    train_test_i_ids = sample(class_i_ids, (n_train+n_test))
    train_i_data = data[train_test_i_ids[1:n_train],]
    test_i_data = 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, t
# 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
                 Predicted Curve: randomforest
                                                                   Predicted Curve: randomforest
 0.80
                                                    0.63
 0.75
                                                  0.60
 0.70
                                                    0.57
```

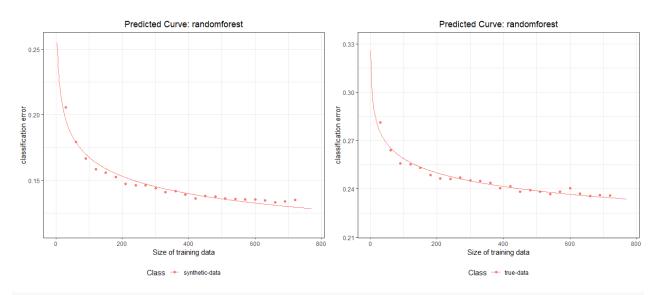
From the results above, even though the values of ARI are different, we can see that the two plots have almost the same trend, which could help us determine the sample size.

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

Size of training data Class - synthetic-data

```
# 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_li
# 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_lis
```

Size of training data



```
# 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
```

