Clustering

December 10, 2021

[238]:
```python
# Import packages
import pyreadr
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import timeit


# Pacakges for dimensional reduction procedure
from sklearn.decomposition import PCA
from ZIFA import ZIFA
from ZIFA import block_ZIFA

# Pacakges for different clustering method
# Hierarchical Clustering
from sklearn.cluster import AgglomerativeClustering
# K Means
from sklearn.cluster import KMeans
# KNN
from sklearn.neighbors import NearestNeighbors
# Gaussian Mixture Model
from sklearn.mixture import GaussianMixture

from sklearn.metrics import accuracy_score


# Set random seed
import random
random.seed(25)
```

0.1 Data Import and Pre-process

[19]:
```python
# Import data from rds file
count = pyreadr.read_r('../Data/Tcell_5type_filtered.rds')
count = count[None]
label = pyreadr.read_r('../Data/Tcell_5type_filtered_labels.rds')
label = label[None]
```

```
[31]: # Extract the read count array
count_array = count.to_numpy()
```

```
[151]: count_array
```

```
[151]: array([[0., 1., 0., …, 0., 0., 0.],
              [0., 0., 0., …, 0., 0., 0.],
              [0., 0., 0., …, 0., 0., 1.],
              …,
              [0., 0., 0., …, 0., 0., 0.],
              [0., 2., 1., …, 0., 1., 2.],
              [0., 0., 0., …, 0., 0., 0.]])
```

```
[195]: # Change labels to integer
new_cluster = dict(zip(list(set(label['Group'])), list(range(5))))
new_label = []
for k in range(len(list(label['Group']))):
    old_label = list(label['Group'])[k]
    new_label.append(new_cluster[old_label])
```

0.2 PCA

```
[35]: # Implement PCA
pca = PCA(n_components=50)
count_array_pca = pca.fit_transform(np.transpose(count_array))
```

```
[36]: # Check the dim of the array after PCA transformation
count_array_pca.shape
```

```
[36]: (2989, 50)
```

0.3 ZIFA

```
[42]: # compute the log count array by log2(1 + count_data)
log_count_array = np.log(1 + count_array)
```

```
[43]: count_array_ZIFA, model_params = block_ZIFA.fitModel(np.
 ↪transpose(log_count_array), 50, p0_thresh=0.9)
```

```
Filtering out all genes which are zero in more than 90.0% of samples. To change
this, change p0_thresh.
Number of blocks has been set to 6
Running block zero-inflated factor analysis with N = 2989, D = 3385, K = 50,
n_blocks = 6
Block sizes [564, 564, 564, 564, 564, 565]
```

```
[45]: # Store the array to avoid multiple running and save time
```

```
# Since it takes more than 40 mins to run this procedure, I save the result to␣
↪a csv file for convenience.
pd.DataFrame(count_array_ZIFA).to_csv("count_array_ZIFA.csv")
```

[44]:
```
# Check the dim of the array after ZIFA transformation
count_array_ZIFA.shape
```

[44]: (2989, 50)

0.4 Hierarchical Clustering

[239]:
```
start = timeit.default_timer()

# Hierarchical Clustering on PCA array
hc_pca = AgglomerativeClustering(n_clusters=5).fit(count_array_pca)
# Obtain Predicted labels
hc_pca_pred = hc_pca.labels_

stop = timeit.default_timer()
# Record Run time
hc_pca_time = stop - start
```

[241]:
```
start = timeit.default_timer()

# Hierarchical Clustering on ZIFA array
hc_ZIFA = AgglomerativeClustering(n_clusters=5).fit(count_array_ZIFA)
# Obtain Predicted labels
hc_ZIFA_pred = hc_ZIFA.labels_

stop = timeit.default_timer()
# Record Run time
hc_ZIFA_time = stop - start
```

0.5 K Means

[242]:
```
start = timeit.default_timer()

# K Means on PCA array
kmeans_pca = KMeans(n_clusters=5, random_state=0).fit(count_array_pca)
# Obtain Predicted labels
kmeans_pca_pred = kmeans_pca.labels_

stop = timeit.default_timer()
# Record Run time
kmeans_pca_time = stop - start
```

[243]:
```
start = timeit.default_timer()

# K Means on ZIFA array
kmeans_ZIFA = KMeans(n_clusters=5, random_state=0).fit(count_array_ZIFA)
# Obtain Predicted labels
kmeans_ZIFA_pred = kmeans_ZIFA.labels_

stop = timeit.default_timer()
# Record Run time
kmeans_ZIFA_time = stop - start
```

0.6 KNN

[119]:
```
def gather_neighbors(tree):
    """
    This function is used to gather neigbors which is the output from TreeBall␣
 ↪algorithm and
    make them in the same cluster.
    """
    tree_list = list(tree)
    cluster = []
    i = len(tree_list)
    while(len(tree_list) > 0):
        cluster.append(np.array(tree_list[-1]))
        n_old = 0
        n_new = len(tree_list)
        while (n_old != n_new):
            # When no update in tree_list, which means that the union of␣
 ↪neighborhoods based on the initial
            # neighborhood is complete. Then break the inner while loop and␣
 ↪initialize with a new neighborhood.
            for j in range(n_new - 1, -1, -1):
                # Use for loop to determine if two neighborhoods share same␣
 ↪data points, union them.
                if len(set(tree_list[j]).intersection(set(cluster[-1]))) > 0:
                    cluster[-1] = np.array(list(set(tree_list[j]).
 ↪union(set(cluster[-1]))))
                    tree_list.pop(j)
            n_old = n_new
            n_new = len(tree_list)

    return cluster
```

[245]:
```
start = timeit.default_timer()

# KNN on PCA array
neigh = NearestNeighbors(n_neighbors=3)
```

```
neigh.fit(count_array_pca)
a = neigh.kneighbors(count_array_pca, return_distance=False)
cluster_pca = gather_neighbors(a)
len(cluster_pca)
```

[245]: 2

[246]:
```
# Obtain Predicted labels
knn_pca = np.zeros(count_array_pca.shape[0])
for i in range(len(cluster_pca)):
    for j in cluster_pca[i]:
        knn_pca[j] = i
knn_pca

stop = timeit.default_timer()
# Record Run time
knn_pca_time = stop - start
```

[247]:
```
start = timeit.default_timer()

# KNN on PCA array
neigh = NearestNeighbors(n_neighbors=3)
neigh.fit(count_array_ZIFA)
b = neigh.kneighbors(count_array_ZIFA, return_distance=False)
cluster_ZIFA = gather_neighbors(b)
len(cluster_ZIFA)
```

[247]: 6

[248]:
```
# Obtain Predicted labels
knn_ZIFA = np.zeros(count_array_ZIFA.shape[0])
for i in range(len(cluster_ZIFA)):
    for j in cluster_ZIFA[i]:
        knn_ZIFA[j] = i

stop = timeit.default_timer()
# Record Run time
knn_ZIFA_time = stop - start
```

0.7 Gaussian Mixure Model

[252]:
```
start = timeit.default_timer()

# Gaussian Mixure Model on PCA array
gm_pca = GaussianMixture(n_components=5, random_state=0).fit(count_array_pca)
# Obtain Predicted labels
gm_pca_pred = gm_pca.predict(count_array_pca)
```

```python

stop = timeit.default_timer()
# Record Run time
gm_pca_time = stop - start
```

[253]:
```python
start = timeit.default_timer()

# Gaussian Mixure Model on ZIFA array
gm_ZIFA = GaussianMixture(n_components=5, random_state=0).fit(count_array_ZIFA)
# Obtain Predicted labels
gm_ZIFA_pred = gm_ZIFA.predict(count_array_ZIFA)

stop = timeit.default_timer()
# Record Run time
gm_ZIFA_time = stop - start
```

0.8 Compute Accuracy and Generate Plots

[211]:
```python
def assign_label(pred, label):
    """
    This function is used to assign label of clusters in pred by the majority␣
↪of cells in it.
    """
    new_cluster = []
    for i in range(len(set(pred))):
        indexes = [j for j,x in enumerate(pred) if x == i]
        counts = np.bincount(label[indexes])
        new_cluster.append(np.argmax(counts))
    new_label = []
    for k in range(len(pred)):
        old_label = pred[k]
        new_label.append(new_cluster[old_label])
    return new_label
```

[218]:
```python
# Assign new labels to clusters using hierarchical clustering on PCA data
hc_pca_pred2 = assign_label(np.array(hc_pca_pred), np.array(new_label))
# accuracy for test data using hierarchical clustering on PCA data
hc_pca_acc = accuracy_score(np.array(new_label), np.array(hc_pca_pred2))
```

[222]:
```python
# Assign new labels to clusters using hierarchical clustering on ZIFA data
hc_ZIFA_pred2 = assign_label(np.array(hc_ZIFA_pred), np.array(new_label))
# accuracy for test data using hierarchical clustering on ZIFA data
hc_ZIFA_acc = accuracy_score(np.array(new_label), np.array(hc_ZIFA_pred2))
```

[223]:
```python
# Assign new labels to clusters using K means on PCA data
kmeans_pca_pred2 = assign_label(np.array(kmeans_pca_pred), np.array(new_label))
# accuracy for test data using K means on PCA data
```

```
kmeans_pca_acc = accuracy_score(np.array(new_label), np.array(kmeans_pca_pred2))
```

[224]:
```
# Assign new labels to clusters using K means on ZIFA data
kmeans_ZIFA_pred2 = assign_label(np.array(kmeans_ZIFA_pred), np.
 ↪array(new_label))
# accuracy for test data using K means on ZIFA data
kmeans_ZIFA_acc = accuracy_score(np.array(new_label), np.
 ↪array(kmeans_ZIFA_pred2))
```

[226]:
```
# Assign new labels to clusters using KNN on PCA data
knn_pca2 = assign_label(np.array(knn_pca).astype('int8'), np.array(new_label))
# accuracy for test data using KNN on PCA data
knn_pca_acc = accuracy_score(np.array(new_label), np.array(knn_pca2).
 ↪astype('int8'))
```

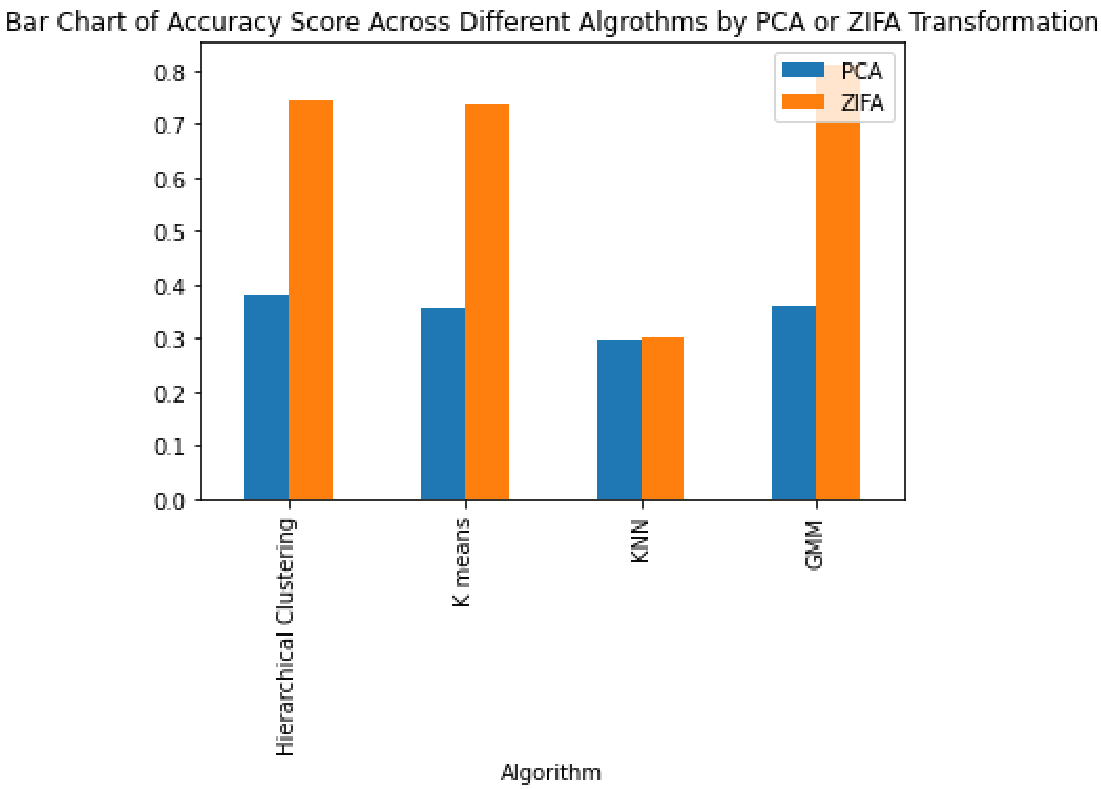
[227]:
```
# Assign new labels to clusters using KNN on ZIFA data
knn_ZIFA2 = assign_label(np.array(knn_ZIFA).astype('int8'), np.array(new_label))
# accuracy for test data using KNN on ZIFA data
knn_ZIFA_acc = accuracy_score(np.array(new_label), np.array(knn_ZIFA2).
 ↪astype('int8'))
```

[231]:
```
# Assign new labels to clusters using GMM on PCA data
gm_pca_pred2 = assign_label(np.array(gm_pca_pred), np.array(new_label))
# accuracy for test data using GMM on PCA data
gm_pca_acc = accuracy_score(np.array(new_label), np.array(gm_pca_pred2))
```

[232]:
```
# Assign new labels to clusters using GMM on ZIFA data
gm_ZIFA_pred2 = assign_label(np.array(gm_ZIFA_pred), np.array(new_label))
# accuracy for test data using GMM on ZIFA data
gm_ZIFA_acc = accuracy_score(np.array(new_label), np.array(gm_ZIFA_pred2))
```

[236]:
```
# Generate Dataframe for plotting
df = pd.DataFrame([['Hierarchical Clustering', hc_pca_acc, hc_ZIFA_acc],
                   ['K means', kmeans_pca_acc, kmeans_ZIFA_acc],
                   ['KNN', knn_pca_acc, knn_ZIFA_acc],
                   ['GMM', gm_pca_acc, gm_ZIFA_acc]],
                  columns=['Algorithm', 'PCA', 'ZIFA'])
# Plot grouped bar chart for Figure 1
df.plot(x='Algorithm',
        kind='bar',
        stacked=False,
        title='Bar Chart of Accuracy Score Across Different Algrothms by PCA or␣
 ↪ZIFA Transformation')
```

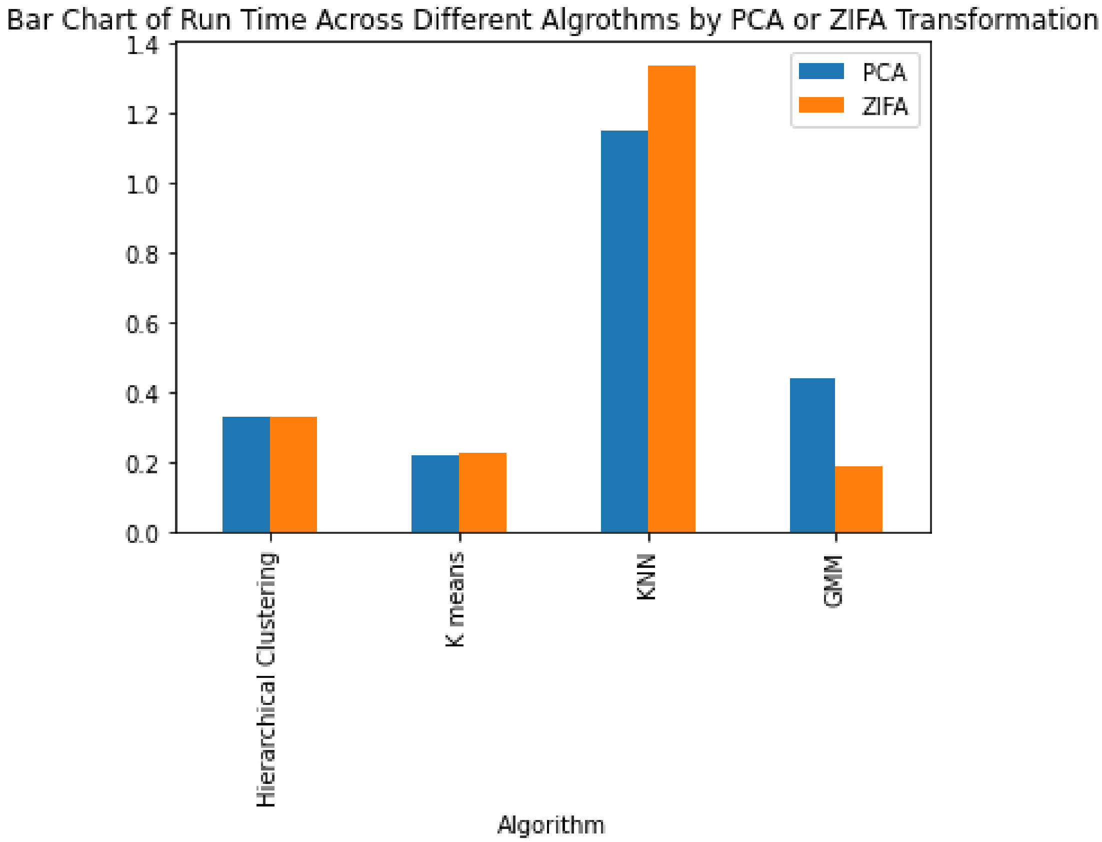
[236]:
```
<AxesSubplot:title={'center':'Bar Chart of Accuracy Score Across Different
Algrothms by PCA or ZIFA Transformation'}, xlabel='Algorithm'>
```



[254]:
```python
# Generate Dataframe for plotting
df = pd.DataFrame([['Hierarchical Clustering', hc_pca_time, hc_ZIFA_time],
                   ['K means', kmeans_pca_time, kmeans_ZIFA_time],
                   ['KNN', knn_pca_time, knn_ZIFA_time],
                   ['GMM', gm_pca_time, gm_ZIFA_time]],
                  columns=['Algorithm', 'PCA', 'ZIFA'])

# Plot grouped bar chart for Figure 2
df.plot(x='Algorithm',
        kind='bar',
        stacked=False,
        title='Bar Chart of Run Time Across Different Algrothms by PCA or ZIFA␣
 ↪Transformation')
```

[254]:
```
<AxesSubplot:title={'center':'Bar Chart of Run Time Across Different Algrothms
by PCA or ZIFA Transformation'}, xlabel='Algorithm'>
```


Bar Chart of Run Time Across Different Algrothms by PCA or ZIFA Transformation
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
PCA
ZIFA
Hierarchical Clustering
K means
KNN
GMM
Algorithm

```
[ ]:
```