Programming 3

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Import Packages

In [39]:
```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.cluster import KMeans
from sklearn import datasets
from sklearn.preprocessing import normalize
from copy import deepcopy

iris = datasets.load_iris()
#X = iris.data
X = norm(iris.data)
y = iris.target
```

KMeans.py

In [143]:
```
# kmeans.py

import numpy as np
from collections import Counter
from sklearn.metrics import f1_score, normalized_mutual_info_score

THRESHOLD = 1e-5

def norm(x):
    """
    >>> Function you should not touch
    """
    max_val = np.max(x, axis=0)
    x = x / max_val
    return x


def rand_center(data, k):
    """
    >>> Function you need to write
```

```python
    >>> Select "k" random points from "data" as the initial centroids.
    """
    n_samples, n_features = np.shape(data)
    centroids = np.zeros((k, n_features))
    for i in range(k):
        centroid = data[np.random.choice(range(n_samples))]
        centroids[i] = centroid
    print(">>> initial centroids")
    print(centroids)
    return centroids


def converged(centroids1, centroids2):
    """
    >>> Function you need to write
    >>> check whether centroids1==centroids
    >>> add proper code to handle infinite loop if it never converges
    """
    diff = np.sum(np.abs(np.sum(centroids1 - centroids2, axis=1)), axis=0)
    if np.equal(centroids1, centroids2).all():
        return True
    elif diff < THRESHOLD:
        return True
    else:
        return False


def euclidean_dist(x1, x2):
    return np.sqrt(np.sum(np.square(x1 - x2), axis=1))


def closest_centroid(val, centroids):
    return np.argmin(np.sqrt(np.sum(np.square(val - centroids), axis=1)))


def update_centroids(data, centroids, k=3):
    """
    >>> Function you need to write
    >>> Assign each data point to its nearest centroid based on the Euclidean distance
    >>> Update the cluster centroid to the mean of all the points assigned to that clu
    """
    n_samples = np.shape(data)[0]
    n_features = np.shape(data)[1]
    clusters = [[] for _ in range(k)]
    labels = np.zeros((n_samples))

    for idx, val in enumerate(data):
        val_label = closest_centroid(val, centroids)
```

```
        clusters[val_label].append(val)
        labels[idx] = val_label
    centroids = np.zeros((k, n_features))
    for idx, cluster_val in enumerate(clusters):
        centroid = np.mean(cluster_val, axis=0)
        centroids[idx] = centroid
    return centroids, labels


def kmeans(data, k=3):
    """
    >>> Function you should not touch
    """
    # step 1:
    centroids = rand_center(data, k)
    converge = False
    iteration = 0
    while not converge:
        old_centroids = np.copy(centroids)
        # step 2 & 3
        centroids, label = update_centroids(data, old_centroids)
        # step 4
        converge = converged(old_centroids, centroids)
        iteration += 1
    print('number of iterations to converge: ', iteration)
    print(">>> final centroids")
    print(centroids)
    return centroids, label


def evaluation(predict, ground_truth):
    """
    >>> use F1 and NMI in scikit-learn for evaluation
    """
    f1 = f1_score(y_true=ground_truth, y_pred=predict, average='weighted')
    nmi = normalized_mutual_info_score(labels_true=ground_truth, labels_pred=predict)
    return f1, nmi


def gini(predict, ground_truth):
    """
    >>> use the ground truth to do majority vote to assign a flower type for each clus
    >>> accordingly calculate the probability of missclassifiction and correct classif
    >>> finally, calculate gini using the calculated probabilities
    """
    labels = np.unique(ground_truth)
    num_labels = len(labels)
    cluster_p, cluster_g = [0 for _ in range(num_labels)],
```

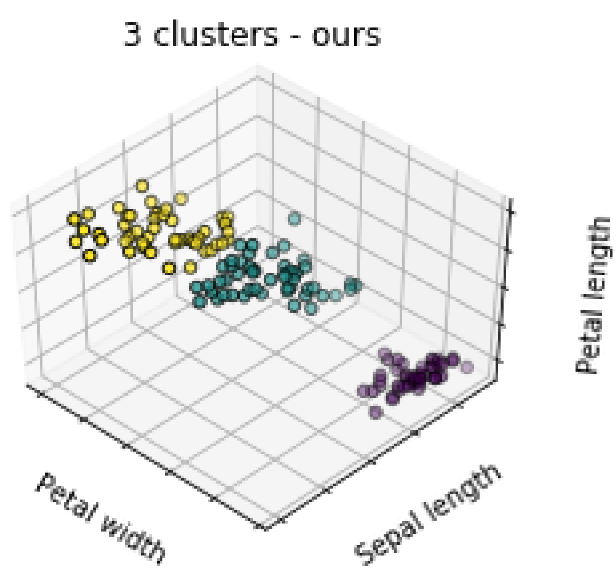
```
                              [0 for _ in range(num_labels)]
    gini_index = 0
    for i in labels:
        cluster_p[i], cluster_g[i] = np.array(predict[predict==i].shape[0]),
                                     np.array(ground_truth[ground_truth==i].shape[0])
        if cluster_p[i]<cluster_g[i]:
            correct_prob = cluster_p[i]/cluster_g[i]
            incorrect_prob = (cluster_g[i] - cluster_p[i])/cluster_g[i]
            gini_index += 1 - np.square(correct_prob) - np.square(incorrect_prob)
    gini_index /= num_labels
    print('Gini Index :', gini_index)
    return gini_index


def SSE(centroids, data):
    """
    >>> Calculate the sum of squared errors for each cluster
    """
    clusters = [[] for _ in centroids]
    num_centroids = len(centroids)
    for val in data:
        clusters[closest_centroid(val, centroids)].append(val)
    sse_each_cluster = [np.sum(np.sum(np.square(clusters[i] - centroids[i]), axis=1))
    print('SSE_each_cluster: ', sse_each_cluster)
    return sse_each_cluster


def plot_result(model):
    fig = plt.figure(1, figsize=(4, 3))
    ax = Axes3D(fig, rect=[0, 0, .95, 1], elev=48, azim=134)
    ax.scatter(X[:, 3], X[:, 0], X[:, 2],
               c=label.astype(np.float), edgecolor='k')
    ax.w_xaxis.set_ticklabels([])
    ax.w_yaxis.set_ticklabels([])
    ax.w_zaxis.set_ticklabels([])
    ax.set_xlabel('Petal width')
    ax.set_ylabel('Sepal length')
    ax.set_zlabel('Petal length')
    ax.set_title('3 clusters - {}'.format(model))
    ax.dist = 12

    plt.show()
```

Q1

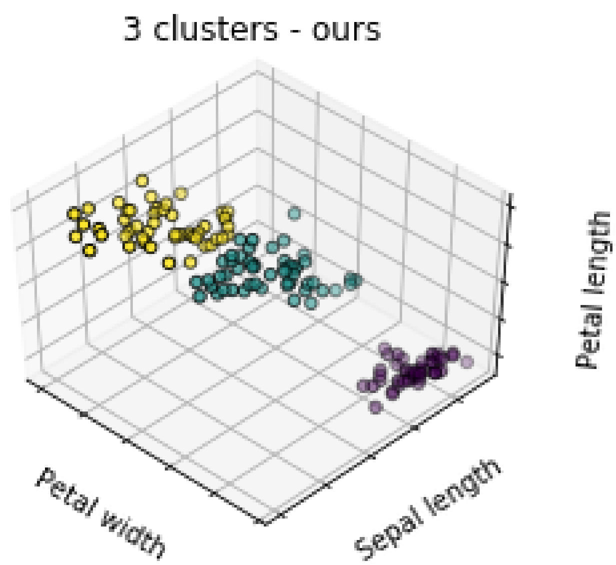
1. Run your own k-Means multiple times (at least 10 times) to find the best three clustering based on SSE (sum of squared errors) and compare it with the result obtained from k-Means in scikit-learn for comparison. Show both clustering results using matplotlib.

```
In [145]: for _ in range(10):
              # this is the function you are supposed to implement in kmeans.py
              centroids, label = kmeans(X,3)
              # this is the function you are supposed to implement in kmeans.py
              evaluation(label, y)
              gini(label, y)
              SSE(centroids, X)
              plot_result('ours')
```

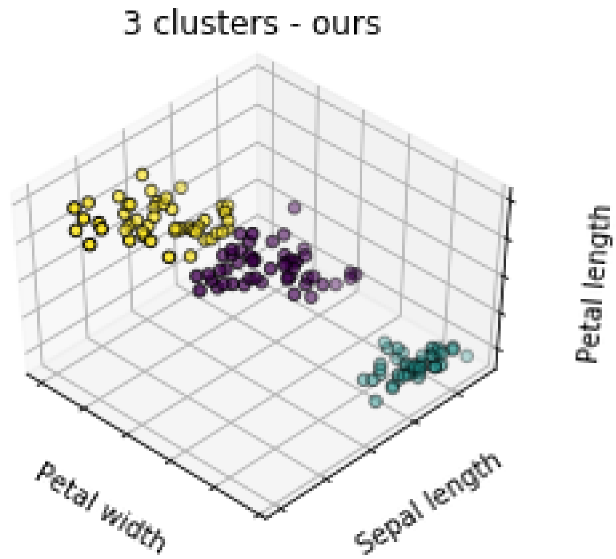
```
>>> initial centroids
[[0.72151899 0.59090909 0.50724638 0.4       ]
 [0.69620253 0.54545455 0.53623188 0.4       ]
 [0.84810127 0.68181818 0.75362319 0.92      ]]
number of iterations to converge:  4
>>> final centroids
[[0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [0.5860971086851517, 1.0302179676457113, 1.2157725785900486]
```



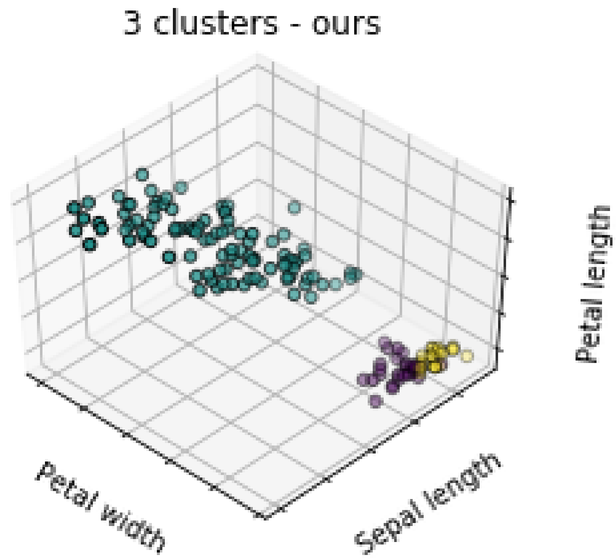
```
>>> initial centroids
[[0.5443038  0.68181818 0.15942029 0.04      ]
 [0.82278481 0.72727273 0.73913043 0.8       ]
 [0.79746835 0.77272727 0.8115942  0.96      ]]
number of iterations to converge:  7
>>> final centroids
[[0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [0.5860971086851517, 1.0302179676457113, 1.2157725785900486]
```



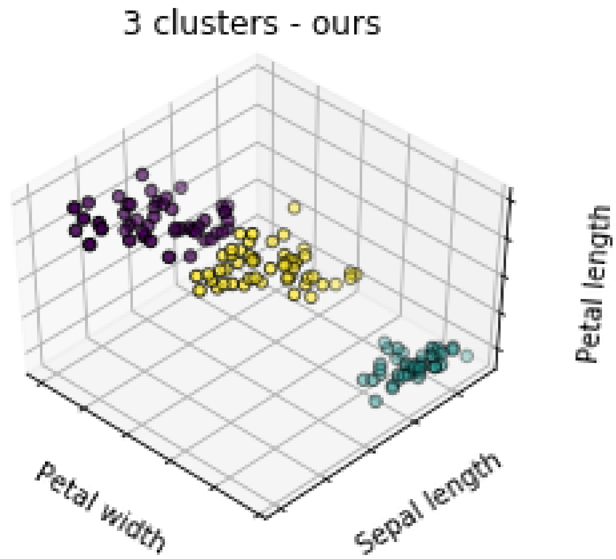

```
>>> initial centroids
[[0.84810127 0.56818182 0.84057971 0.72      ]
 [0.64556962 0.75       0.24637681 0.2       ]
 [0.78481013 0.77272727 0.7826087  0.92      ]]
number of iterations to converge:  7
>>> final centroids
[[0.74853944 0.62237762 0.62263099 0.53      ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.0302179676457113, 0.5860971086851517, 1.2157725785900486]
```



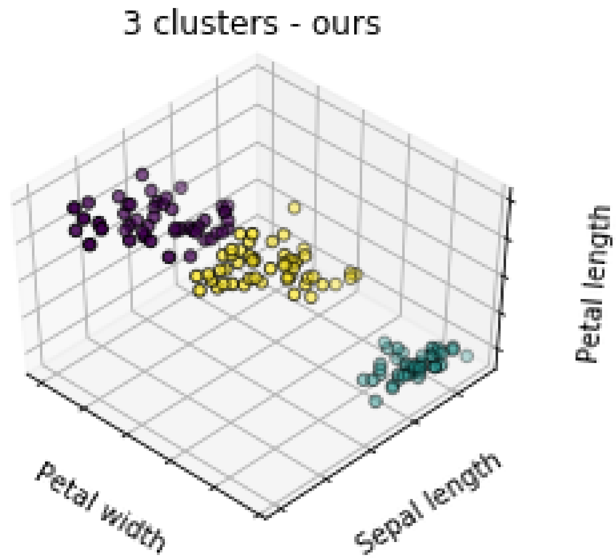

```
>>> initial centroids
[[0.62025316 0.70454545 0.2173913  0.04      ]
 [0.72151899 0.65909091 0.60869565 0.52      ]
 [0.60759494 0.68181818 0.20289855 0.04      ]]
number of iterations to converge:  7
>>> final centroids
[[0.66229656 0.8336039  0.21532091 0.11428571]
 [0.79265823 0.65272727 0.71101449 0.6704    ]
 [0.5972382  0.70454545 0.20816864 0.07636364]]
Gini Index : 0.3285333333333333
SSE_each_cluster:  [0.21307645052258836, 5.538389212891668, 0.09732480213098582]
```



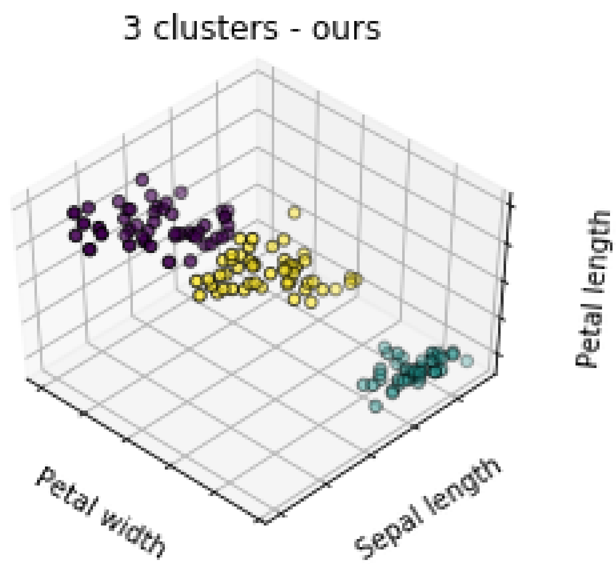

```
>>> initial centroids
[[0.86075949 0.72727273 0.85507246 0.92      ]
 [0.82278481 0.68181818 0.75362319 0.8       ]
 [0.87341772 0.70454545 0.73913043 0.92      ]]
number of iterations to converge:  10
>>> final centroids
[[0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.2157725785900486, 0.5860971086851517, 1.0302179676457113]
```



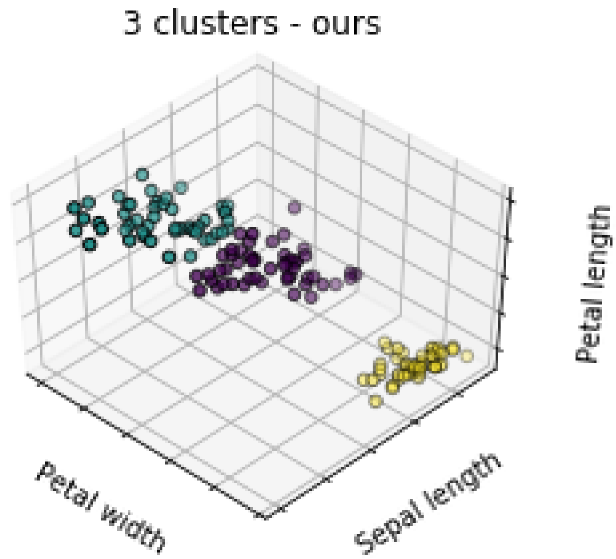

```
>>> initial centroids
[[0.91139241 0.68181818 0.84057971 0.64      ]
 [0.72151899 1.         0.2173913  0.16      ]
 [0.70886076 0.65909091 0.52173913 0.52      ]]
number of iterations to converge:  4
>>> final centroids
[[0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.2157725785900486, 0.5860971086851517, 1.0302179676457113]
```



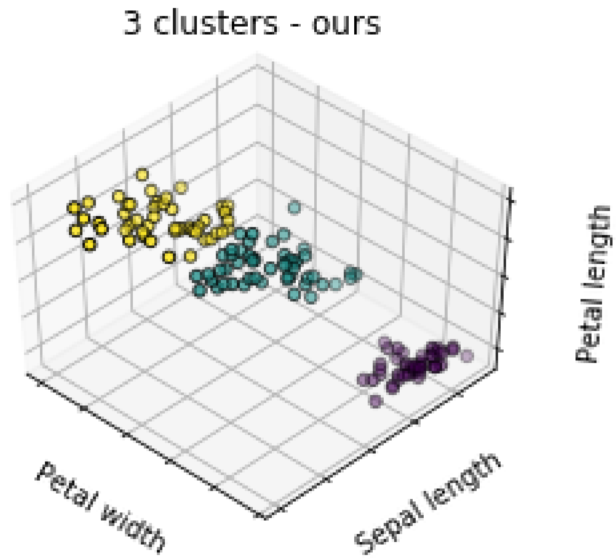

```
>>> initial centroids
[[0.84810127 0.68181818 0.75362319 0.92      ]
 [0.63291139 0.77272727 0.2173913  0.08      ]
 [0.83544304 0.68181818 0.63768116 0.56      ]]
number of iterations to converge:  4
>>> final centroids
[[0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.2157725785900486, 0.5860971086851517, 1.0302179676457113]
```



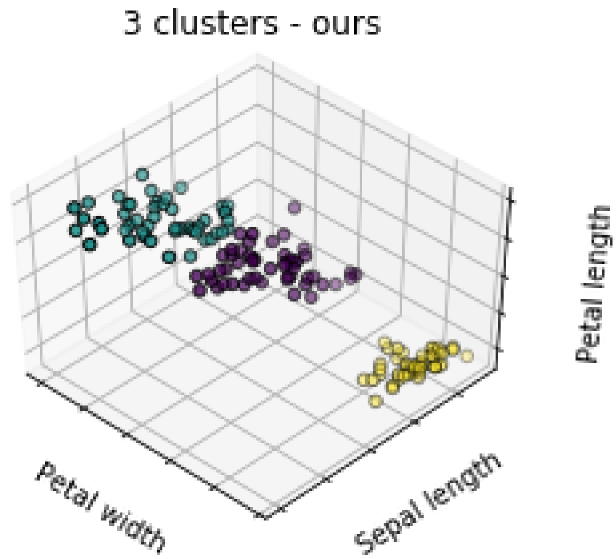

```
>>> initial centroids
[[0.72151899 0.65909091 0.60869565 0.52      ]
 [0.84810127 0.70454545 0.8115942  0.96      ]
 [0.6835443  0.77272727 0.24637681 0.08      ]]
number of iterations to converge:  4
>>> final centroids
[[0.74853944 0.62237762 0.62263099 0.53      ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.0302179676457113, 1.2157725785900486, 0.5860971086851517]
```




```
>>> initial centroids
[[0.69620253 0.52272727 0.57971014 0.52      ]
 [0.79746835 0.52272727 0.63768116 0.52      ]
 [0.83544304 0.68181818 0.63768116 0.56      ]]
number of iterations to converge:  5
>>> final centroids
[[0.63367089 0.77681818 0.21217391 0.0976    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [0.5860971086851517, 1.0302179676457113, 1.2157725785900486]
```



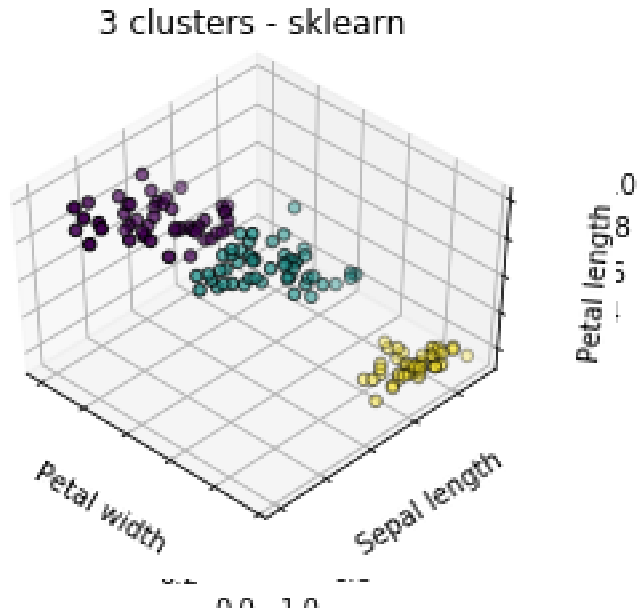

```
>>> initial centroids
[[0.73417722 0.61363636 0.73913043 0.76      ]
 [0.86075949 0.72727273 0.85507246 0.92      ]
 [0.60759494 0.77272727 0.27536232 0.08      ]]
number of iterations to converge:  7
>>> final centroids
[[0.74853944 0.62237762 0.62263099 0.53      ]
 [0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.0302179676457113, 1.2157725785900486, 0.5860971086851517]
```



sklearn

```
est = KMeans(n_clusters=3)
fig = plt.figure(1, figsize=(4, 3))
ax = Axes3D(fig, rect=[0, 0, .95, 1], elev=48, azim=134)
est.fit(X)
labels = est.labels_

# this is the function you are supposed to implement in kmeans.py
evaluation(labels, y)
gini(labels, y)
plot_result('sklearn')
```

```
Gini Index : 0.025600000000000008
```



Q2

2. Use the results obtained in (1) to explain why it's important to choose proper initial centroids.

From the result of question 1 we can observe in one case that when we choose the initial centroids as :

```
[[0.62025316 0.70454545 0.2173913  0.04      ]
 [0.72151899 0.65909091 0.60869565 0.52      ]
 [0.60759494 0.68181818 0.20289855 0.04      ]]
```

the evaluation parameters we get are:

- Gini Index : 0.3285333333333333
- SSE_each_cluster:
    * [0.21307645052258836, 5.538389212891668, 0.09732480213098582]

There is no feasible way to guarantee finding the optimal solution because the clustering analysis is a NP hard problem, heuristics approaches are needed to get an outcome that's more likely to be optimal. So there's a chance that with poorly chosen initial centroids, the results might be suboptimal.

Q3

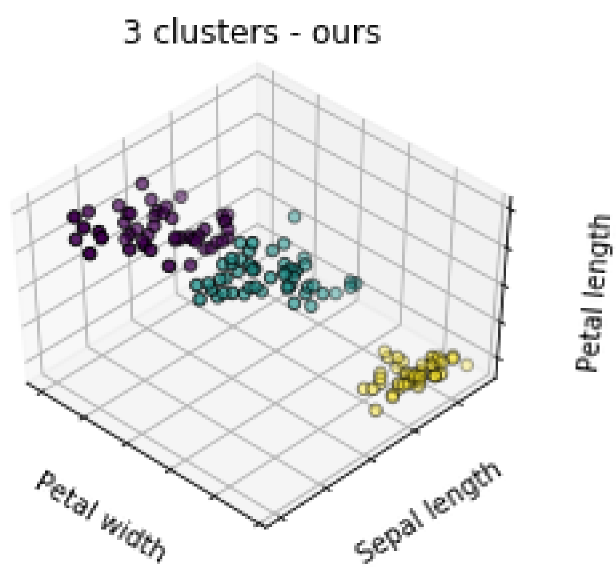
3. Between the best clusterings you obtained via scikit-learn and your own k-Means implementation, which clustering is better? Please make comparison in terms of Impurity (Gini

Index) of the clusterings. To compute. Gini Index for a clustering, use the ground truth (i.e., flower types of data points) to do majority vote in order to assign a flower type for each cluster. Accordingly, calculate the probability of misclassification and correct classification. Finally, calculate Gini Index for a clustering using the calculated probabilities.

our Kmeans

```
In [147]: # this is the function you are supposed to implement in kmeans.py
          centroids, label = kmeans(X,3)
          # this is the function you are supposed to implement in kmeans.py
          evaluation(label, y)
          gini(label, y)
          SSE(centroids, X)
          plot_result('ours')
```

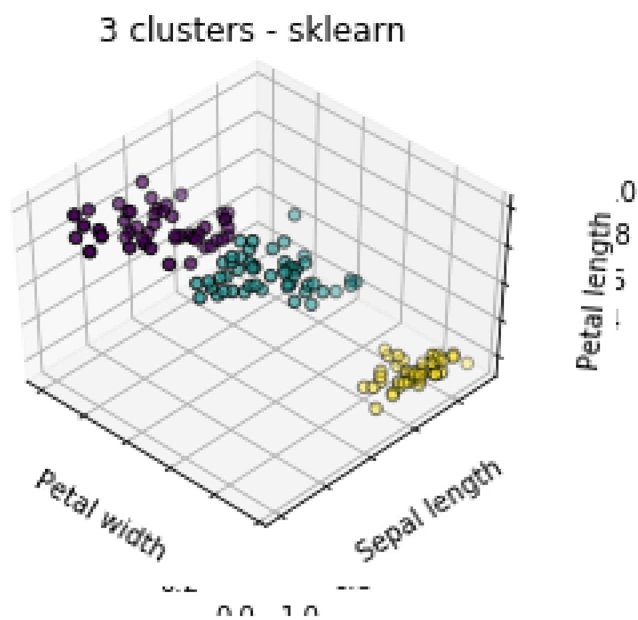
```
>>> initial centroids
[[0.70886076 0.68181818 0.65217391 0.6       ]
 [0.6835443  0.68181818 0.65217391 0.6       ]
 [0.72151899 1.         0.2173913  0.16      ]]
number of iterations to converge:  6
>>> final centroids
[[0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.2157725785900486, 1.0302179676457113, 0.5860971086851517]
```



sklearn

```
In [152]: est = KMeans(n_clusters=3)
          fig = plt.figure(1, figsize=(4, 3))
          ax = Axes3D(fig, rect=[0, 0, .95, 1], elev=48, azim=134)
          est.fit(X)
          labels = est.labels_

          # this is the function you are supposed to implement in kmeans.py
          evaluation(labels, y)
          gini(labels, y)
          plot_result('sklearn')
```

```
Gini Index : 0.025600000000000008
```



Discussion

Comparing the evaluation of our kmeans and the kmeans built in the sklearn package, the Gini Index of the best case in the 10 tests run with our kmeans is equivalent to the Gini Index calculated from sklearn.

Q4

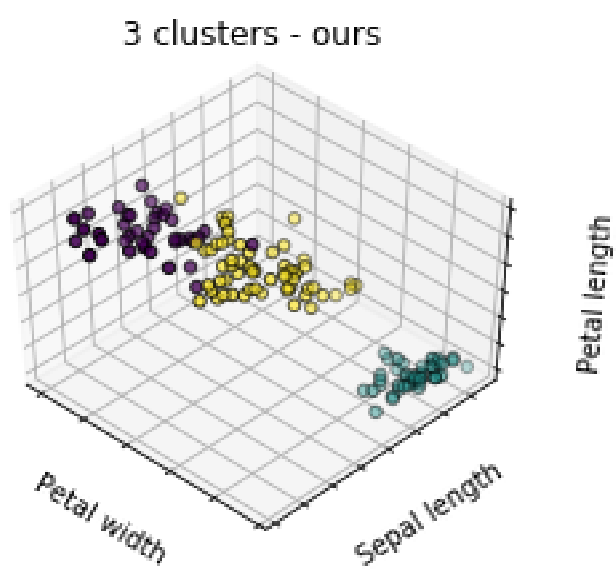
4. In lab3.py, the data points are normalized (see line 12) by default as a data preprocessing step. What happens if you use the raw data (line 11) without any data preprocessing? Between normalized and unnormalized datasets, which one obtains better clustering? Please make comparison in terms of Impurity (Gini Index) of the clusterings and computational cost (number of iterations to converge).

un-normalize

```
In [158]: X = iris.data
```

```
In [161]: # this is the function you are supposed to implement in kmeans.py
          centroids, label = kmeans(X,3)
          # this is the function you are supposed to implement in kmeans.py
          evaluation(label, y)
          gini(label, y)
          SSE(centroids, X)
          plot_result('ours')
```

```
>>> initial centroids
[[7.1 3.  5.9 2.1]
 [6.  2.9 4.5 1.5]
 [6.5 3.  5.5 1.8]]
number of iterations to converge:  8
>>> final centroids
[[6.85       3.07368421 5.74210526 2.07105263]
 [5.006      3.418      1.464      0.244     ]
 [5.9016129  2.7483871  4.39354839 1.43387097]]
Gini Index : 0.1216
SSE_each_cluster:  [23.87947368421052, 15.240400000000001, 39.82096774193548]
```

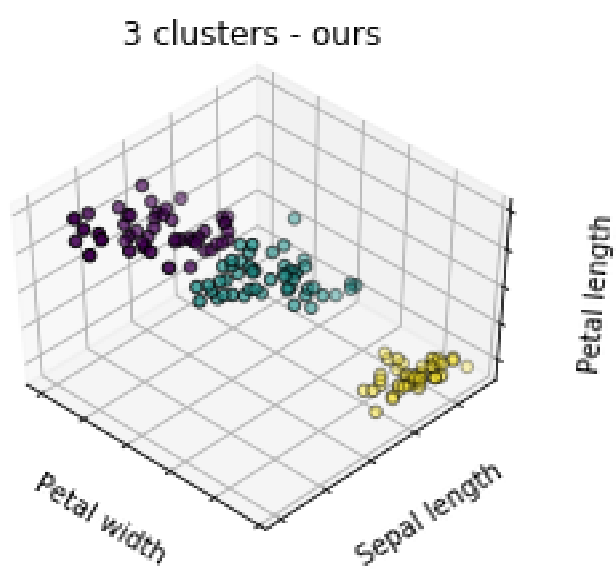


normalize

```
In [162]: X = norm(iris.data)
```

```
In [169]: # this is the function you are supposed to implement in kmeans.py
          centroids, label = kmeans(X,3)
          # this is the function you are supposed to implement in kmeans.py
          evaluation(label, y)
          gini(label, y)
          SSE(centroids, X)

          plot_result('ours')
```

```
>>> initial centroids
[[0.73417722 0.61363636 0.73913043 0.76      ]
 [0.83544304 0.68181818 0.63768116 0.56      ]
 [0.70886076 0.65909091 0.52173913 0.52      ]]
number of iterations to converge:  5
>>> final centroids
[[0.84045359 0.68560606 0.80676329 0.8225    ]
 [0.74853944 0.62237762 0.62263099 0.53      ]
 [0.63367089 0.77681818 0.21217391 0.0976    ]]
Gini Index : 0.025600000000000008
SSE_each_cluster:  [1.2157725785900486, 1.0302179676457113, 0.5860971086851517]
```



Discussion

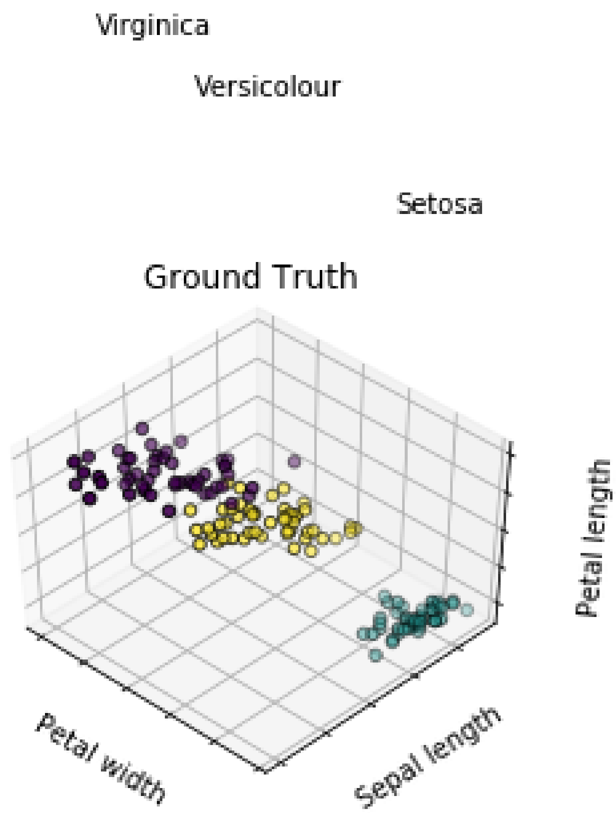
From the evaluation results, we can see that the normalized dataset obtains better clustering, reducing the Gini Index by approximately 0.096 from 0.1216 to 0.0256. And with regard to the computational cost, the number of iterations consumed to for the algorithm trained by unnormalized dataset to converge is 8 and the number of iterations for the algorithm trained by normalized dataset is 5 (*however by running the test for a few times, the numbers of iterations took for both unnormalized and normalized dataset to converge are mostly similar and not significantly different*)

Q5

5. By comparing the clusterings in (3) and (4) against the ground truth, explain whether Impurity is a reasonable quality measure for clustering?

ground truth visualization

In [170]:
```
fig = plt.figure(1, figsize=(4, 3))
ax = Axes3D(fig, rect=[0, 0, .95, 1], elev=48, azim=134)

for name, label in [('Setosa', 0),
                    ('Versicolour', 1),
                    ('Virginica', 2)]:
    ax.text3D(X[y == label, 3].mean(),
              X[y == label, 0].mean(),
              X[y == label, 2].mean() + 2, name,
              horizontalalignment='center',
              bbox=dict(alpha=.2, edgecolor='w', facecolor='w'))
y = np.choose(y, [1, 2, 0]).astype(np.float)
ax.scatter(X[:, 3], X[:, 0], X[:, 2], c=y, edgecolor='k')

ax.w_xaxis.set_ticklabels([])
ax.w_yaxis.set_ticklabels([])
ax.w_zaxis.set_ticklabels([])
ax.set_xlabel('Petal width')
ax.set_ylabel('Sepal length')
ax.set_zlabel('Petal length')
ax.set_title('Ground Truth')
ax.dist = 12

plt.show()
```



Discussion

Impurity is a reasonable quality measure for clustering from the clusterings we got from (3) and (4). Because:

- Impurity (in this case, the Gini Index) could be used as evaluation criteria for the algorithm to determine its optimality. Clustering with smaller Gini Index is more optimal than the clustering with larger Gini Index:
    * In question 3, Gini Index is used for comparison of clusterings obtained between our KMeans and the one from sklearn package. From the result that the Gini Index of the best clustering we got from our kmeans algorithm and the sklearn package are the same, we could make an assumption that the optimality of our kmeans is close to that of kmeans. And from the visualization of both ours and sklearn compared with the ground truth, we are able to confirm our assumption.
    * In question 4, Gini Index is used for comparison of clusterings obtained between KMeans models trained with normalized and unnormalized dataset. From the result that the Gini Index of our kmeans algorithm trained with the normalized dataset is smaller than the one trained with un-normalized dataset, we could make an assumption that the optimality of our kmeans trained with normalized dataset is better than

that trained with un-normalized dataset. And from the visualization of both with the ground truth, we are also able to confirm our assumption.