实验五：层次聚类

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实验要求

基本要求

a) 实现single-linkage层次聚类算法； b) 实现complete-linkage层次聚类算法；

中级要求

a) 实现average-linkage层次聚类算法； b) 将上述三种算法的性能进行简要对比；

高级要求

通过变换聚类簇的个数，测试上述三种算法的性能，并给出分析。

1. 生成数据集

数据包含2000个样例，每个样例的前3列表示特征，第4列表示标签。

In [1]:
```
from matplotlib import pyplot as plt
import numpy as np
from sklearn.datasets import make_blobs
from sklearn.metrics.cluster import adjusted_rand_score
def create_data(centers,num=100,std=0.7):
    '''
    生成用于聚类的数据集
    :param centers: 聚类的中心点组成的数组。如果中心点是二维的，则产生的每个样本都是
    :param num: 样本数
    :param std: 每个簇中样本的标准差
    :return: 用于聚类的数据集。是一个元组，第一个元素为样本集，第二个元素为样本集的真
    '''
    X, labels_true = make_blobs(n_samples=num, centers=centers, cluster_std=std)
    return  X,labels_true

centers=[[1,1,1],[1,3,3],[3,6,5],[2,6,8]]# 用于产生聚类的中心点, 聚类中心的维度代表产
X,labels_true= create_data(centers,2000,0.5) # 产生用于聚类的数据集, 聚类中心点的个数
np.savetxt('D:/Program Files/JupyterSpace/ML/lab5/data.dat',X)
np.savetxt('D:/Program Files/JupyterSpace/ML/lab5/label.dat',labels_true)
print("generate data finish!")
```

```
generate data finish!
```

2. 初级&中级要求：实现single-linkage、complete-linkage、average-linkage层次聚类算法

In [2]:
```
import numpy as np
```

```python
MAX_NUM = 1e3

# method
def singleLinkage(X):
    # your code
    Minres = []
    for i in range(len(X[0])):
        Minres.append(MAX_NUM)
    for i in range(len(X[0])):
        if X[0][i] < Minres[i]:
            Minres[i] = X[0][i]
        if X[1][i] < Minres[i]:
            Minres[i] = X[1][i];
    return Minres

def completeLinkage(X):
    # your code
    Maxres = []
    for i in range(len(X[0])):
        Maxres.append(0)
    for i in range(len(X[0])):
        if X[0][i] > Maxres[i]:
            Maxres[i] = X[0][i]
        if X[1][i] > Maxres[i]:
            Maxres[i] = X[1][i];
    return Maxres

def averageLinkage(setList,dest,src,allDist):
    # your code
    Avgres = []
    for clu in range(len(setList)):
        if clu == dest or clu == src:
            Avgres.append(0)
            continue
        sumdistance = 0
        for other_cluster_element in setList[clu]:
            for dest_cluster_element in setList[dest]:
                sumdistance += allDist[dest_cluster_element][other_cluster_element]
            for src_cluster_element in setList[src]:
                sumdistance += allDist[src_cluster_element][other_cluster_element]
        res = sumdistance/((len(setList[dest])+len(setList[src]))*len(setList[clu]))
        Avgres.append(res)
    return Avgres

class AgglomerativeClustering:
    def __init__(self):
        # 对每次的合并进行记录
        self.steps=[]

    def fit(self,datas,method):
        self.dataCnt = datas.shape[0]# dataCnt为总数据条数
        # 预处理各点之间的距离
        allDist = np.zeros((self.dataCnt,self.dataCnt))# allDist为各点之间的距离
        for i in range(self.dataCnt):
            for j in range(i):
                allDist[i][j] = allDist[j][i] = np.sum((datas[i]-datas[j])**2)
        setList, clusterCount = [[i] for i in range(self.dataCnt)], self.dataCnt
        # setList为这一类有哪些数据，clusterCount为聚类个数(初始化为数据条数)
        print("calculate distance finish!")

        # 聚类间距离矩阵
        clusterDist = np.zeros((self.dataCnt,self.dataCnt))+MAX_NUM# clusterDist为聚
        for i in range(clusterCount):
            for j in range(i+1,clusterCount):
```

```
            clusterDist[i][j] = clusterDist[j][i] = allDist[i][j]
        print("calculate cluster distance finish!")

        while clusterCount != 1:# 反复聚类直到只剩下一类
            # 最相似的两个聚类
            res = np.argmin(clusterDist)# res为距离最短的两类(i类和j类)的下标(i,j)
            dest,src = int(res/clusterCount),res%clusterCount# dest为i类, src为j类
            # steps进行一次记录
            self.steps.append((setList[dest][0],setList[src][0]))# steps用于记录每次
            # 聚类间距离矩阵更新
            if(method == averageLinkage):
                modify = method(setList,dest,src,allDist)
            else:
                modify = method(clusterDist[[dest,src]])
            clusterDist[dest] = modify# 所有其他类到新类的距离(一排)
            clusterDist[:,dest] = modify# 所有其他类到新类的距离(一列)
            clusterDist = np.delete(clusterDist,src,axis=0)
            clusterDist = np.delete(clusterDist,src,axis=1)
            clusterDist[dest][dest] = MAX_NUM
            # 聚类更新
            setList[dest] = setList[dest] + setList[src]
            del setList[src]
            clusterCount -= 1# 总类数-1
            if (self.dataCnt - clusterCount) % (self.dataCnt / 20) == 0:
                print(clusterCount, " clusters left.")# 打印还剩多少类
        print("cluster finish !")

    def label(self,k):
        root = list(range(self.dataCnt))
        def find_root(n):
            if root[root[n]] == root[n]:
                return root[n]
            root[n]=find_root(root[n])
            return root[n]
        for i in range(self.dataCnt-k): # 根据steps记录产生非连通图
            src,dest = self.steps[i]
            root[find_root(dest)] = find_root(src)
        cluster, clusterNum = [0 for i in range(self.dataCnt)], 0
        for i in range(self.dataCnt): # 将根节点标注为新的cluster
            if i == root[i]: # i是根
                clusterNum += 1
                cluster[i] = clusterNum
        for i in range(self.dataCnt): # 将非根节点标注为根节点的cluster
            if i != root[i]: # i不是根
                cluster[i] = cluster[find_root(i)]
        return cluster
```

In [3]:

```
from itertools import permutations
def accuracy_cal(labels_true,labels_predict,k):
    labels_reshuffle = [0 for i in range(len(labels_true))]
    combination = list(permutations([i for i in range(1,k+1)],k))
    acclis = []
    for i in range(len(combination)):# 每个组合都试一下, 算出acc
        comindex = 0
        for j in range(1,k+1):#修改每类的label
            for index in range(len(labels_true)):# 把所有label为j的都改成combinatio
                if labels_true[index] == j:
                    labels_reshuffle[index] = combination[i][comindex]
            comindex += 1
        # 计算acc
        acc = 0
        for j in range(len(labels_reshuffle)):
            if(labels_reshuffle[j] == labels_predict[j]):
```

```python
                acc += 1
        acclis.append(acc/len(labels_reshuffle))
#     print("acclis is :{0}".format(acclis))
    return max(acclis)
```

In [4]:
```python
def plot_data(*data):
    '''
    绘制用于聚类的数据集
    :param data: 可变参数。它是一个元组。元组元素依次为：第一个元素为样本集，第二个元
    :return: None
    '''
    X,labels_true,labels_predict,cnt=data
    fig=plt.figure()
    ax=fig.add_subplot(1,1,1)
    colors='rgbyckm' # 每个簇的样本标记不同的颜色
    markers='o^sP*DX'
    for i in range(len(labels_true)):
        predict=labels_predict[i]
        ax.scatter(X[i,0],X[i,1],label="cluster %d"%labels_true[i],
        color=colors[predict%len(colors)],marker=markers[labels_true[i]%len(markers)

METHOD_APPLY = [singleLinkage,completeLinkage,averageLinkage]

cnt=0
for method in METHOD_APPLY:
    model = AgglomerativeClustering()
    model.fit(X,method)
    k=4
    labels_predict = model.label(k)
    acc = adjusted_rand_score(labels_predict, labels_true)
    print("accuracy for {0} is:{1}".format(str(method),acc))
    plot_data(X,labels_true,labels_predict,cnt)
    cnt+=1
    print("-------Segmentation-------")
```

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calculate distance finish!
calculate cluster distance finish!
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cluster finish !
accuracy for <function singleLinkage at 0x000001D325121EE0> is:0.4991242803198932
-------Segmentation-------
calculate distance finish!
calculate cluster distance finish!
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cluster finish !
accuracy for <function completeLinkage at 0x000001D329915EE0> is:0.9906915190011604
-------Segmentation-------
calculate distance finish!
calculate cluster distance finish!
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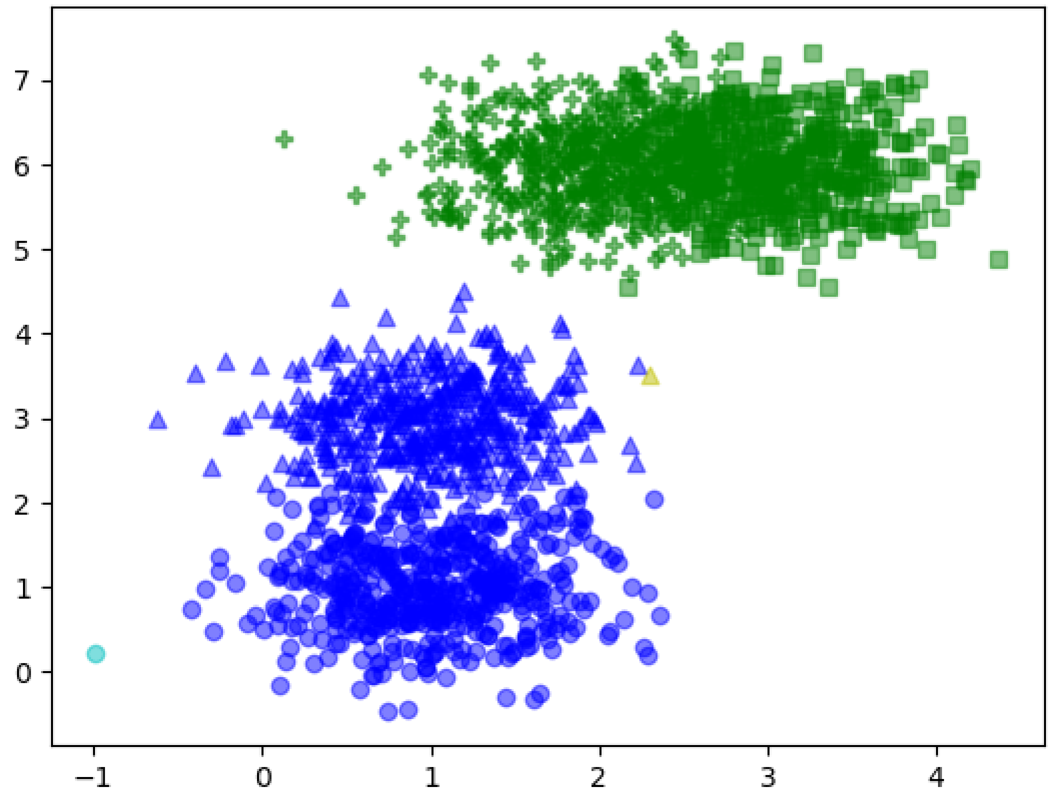
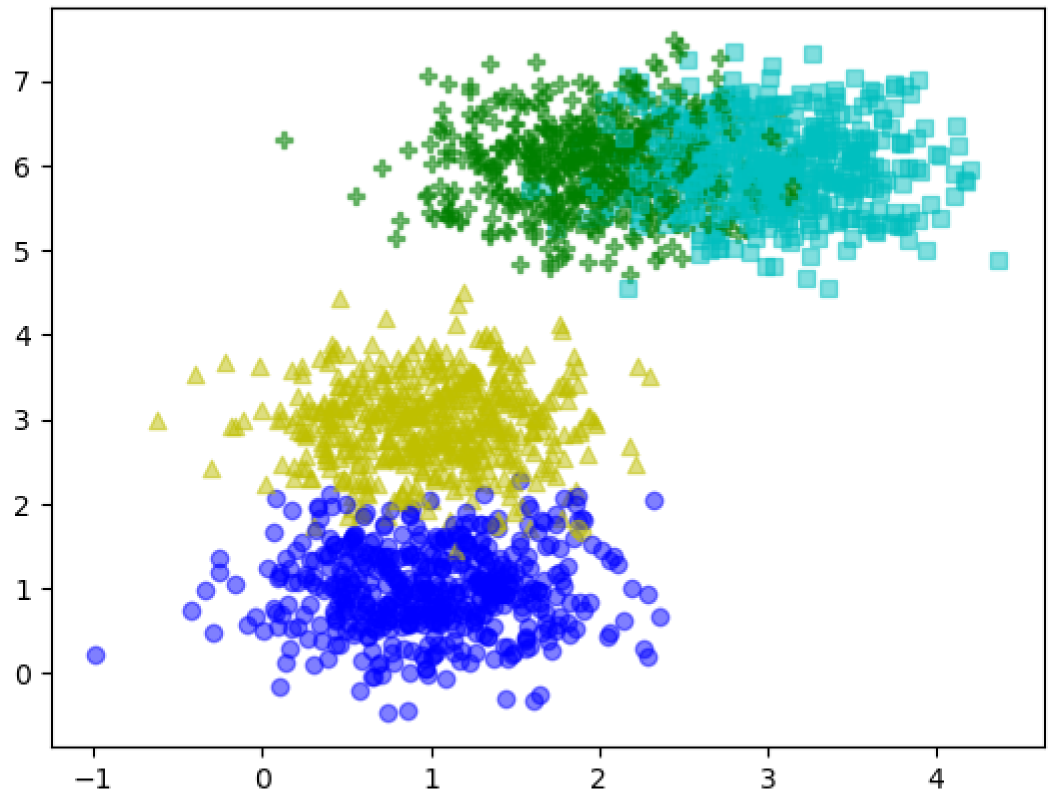
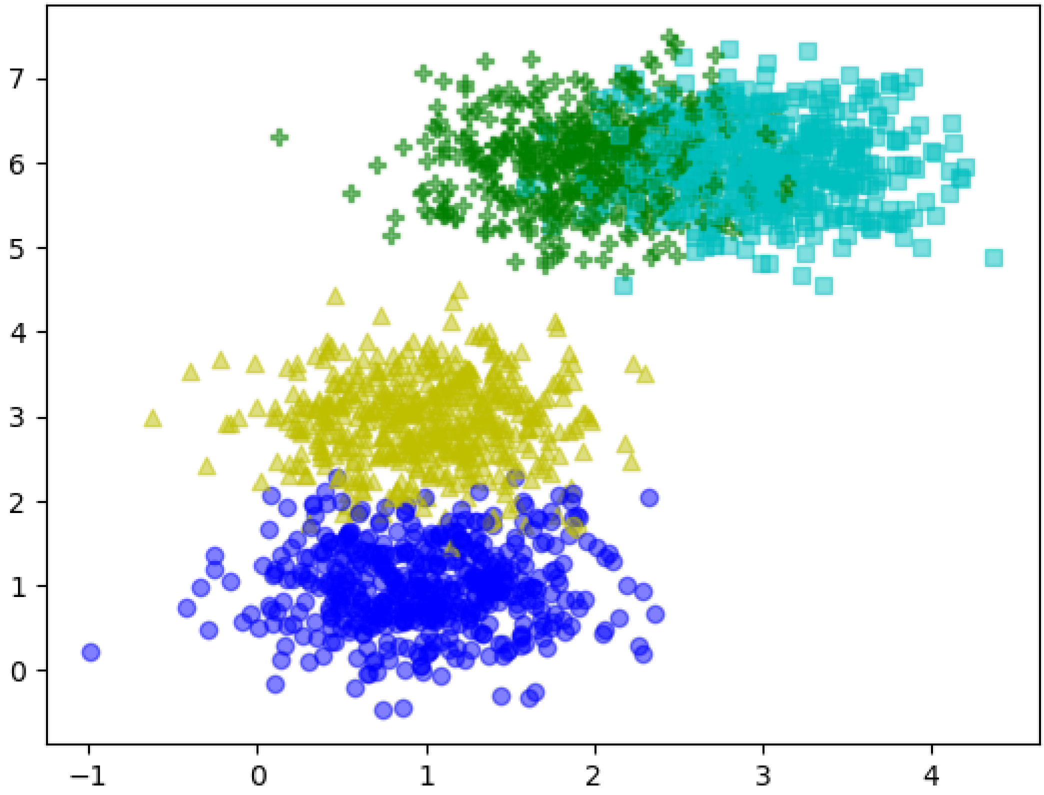
cluster finish !
accuracy for <function averageLinkage at 0x000001D329915F70> is:0.9933460896657262
-------Segmentation-------
```







3. 中级要求：性能比较

列出三种算法的accuracy表格如下：

方法	accuracy
singleLinkage	0.4991
completeLinkage	0.9907
averageLinkage	0.9762

可以看出，singleLinkage算法最差，从聚类图中也可看出它常常将大部分数据分为2类或3类，第3/4类只有极少量的点；completeLinkage和averageLinkage算法明显表现很好。 原因解释如下：

- singleLinkage容易造成两个聚类明明从整体上看相隔很远，但由于其中个别点的距离较近就被合并了，且合并后这种情况会恶化，类似链式效应，这也是为什么singleLinkage表现出容易合并两个明显不同但存在相交的类。
- 上述两种聚类方法的共同问题就是只考虑了某个极端的属性(如最近距离和最远距离)，而没有考虑类内数据的整体特点。averageLinkage把两个集合中的点两两距离全部放在一起求平均值，考虑了所有点对，更全面，**在改变方差进行实验时会发现averageLinkage相较completeLinkage更稳健。**

4. 高级要求

In [7]:
```
acclis = [[],[],[]]# 二维list，第二维表示不同方法，第一维表示不同clusternum
centerlis = [[1,1,1],[1,3,3],[3,6,5],[2,6,8],[2,5,6],[3,4,7],[4,7,8]]
for clunum in range(2,8):
    centers=[centerlis[i] for i in range(clunum)]# 用于产生聚类的中心点, 聚类中心的
    X,labels_true= create_data(centers,2000,0.5) # 产生用于聚类的数据集，聚类中心点的
    for methodindex in range(len(METHOD_APPLY)):
```

```
        model = AgglomerativeClustering()
        model.fit(X,METHOD_APPLY[methodindex])
        labels_predict = model.label(clunum)
        acclis[methodindex].append(adjusted_rand_score(labels_predict, labels_true))
#         acclis[methodindex].append(accuracy_cal(labels_true,labels_predict,clunum)
#         print("accuracy for {0} is:{1},with clunum={2}".format(str(METHOD_APPLY[me
    print("-------Segmentation-------")
```

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cluster finish !
-------Segmentation-------
```
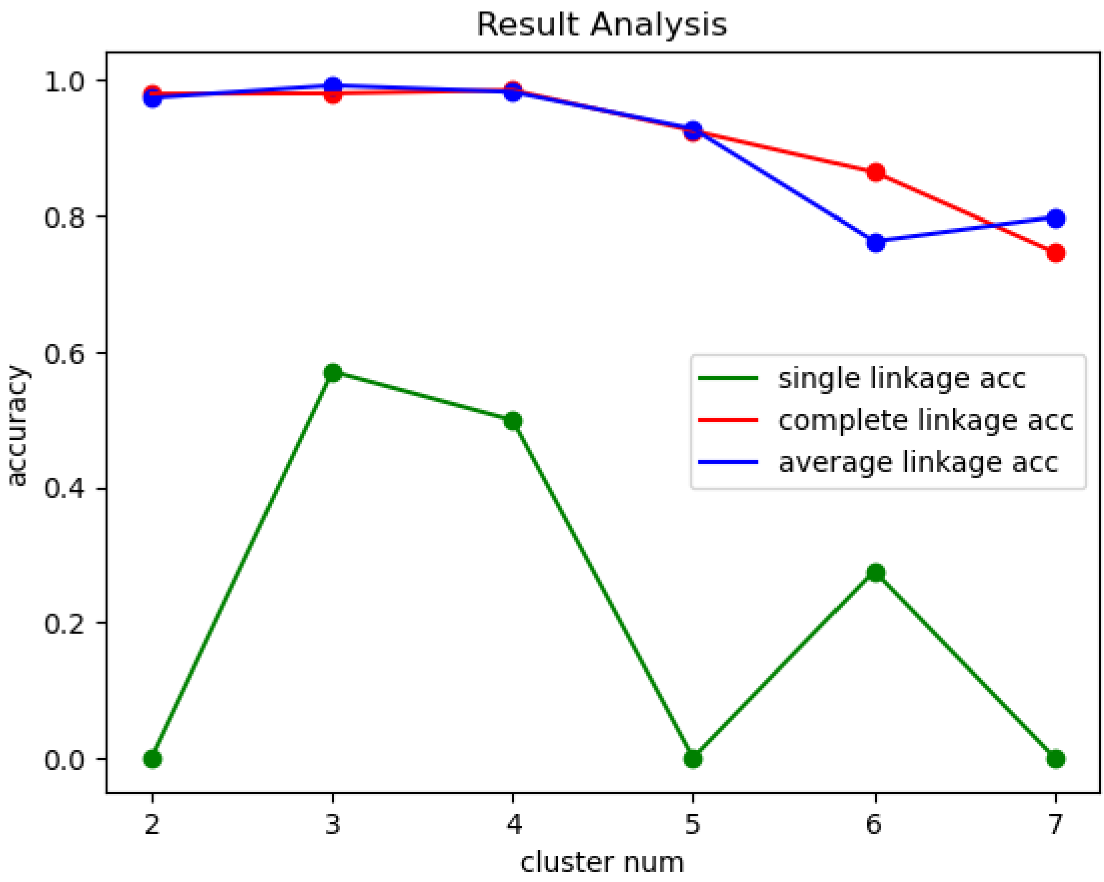

In [8]:

```python
k = [i for i in range(2, 8)]
plt.title('Result Analysis')
plt.plot(k, acclis[0], color='green', label='single linkage acc')
plt.plot(k, acclis[1], color='red', label='complete linkage acc')
plt.plot(k, acclis[2], color='blue', label='average linkage acc')
plt.scatter(k, acclis[0],color='green')
plt.scatter(k, acclis[1], color='red')
plt.scatter(k, acclis[2], color='blue')
plt.legend()  # 显示图例

plt.xlabel('cluster num')
plt.ylabel('accuracy')
plt.show()
```



- acc： 从acc曲线可以看出，complete linkage和average linkage效果远优于single linkage。average linkage和complete linkage不相上下，但总体而言average linkage更加稳健。这是因为complete linkage虽然解决了single linkage中链式反应的问题，但对离群点的处理能力不足，而average linkage考虑了所有情况，更加全面，故效果最好。
- 时间复杂度：值得一提的是，运行复杂度方面average linkage高于另外两种算法，这是因为它每次计算都要考虑全部的组合情况，而single linkage和complete linkage只需找出两类中较小/大的那个distance即可。

因此，模型选择时需要在时间和空间上折中。