Assignment 4

Group Members

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In [1]:
```
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
import numpy as np
from KDTree_rec import *
from sklearn.manifold import TSNE
from matplotlib.pyplot import figure
from sklearn.decomposition import PCA
from sklearn.manifold import Isomap
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
```

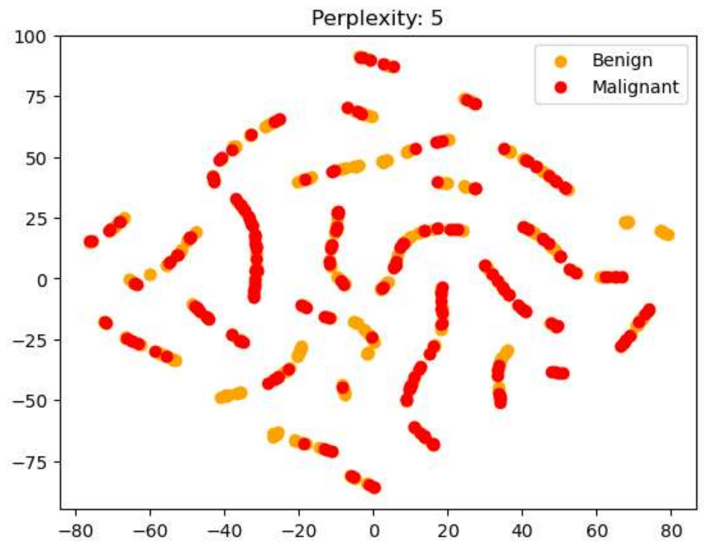
Ex.1: ISOMAP and t-SNE

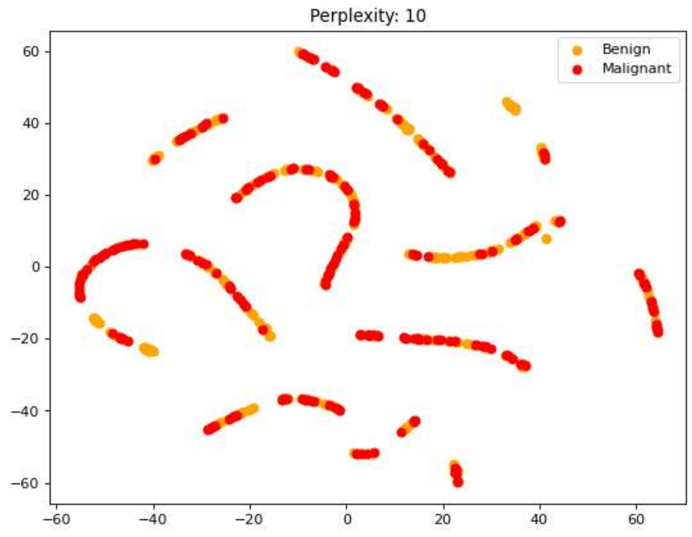
a)

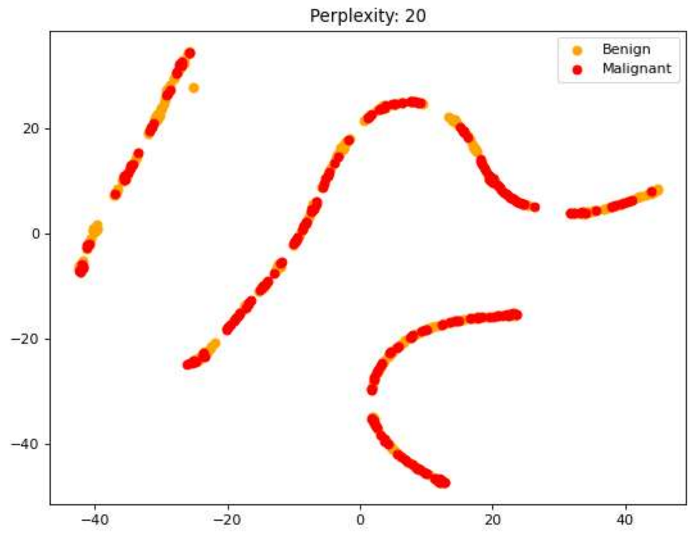
In [2]:
```
df = pd.read_excel("breast-cancer-wisconsin.xlsx")

dF=df.interpolate()
```

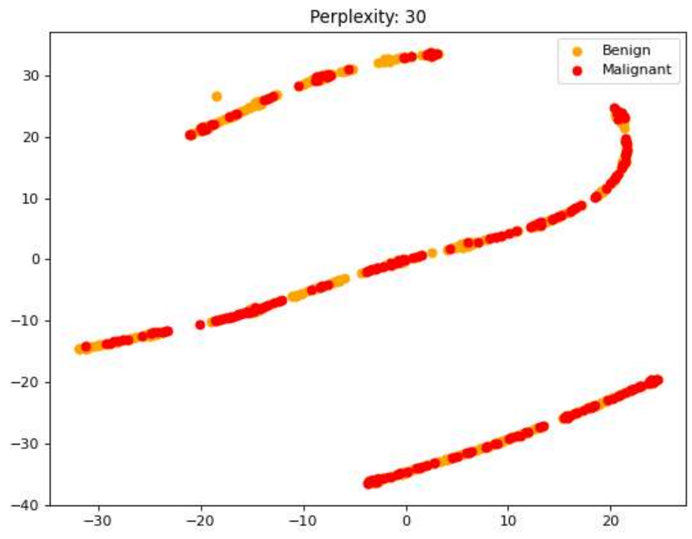
t-SNE with a random initial distribution

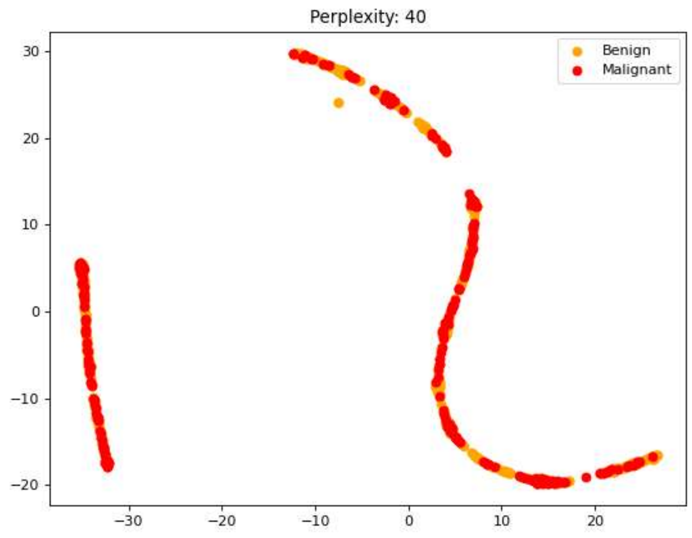
In [3]:
```
benign_df = dF[dF['class'] == 2]
malignant_df= dF[dF['class'] == 4]

X = np.concatenate((benign_df.drop('class', axis=1), malignant_df.drop('class', axis=1)), axis=0)
y = np.concatenate((np.zeros(benign_df.shape[0]), np.ones(malignant_df.shape[0])))
perplexities = [5, 10, 20, 30, 40, 50]

for i, perplexity in enumerate(perplexities):
    tsne = TSNE(n_components=2, perplexity=perplexity, init='random')
    Y = tsne.fit_transform(X)
    plt.scatter(Y[y==0, 0], Y[y==0, 1], c='orange', label='Benign')
    plt.scatter(Y[y==1, 0], Y[y==1, 1], c='red', label='Malignant')
    plt.title("Perplexity: {}".format(perplexity))
    plt.legend()
    figure(figsize=(8, 6), dpi=80)
plt.show()
```

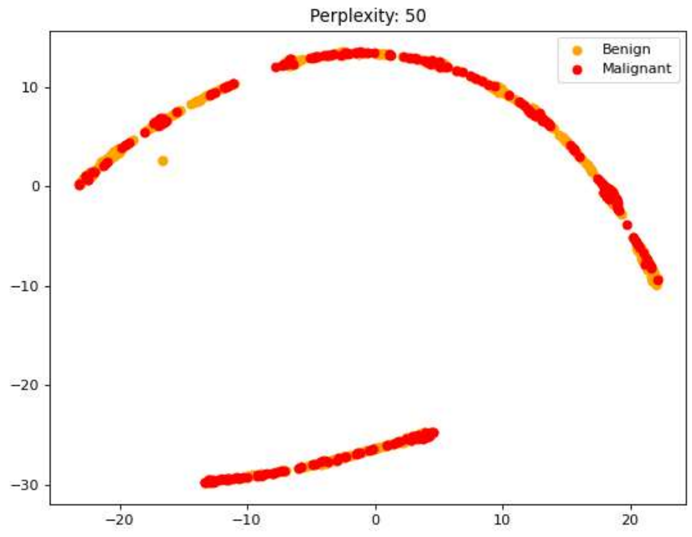



Perplexity: 10
Benign
Malignant


Perplexity: 20
Benign
Malignant


Perplexity: 30
Benign
Malignant

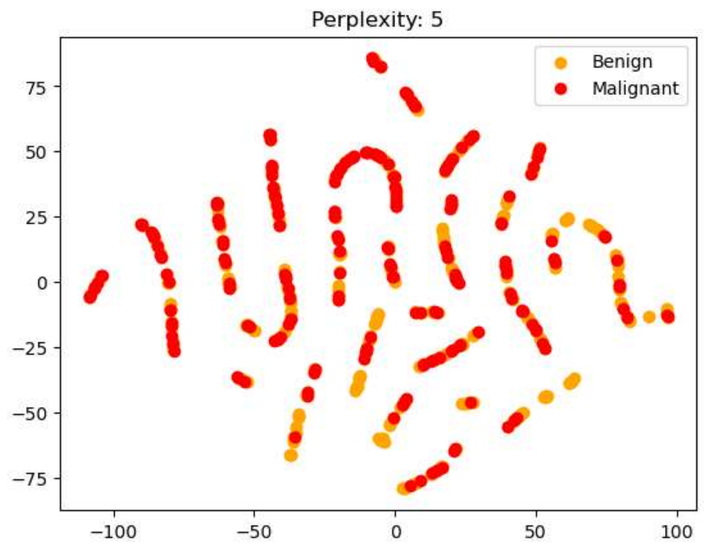


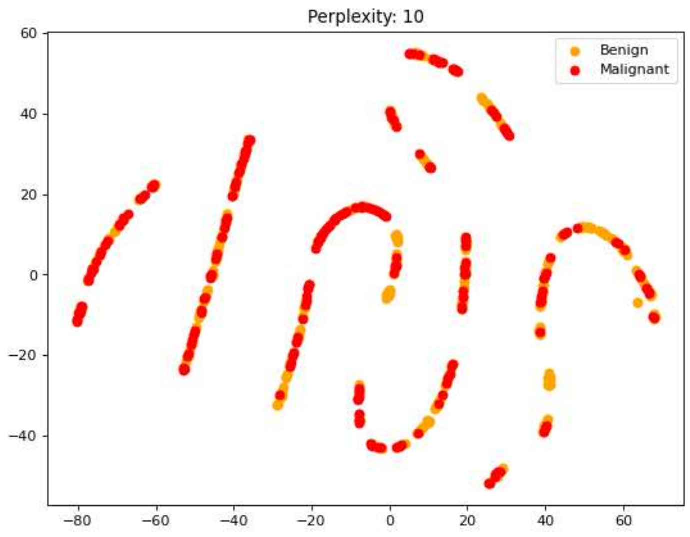


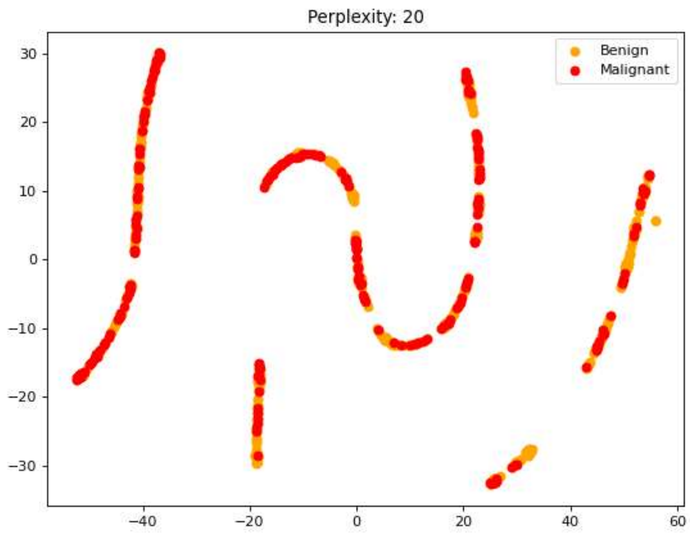
```
<Figure size 640x480 with 0 Axes>
```

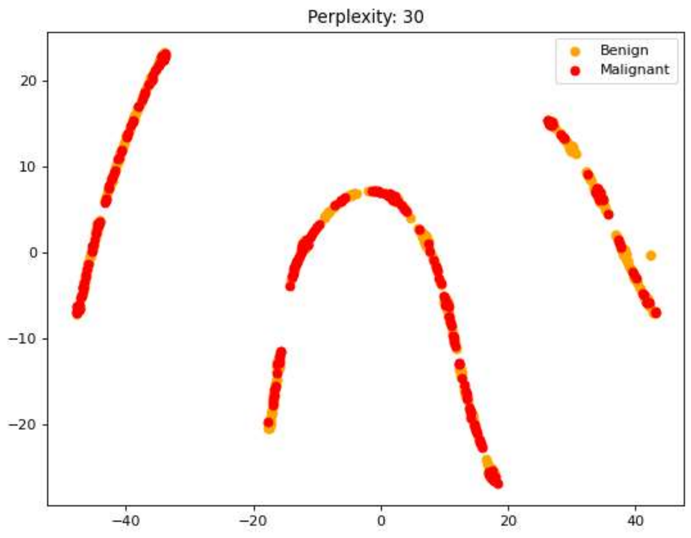
t-SNA with PCA as the initial distribution

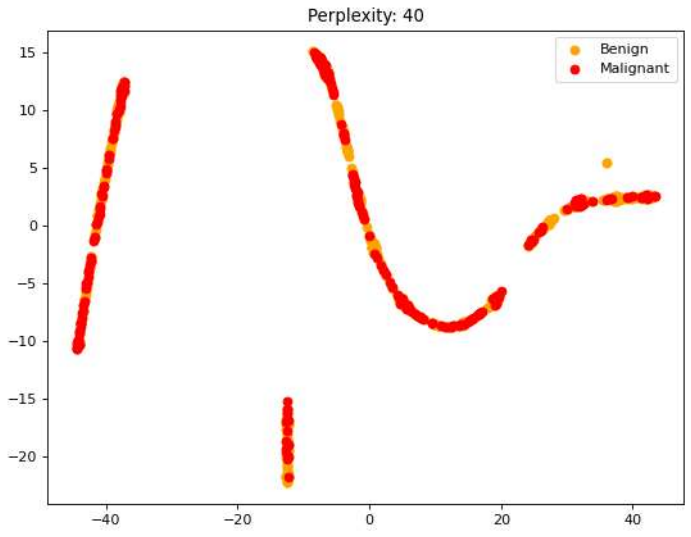
```
In [4]: benign_df = dF[dF['class'] == 2]
        malignant_df = dF[dF['class'] == 4]

        X = np.concatenate((benign_df.drop('class', axis=1), malignant_df.drop('class', axis=1)), axis=0)
        y = np.concatenate((np.zeros(benign_df.shape[0]), np.ones(malignant_df.shape[0])))

        perplexities = [5, 10, 20, 30, 40, 50]

        for i, perplexity in enumerate(perplexities):

            tsne = TSNE(n_components=2, perplexity=perplexity, init='pca')
            Y = tsne.fit_transform(X)
            plt.scatter(Y[y==0, 0], Y[y==0, 1], c='orange', label='Benign')
            plt.scatter(Y[y==1, 0], Y[y==1, 1], c='red', label='Malignant')
            plt.title("Perplexity: {}".format(perplexity))
            plt.legend()
            figure(figsize=(8, 6), dpi=80)
        plt.show()
```

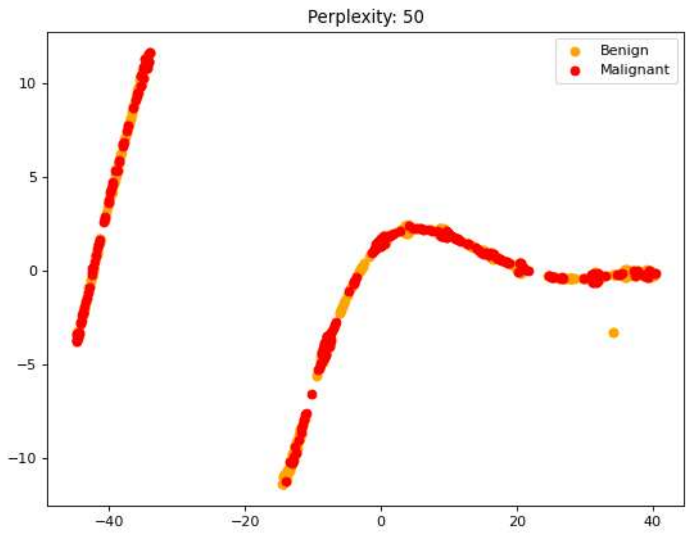

Perplexity: 5
Benign
Malignant
75
50
25
0
−25
−50
−75
−100
−50
0
50
100


Perplexity: 10
Benign
Malignant
60
40
20
0
−20
−40
−80
−60
−40
−20
0
20
40
60


Perplexity: 20
Benign
Malignant
30
20
10
0
−10
−20
−30
−40
−20
0
20
40
60







```
<Figure size 640x480 with 0 Axes>
```

Analysis of both initial distributions

By comparing the diagrams with random initial distribution with pca initial distribution, we can see that the data is overlapping greatly in each cluster. As we increase the value of perplexity, the numbers of individual small clusters start reducing. For the perplexity=50, only two clusters can be observed. The initial distribution didn't matter as we can see that both random and pca initial distribution were able to achieve 2 clear clusters at the perplexity=50.

b)

```
In [5]: df1=pd.read_excel("Data_Cortex_Nuclear.xls")
```

```
In [6]: df2=df1.interpolate()
```

```
In [7]: print(df2.isnull().sum())
```

```
MouseID      0
DYRK1A_N     0
ITSN1_N      0
BDNF_N       0
NR1_N        0
            ..
CaNA_N       0
Genotype     0
Treatment    0
Behavior     0
class        0
Length: 82, dtype: int64
```

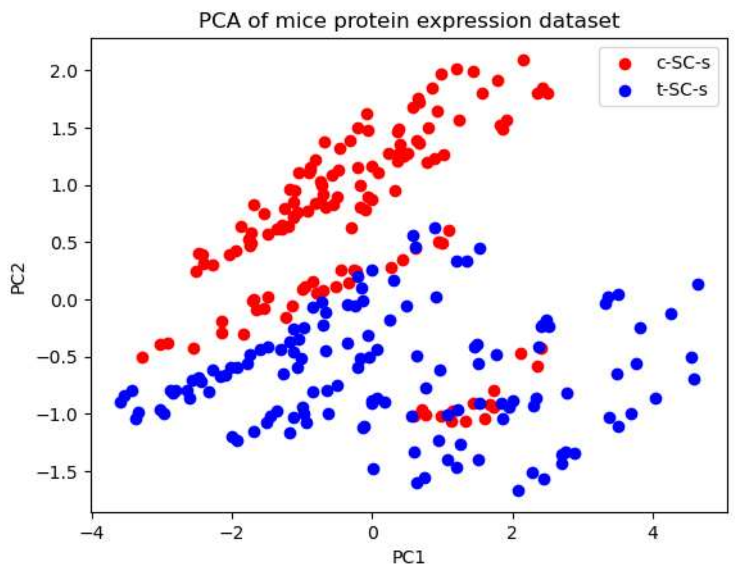
In [8]:
```
data_filtered = df2.loc[(df2['class'] == 'c-SC-s') | (df2['class'] == 't-SC-s')]
df_fltr= data_filtered.drop(columns=['MouseID', 'class','Behavior','Treatment','Genotype'])
df_fltr
```

Out[8]:

	DYRK1A_N	ITSN1_N	BDNF_N	NR1_N	NR2A_N	pAKT_N	pBRAF_N	pCAMKII_N	pCREB_N	pELK_N	...	SHH_N	BAD_N	BCL2_N	pS6_N	pCFOS_N
435	0.304966	0.477769	0.319786	2.596944	4.447364	0.227196	0.176165	4.218640	0.203972	1.279603	...	0.253098	0.137671	0.132904	0.136876	0.126152
436	0.298968	0.480565	0.315214	2.626784	4.473428	0.232007	0.175068	4.259338	0.201488	1.329335	...	0.263292	0.142504	0.134201	0.145857	0.142504
437	0.303297	0.485640	0.321380	2.606443	4.681811	0.228233	0.173986	4.226105	0.208479	1.433825	...	0.249487	0.143534	0.133823	0.153798	0.142271
438	0.303962	0.454134	0.314818	2.414511	4.004704	0.229781	0.182016	3.950606	0.196309	1.221277	...	0.246382	0.140363	0.135732	0.128497	0.125603
439	0.302761	0.473041	0.322587	2.527886	4.099685	0.242727	0.180656	4.016491	0.197517	1.299055	...	0.251730	0.150038	0.131296	0.132161	0.142253
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
1075	0.254860	0.463591	0.254860	2.092082	2.600035	0.211736	0.171262	2.483740	0.207317	1.057971	...	0.275547	0.190483	0.172645	0.115806	0.183324
1076	0.272198	0.474163	0.251638	2.161390	2.801492	0.251274	0.182496	2.512737	0.216339	1.081150	...	0.283207	0.190463	0.172645	0.113614	0.175674
1077	0.228700	0.395179	0.234118	1.733184	2.220852	0.220665	0.161435	1.989723	0.185164	0.884342	...	0.290843	0.216682	0.172645	0.118948	0.158296
1078	0.221242	0.412894	0.243974	1.876347	2.384088	0.208897	0.173623	2.086028	0.192044	0.922595	...	0.306701	0.222263	0.172645	0.125295	0.196296
1079	0.302626	0.461059	0.256564	2.092790	2.594348	0.251001	0.191811	2.361816	0.223632	1.064085	...	0.292330	0.227606	0.172645	0.118899	0.187556

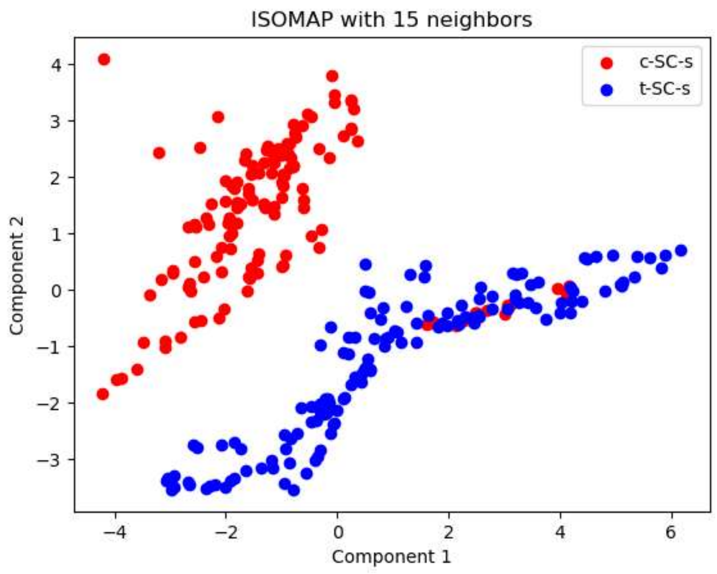
270 rows × 77 columns

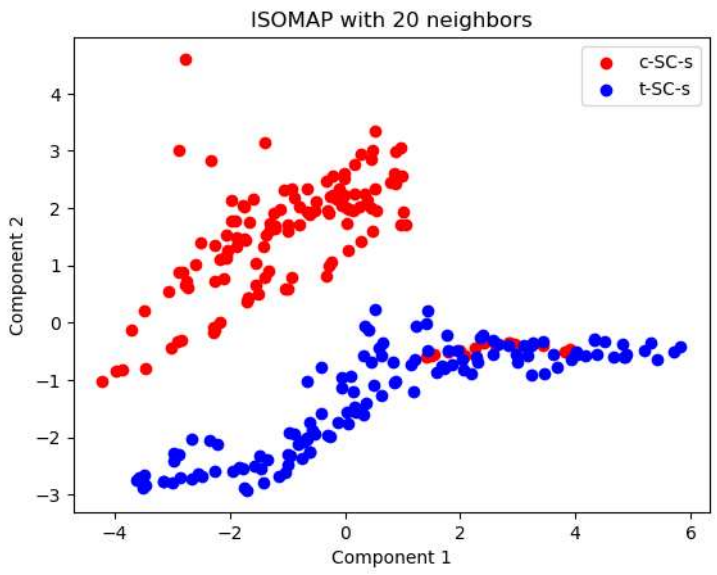
In [9]:
```
X = df_fltr
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X)
plt.scatter(X_pca[data_filtered['class'] == 'c-SC-s', 0], X_pca[data_filtered['class'] == 'c-SC-s', 1], c='red', label='c-SC-s')
plt.scatter(X_pca[data_filtered['class'] == 't-SC-s', 0], X_pca[data_filtered['class'] == 't-SC-s', 1], c='blue', label='t-SC-s')
plt.legend()
plt.xlabel('PC1')
plt.ylabel('PC2')
plt.title('PCA of mice protein expression dataset')
plt.show()
```

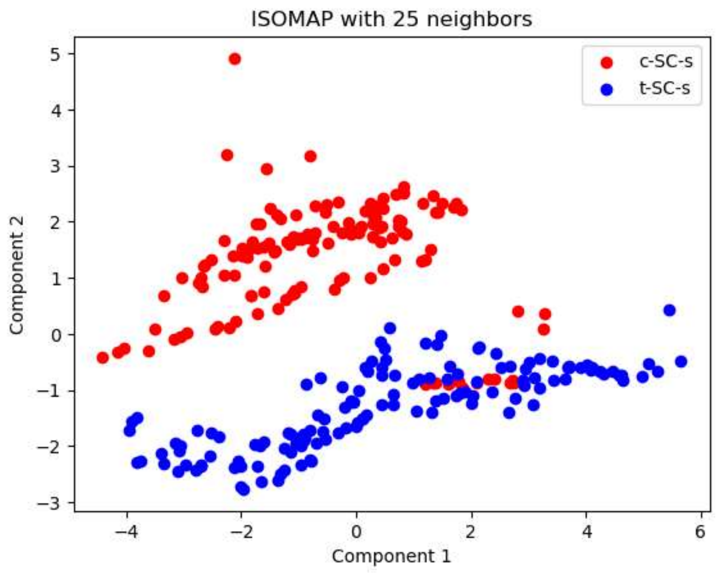


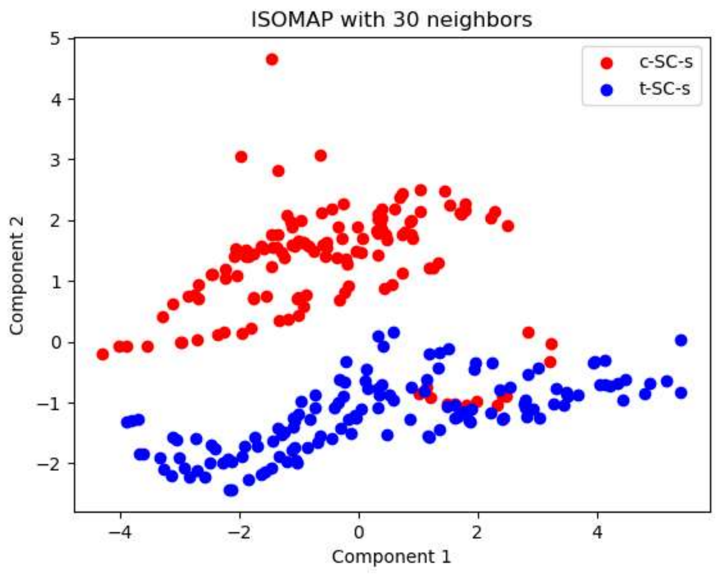
ISOMAP with different settings

In [10]:
```
n_neighbors = [ 15, 20, 25, 30]
for n in n_neighbors:
    isomap = Isomap(n_neighbors=n, n_components=2)
    X_isomap = isomap.fit_transform(X)
    plt.scatter(X_isomap[data_filtered['class'] == 'c-SC-s', 0], X_isomap[data_filtered['class'] == 'c-SC-s', 1], c='red', label='c-SC-s')
    plt.scatter(X_isomap[data_filtered['class'] == 't-SC-s', 0], X_isomap[data_filtered['class'] == 't-SC-s', 1], c='blue', label='t-SC-s')
    plt.legend()
    plt.xlabel('Component 1')
    plt.ylabel('Component 2')
    plt.title('ISOMAP with {} neighbors'.format(n))
    plt.show()
```


ISOMAP with 15 neighbors
c-SC-s
t-SC-s
Component 1
Component 2

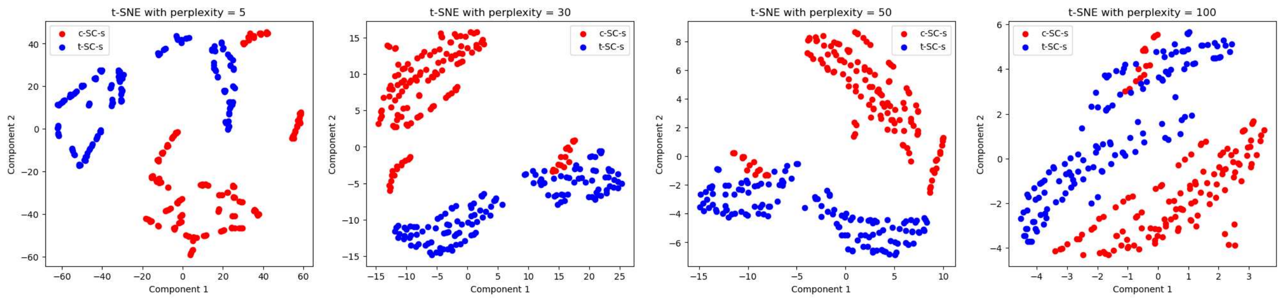

ISOMAP with 20 neighbors
c-SC-s
t-SC-s
Component 1
Component 2


ISOMAP with 25 neighbors
c-SC-s
t-SC-s
Component 1
Component 2



t-SNE with different settings

In [11]:
```python
perplexities = [5, 30, 50, 100]
plt.figure(figsize=(25, 5))

for i, perplexity in enumerate(perplexities):
    tsne = TSNE(n_components=2, perplexity=perplexity)
    X_tsne = tsne.fit_transform(X)

    plt.subplot(1, len(perplexities), i+1)
    plt.scatter(X_tsne[data_filtered['class'] == 'c-SC-s', 0], X_tsne[data_filtered['class'] == 'c-SC-s', 1], c='red', label='c-SC-s')
    plt.scatter(X_tsne[data_filtered['class'] == 't-SC-s', 0], X_tsne[data_filtered['class'] == 't-SC-s', 1], c='blue', label='t-SC-s')
    plt.legend()
    plt.xlabel('Component 1')
    plt.ylabel('Component 2')
    plt.title('t-SNE with perplexity = {}'.format(perplexity))

plt.show()
```



Yes

The t-SNE help us to separate the groups better than with PCA or ISOMAP.

Ex.2: Shrinkage in Linear Discriminant Analysis

b)

In [12]:
```python
df5=pd.read_csv("LDA-input.csv")
df5
```

Out[12]:

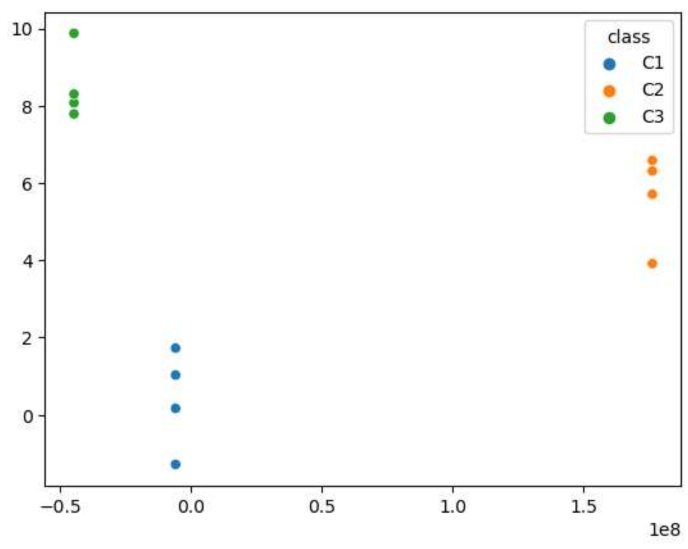
	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	class
0	-0.270712	0.104848	0.250528	-0.925200	0.567144	-1.040180	-0.153676	0.789852	-1.226216	-0.948007	C1
1	-0.569654	-0.977150	-0.770632	-0.033711	-1.032859	1.142427	-0.609778	1.469416	1.492679	0.707125	C1
2	-1.858490	-1.370624	-0.330106	-1.515290	1.200060	-1.822619	0.269385	-0.446424	1.114314	-1.380803	C1
3	1.015425	0.224081	-0.644551	0.661532	1.292965	-0.895312	-0.568311	-2.111618	-0.818308	-0.962384	C1
4	5.124502	0.108509	-0.439301	-0.713560	0.934181	0.058656	1.609714	0.859907	-0.985203	-0.958368	C2
5	5.449109	-0.942463	0.158909	0.388076	0.437338	0.418230	-0.732185	-1.428283	-2.009217	-0.233440	C2
6	6.803952	-1.948671	1.367851	-1.858739	-1.233951	-0.507570	1.407171	-0.941097	0.873505	1.135100	C2
7	6.165984	0.049214	0.510947	0.631299	0.887702	0.057652	-0.329544	-2.832079	-1.182554	-0.054846	C2
8	4.248352	6.510343	-0.171336	-0.458055	-1.338782	1.320063	-1.409329	-1.098297	-0.486751	-1.000971	C3
9	4.773877	4.555783	-0.548712	1.080016	-0.752434	1.158795	0.750871	-1.262713	-0.790701	-0.170789	C3
10	1.380615	4.642895	-0.634127	-0.561483	-1.025565	-0.254553	0.396176	0.516693	0.751490	1.148879	C3
11	3.238620	3.248823	0.310664	-1.081209	0.036498	-0.294449	-0.270871	-0.128858	-1.018221	-1.917969	C3

In [13]:

```python
clf = LinearDiscriminantAnalysis(solver='eigen')
x=df5.iloc[:,0:10].values
y=df5.iloc[:,10].values
cclf= clf.fit_transform(x,y)
xs5= cclf[:,0]
ys5= cclf[:,1]
sns.scatterplot(data=df5, x=xs5,y=ys5, hue="class")
```

Out[13]:

```
<Axes: >
```



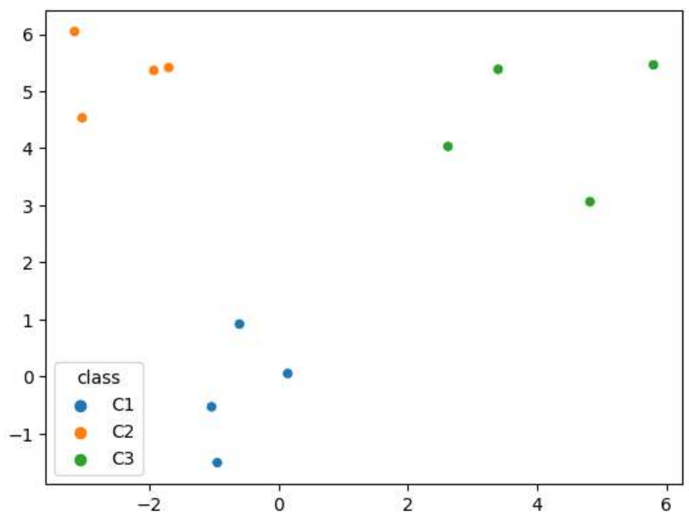
c)

In [14]:

```python
clf2 = LinearDiscriminantAnalysis(solver='eigen',shrinkage='auto')
cclf2= clf2.fit_transform(x,y)
xs52= cclf2[:,0]
ys52= cclf2[:,1]
sns.scatterplot(data=df5, x=xs52,y=ys52, hue="class")
```

Out[14]:

```
<Axes: >
```



We prefer this graph over before one as the sample covariance matrix was estimated poorly before as the graph features small number of samples. So, we can see that after using shrinkage parameter, it improves the Graph.

Ex.3: Pitfalls in t-SNE

a)

First we executed the t-SNE with three clusters each conating equal number of point. with 10 points per class, dimension = 50 and perplexity = 29. we obseserved that clusters were separated from each other but overlapping within eachother(inside clusters). then we run it with perplexity = 30. here we observed that the clusters were not much separated from eachother and also were not overlapping within eachother.

the reason of this big difference is because the lower values of perplexity controls the structure within clusters while the higher values of perplexity controls the structure between clusters.

we observed perplexity to be directly propotional to points per clusters, as when we increased the points per cluster from 10 to 11 with perplexity = 30, we obtained clusters separated from eachother but overlapping within eachother again.

b)

it is beacuse the points that are near the boundry could be local to each other in the higher dimension and when t-SNE mapps them into 2D it is trying to preserve both local and global structure of data. so, the points that are local to each other in higher dimension, appear closer in 2D square.

c)

The Square grid is breaking into smaller clusters because when perplexity is set to 2, t-SNE is focusing on perserving the small number of nearby points and is not able to preserve the overall global structure. thus, it is forming small clusters while breaking the grid.

d)

From perplexity value from 7 to onwards the resulting visualization start resembling the input data set. and for this we have tried 7 perplexity multiple times just to be sure. it gave use same visualization as input data set. any lower then 7 the circle get deshaped. larger the perplexity, the more global information or structure will be preserved in the dimensionality reduction. and for different data sets value of perplexity can vary.

Ex.4: KD Trees

a)

In [15]:
```
Array = np.array([(2,3),(3,8),(7,7),(4,5),(5,8),(3,5),(8,1),(8,2),(9,5),(9,8)])
query = [4 ,7]
KD = kdtree(Array)
```

In [16]:
```
temp = one_NN_rec(KD,0,query,KD.location,10)
```

```
3.0 3.0
2.0 2.0
1.4142135623730951 1.4142135623730951
```

b)

In [17]:
```
kNN_rec(KD,0,query,KD.location,3,10)
```

```
[7 7] 3.0
temp  temp1 (3.0, array([7, 7]), [array([7, 7]), array([7, 7])]) (3.0, array([7, 7]), [array([7, 7]), array([7, 7])])
[4 5] 2.0
temp  temp1 (2.0, array([4, 5]), [array([7, 7]), array([4, 5])]) (2.0, array([4, 5]), [array([7, 7]), array([4, 5])])
temp  temp1 (2.0, array([4, 5]), [array([4, 5])]) (2.0, array([4, 5]), [array([4, 5])])
[5 8] 1.4142135623730951
temp  temp1 (1.4142135623730951, array([5, 8]), [array([4, 5]), array([5, 8])]) (1.4142135623730951, array([5, 8]), [array([4, 5]), array
([5, 8])])
temp  temp1 (1.4142135623730951, array([5, 8]), [array([5, 8])]) (1.4142135623730951, array([5, 8]), [array([5, 8])])
```

Out[17]:
```
(1.4142135623730951,
 array([5, 8]),
 [array([7, 7]), array([7, 7]), array([5, 8])])
```