Section 15 Unsupervised Learning: Clustering

In addition to **dimension reduction**, another typical task of unsupervised machine learning is **clustering**: assigning the data samples into several groups (called clusters) based on their similarity -- similar samples should be in the same cluster, and dissimilar samples should be in different clusters.

Caution: Don't confuse clustering (unsupervised) with classification (supervised)!

K-Means Clustering

Mathematical Description: Given a set of observations $(x^{(1)}, x^{(2)}, \dots, x^{(n)})$, where each observation is a p-dimensional real vector, k-means clustering aims to partition the n samples into $K(\leq n)$ sets $S = S_1, S_2, \dots, S_K$ so as to minimize the within-cluster sum of squares (i.e. variance). Formally, the objective is to find the best parition of groups such that minimize the "loss function" of S

$$\min_S \sum_{i=1}^{K} \sum_{x \in S_i} \|x - \mu_i\|^2$$

where μ_i is the mean of points in S_i.

How to solve it: The exact solution to the K-means problem is NP hard. In practical, the common approach is to apply Lloyd's algorithm to find the heuristic solutions (local minimum).

In the iterative algorithm, each iteration contains two steps:

- (**assignment step**) Given the cluster center, update the cluster of data according to its nearest cluster center.
- (**update step**) Given the cluster assignment, update the cluster centers by calculating the means within each cluster.

The algorithm may converge if no further adjustments can be made.

Because the algorithm may stuck in local minimums, the practical strategy is to randomly initialize the algorithm, and run multiple parallel programs to find the best partition with smallest "loss function ".

Caution: Don't confuse K-means clustering with kNN classification!

Below we will apply the functions in scikit-learn. Note that to visualize the results of k-means on high-dimensional data, it is often combined with dimension reductions. Another pratical strategy is to use dimension reduction to pre-process the data, and apply clustering on the reduced datasets.

It is also worth noting that in practice, determining true number of clusters (K) is a very hard problem.

In [1]:
```
import pandas as pd
from sklearn.datasets import load_iris

#This cell is completely optional and is provided for context

iris = load_iris(as_frame=True)
df_iris = pd.DataFrame(iris.data,columns=iris.feature_names)
df_iris['target'] = pd.Series(iris.target)
df_iris.head()
```

Out[1]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
0	5.1	3.5	1.4	0.2	0
1	4.9	3.0	1.4	0.2	0
2	4.7	3.2	1.3	0.2	0
3	4.6	3.1	1.5	0.2	0
4	5.0	3.6	1.4	0.2	0

In [2]:
```
#from sklearn.datasets import load_iris
X,y = load_iris(return_X_y = True)

from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=3, random_state=0)
y_km = kmeans.fit_predict(X)
```

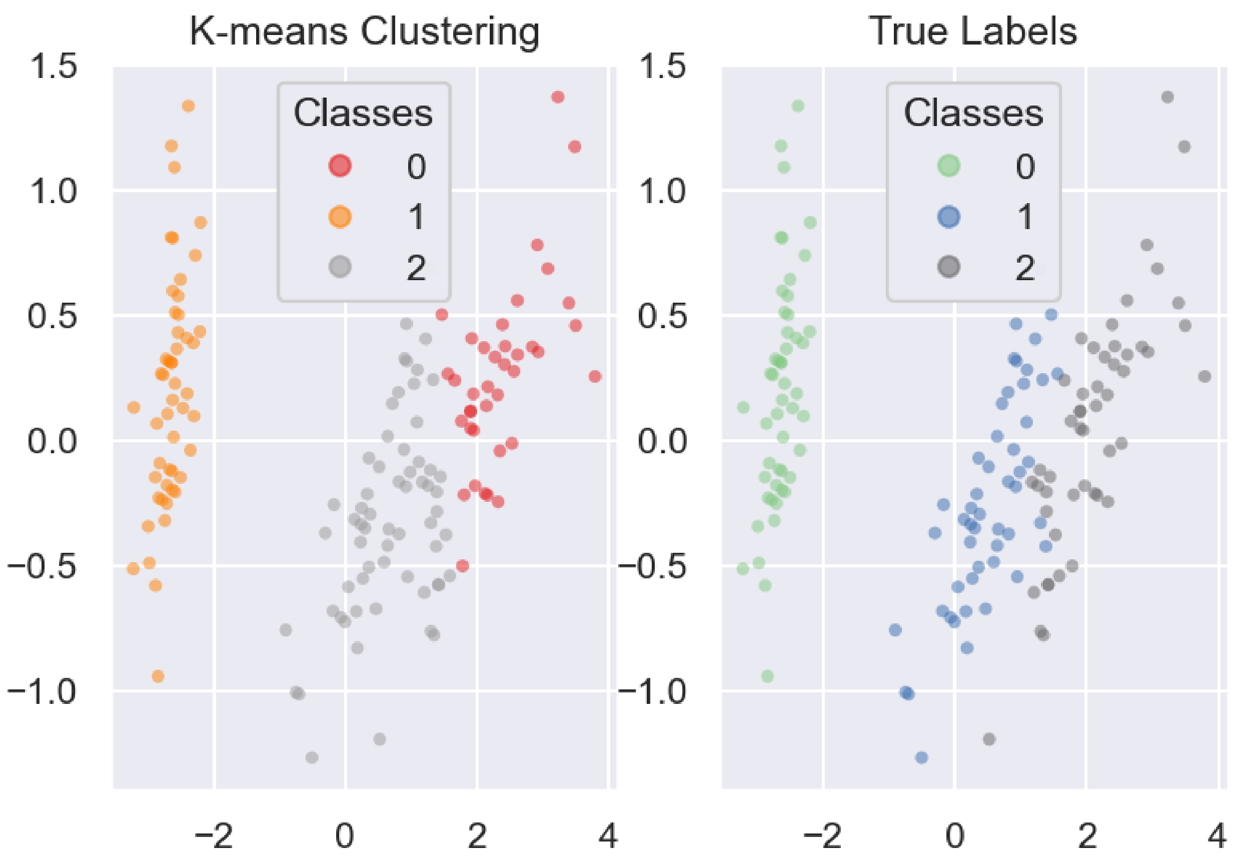
In [3]:
```
y_km
```

Out[3]:
```
array([1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 2, 2, 0, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 0, 2, 0, 0, 0, 0, 2, 0, 0, 0,
       0, 0, 0, 2, 2, 0, 0, 0, 0, 2, 0, 2, 0, 2, 0, 0, 2, 2, 0, 0, 0, 0,
       0, 2, 0, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 0, 2, 0, 0, 2])
```

In [4]:
```
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X)
```

In [5]:
```
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()
fig, (ax1, ax2) = plt.subplots(1, 2,dpi=150)

fig1 = ax1.scatter(X_pca[:, 0], X_pca[:, 1],c=y_km, s=15, edgecolor='none', alpha=0.5,c
fig2 = ax2.scatter(X_pca[:, 0], X_pca[:, 1],c=y, s=15, edgecolor='none', alpha=0.5,cmap
ax1.set_title('K-means Clustering')
legend1 = ax1.legend(*fig1.legend_elements(), loc="best", title="Classes")
ax1.add_artist(legend1)
ax2.set_title('True Labels')
legend2 = ax2.legend(*fig2.legend_elements(), loc="best", title="Classes")
ax2.add_artist(legend2)
```

```
Out[5]: <matplotlib.legend.Legend at 0x20233035c40>
```



To quantitatively measure the performace, it is not a good idea to naively compute "accuracy" as in the classification case, because permutation of the label values does not affect clustering results, while severely affects the "accuracy". There are many good measures considering such effects in the clustering.

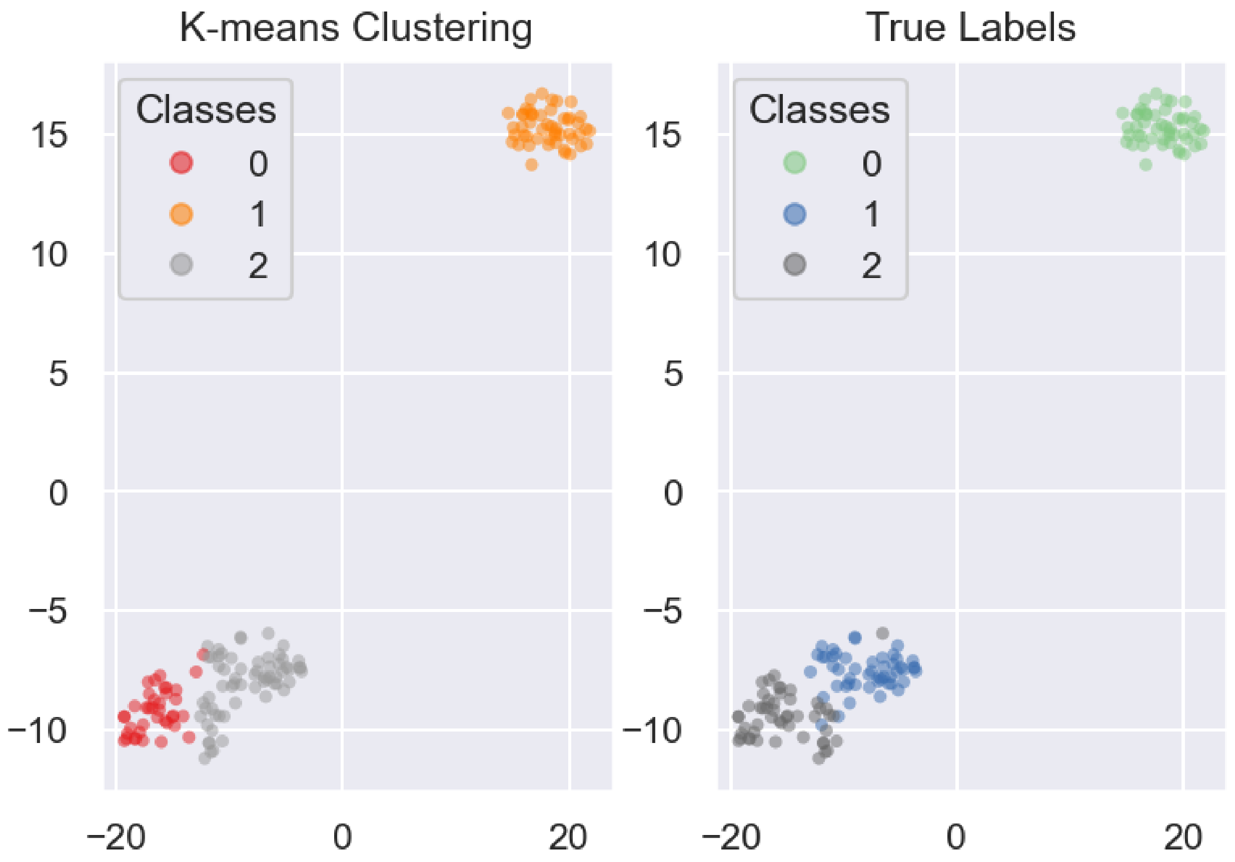
```
In [6]: from sklearn import metrics
        metrics.adjusted_rand_score(y_km, y)
```

```
Out[6]: 0.7302382722834697
```

```
In [7]: from sklearn.manifold import TSNE
        tsne = TSNE(random_state=0, n_jobs = -1) #t-distributed stochastic neighbor embedding
        X_tsne = tsne.fit_transform(X)


        fig, (ax1, ax2) = plt.subplots(1, 2,dpi=150)

        fig1 = ax1.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y_km, s=15, edgecolor='none', alpha=0.5
        fig2 = ax2.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y, s=15, edgecolor='none', alpha=0.5,cm

        ax1.set_title('K-means Clustering')
        #Colors from y_km, our fit at the top of this notebook

        legend1 = ax1.legend(*fig1.legend_elements(), loc="best", title="Classes")
        ax1.add_artist(legend1)
        ax2.set_title('True Labels')
```

```
legend2 = ax2.legend(*fig2.legend_elements(), loc="best", title="Classes")
ax2.add_artist(legend2)
```

Out[7]:
```
<matplotlib.legend.Legend at 0x202335cb280>
```



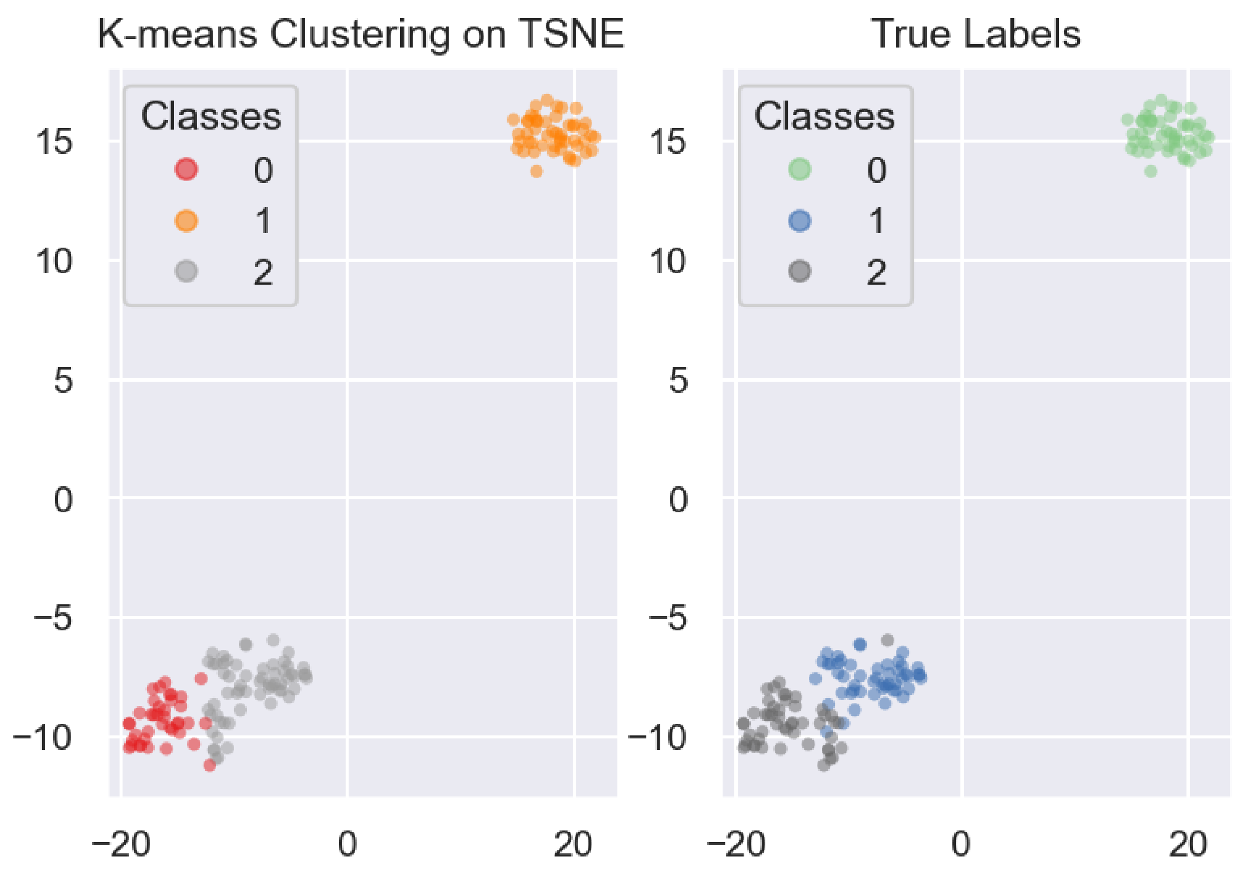
How about clustering on TSNE results?

In [8]:
```
y_km_tsne = kmeans.fit_predict(X_tsne)
metrics.adjusted_rand_score(y_km_tsne, y)
```

Out[8]:
```
0.7726314170414115
```

In [9]:
```
fig, (ax1, ax2) = plt.subplots(1, 2,dpi=150)

fig1 = ax1.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y_km_tsne, s=15, edgecolor='none', alph
fig2 = ax2.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y, s=15, edgecolor='none', alpha=0.5,cm

ax1.set_title('K-means Clustering on TSNE')
#colors from y_km_tsne in the cell above this one. Compare the colorings of the diagram

legend1 = ax1.legend(*fig1.legend_elements(), loc="best", title="Classes")
ax1.add_artist(legend1)
ax2.set_title('True Labels')
legend2 = ax2.legend(*fig2.legend_elements(), loc="best", title="Classes")
ax2.add_artist(legend2)
```

Out[9]:
```
<matplotlib.legend.Legend at 0x20233124a90>
```



Can we try other clustering methods?

```
In [10]:
from sklearn.mixture import GaussianMixture
gm = GaussianMixture(n_components = 3,random_state=0)
y_gm = gm.fit_predict(X)
```

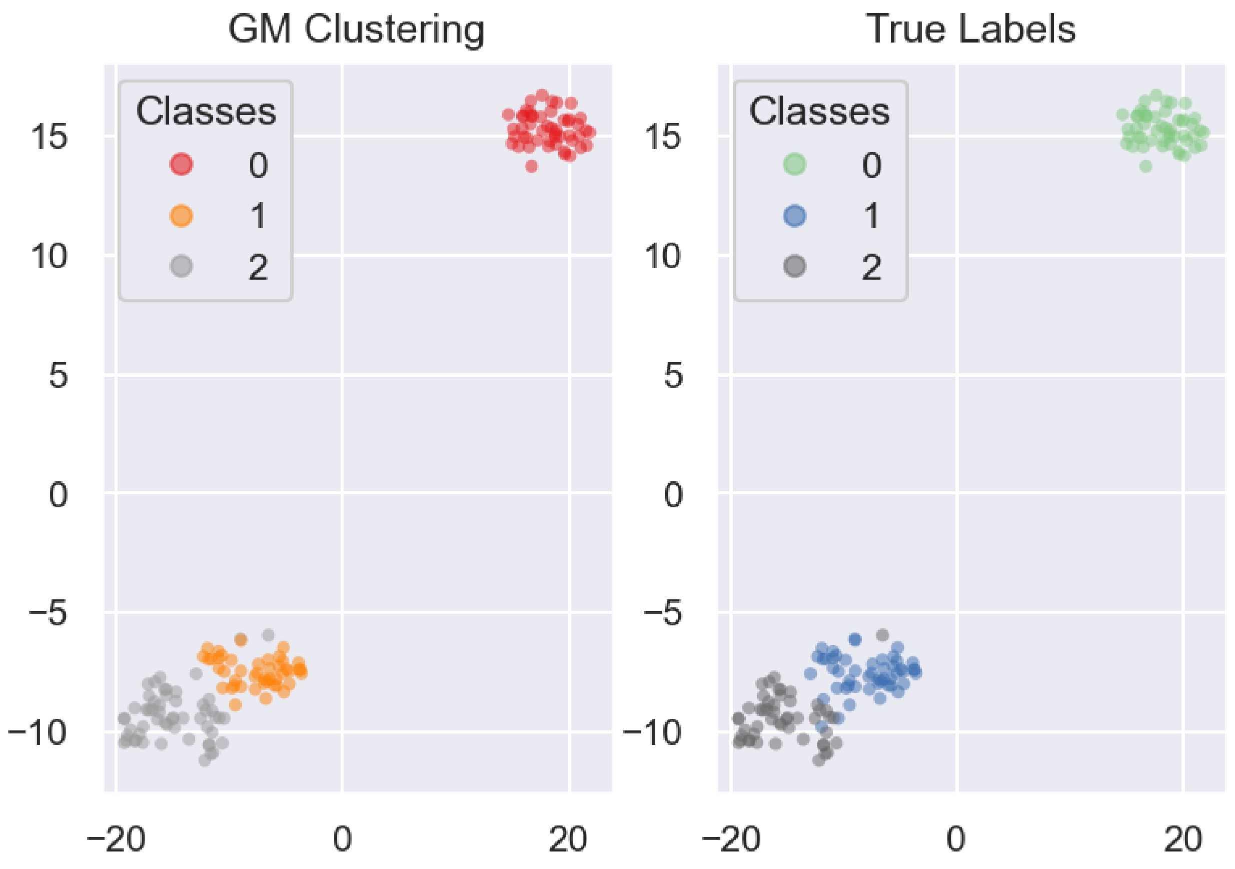
More information on Gaussian Mixture models

```
In [11]:
metrics.adjusted_rand_score(y_gm, y)
```

```
Out[11]: 0.9038742317748124
```

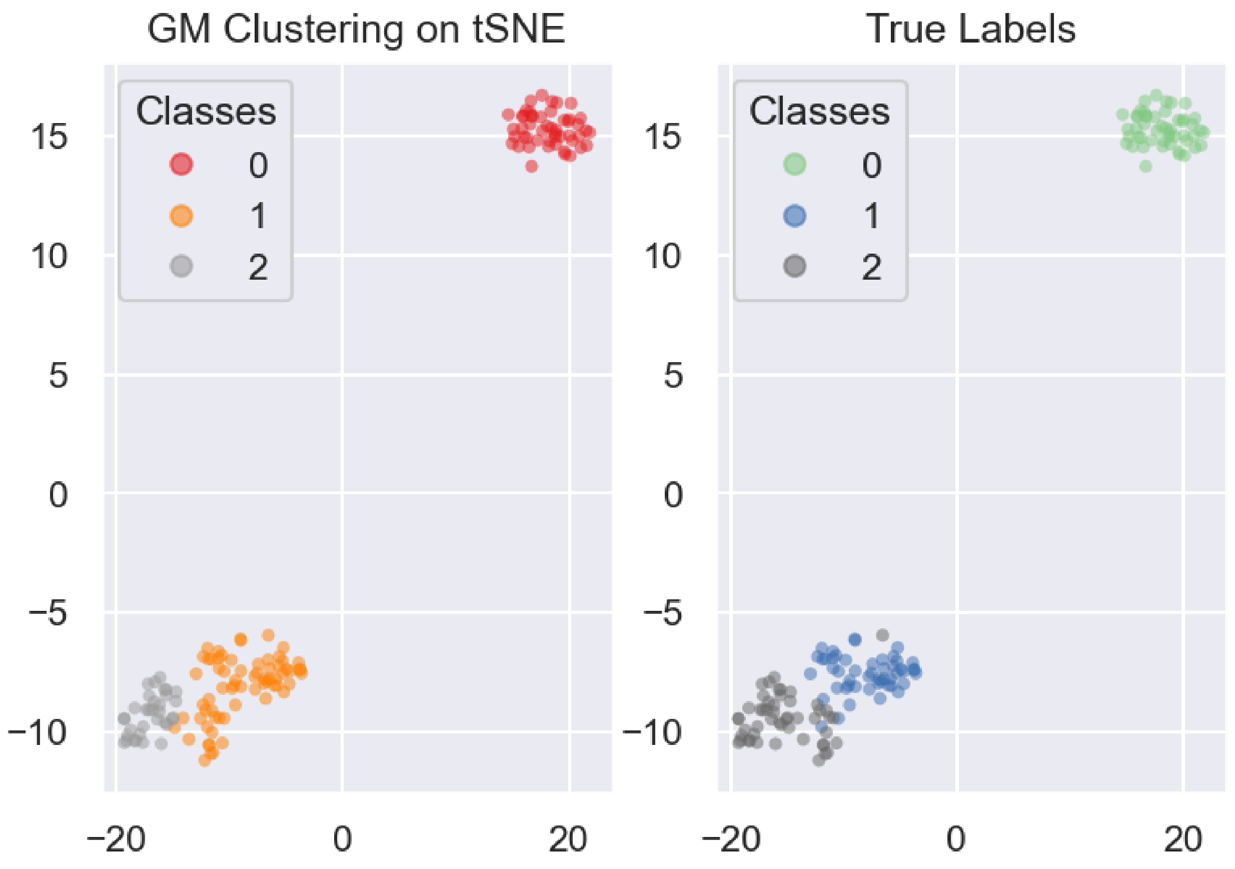
```
In [12]:
fig, (ax1, ax2) = plt.subplots(1, 2,dpi=150)

fig1 = ax1.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y_gm, s=15, edgecolor='none', alpha=0.5
fig2 = ax2.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y, s=15, edgecolor='none', alpha=0.5,cm
ax1.set_title('GM Clustering')
legend1 = ax1.legend(*fig1.legend_elements(), loc="best", title="Classes")
ax1.add_artist(legend1)
ax2.set_title('True Labels')
legend2 = ax2.legend(*fig2.legend_elements(), loc="best", title="Classes")
ax2.add_artist(legend2)
```

```
Out[12]: <matplotlib.legend.Legend at 0x2023322e040>
```



```
In [13]: y_gm_tsne = gm.fit_predict(X_tsne)
         metrics.adjusted_rand_score(y_gm_tsne, y) #Applying tsne to every model doesn't always

Out[13]: 0.7195837484778037
```

```
In [14]: fig, (ax1, ax2) = plt.subplots(1, 2,dpi=150)

         fig1 = ax1.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y_gm_tsne, s=15, edgecolor='none', alph
         fig2 = ax2.scatter(X_tsne[:, 0], X_tsne[:, 1],c=y, s=15, edgecolor='none', alpha=0.5,cm
         ax1.set_title('GM Clustering on tSNE')
         legend1 = ax1.legend(*fig1.legend_elements(), loc="best", title="Classes")
         ax1.add_artist(legend1)
         ax2.set_title('True Labels')
         legend2 = ax2.legend(*fig2.legend_elements(), loc="best", title="Classes")
         ax2.add_artist(legend2)

Out[14]: <matplotlib.legend.Legend at 0x202341e4820>
```



Explore yourself and you may upload your results to Kaggle!