

비지도학습 - 군집분석

K-means clustering

$m^{(k)}$, i 차원 $x = (x_0, \dots, x_i)$

1. 그룹 평균 $m^{(k)}$ 초기화
2. 그룹 할당 ($\text{argmin}[dm, x]$)
3. 평균 업데이트
4. 반복

가중치를 주지 않아 밀도 차이가 있을 경우 클러스터링이 잘 되지 않음. 초기 K 값은 사용자가 정해야 함.

```
In [11]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import make_blobs
```

```
In [15]: X, y = make_blobs(n_samples=100, n_features =2, centers=5, random_state=10)
```

```
In [17]: print(X.shape, y.shape)

(100, 2) (100,)
```

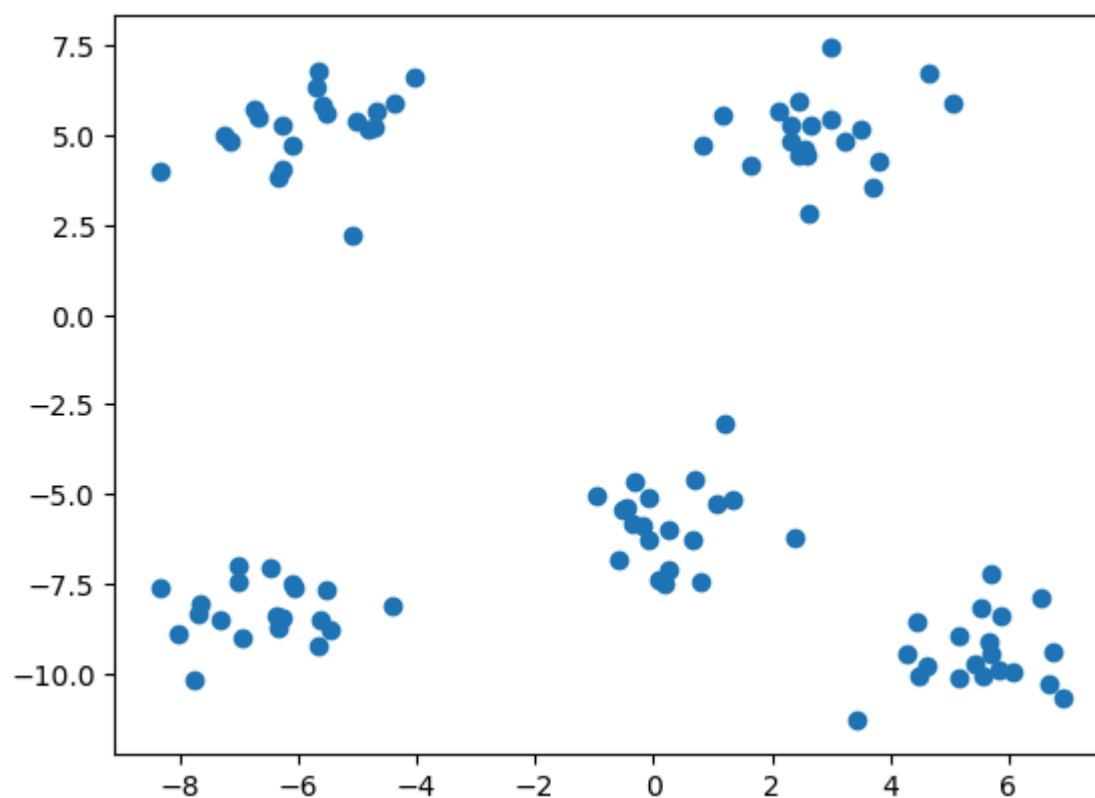
```
In [27]: X[:10]
```

```
Out[27]: array([[ -5.57785425,   5.87298826],
 [   1.62783216,   4.17806883],
 [ -6.95088443,  -9.02459449],
 [ -0.95276902,  -5.03431566],
 [   6.55010412,  -7.9123388 ],
 [ -6.67870531,   5.52444477],
 [ -5.52802829,   5.62491189],
 [ -8.03866378,  -8.91215049],
 [   5.55912116, -10.06110303],
 [ -7.26457869,   4.98882111]])
```

```
In [31]: y[:20]
```

```
Out[31]: array([3, 1, 4, 2, 0, 3, 3, 4, 0, 3, 4, 3, 0, 2, 0, 3, 1, 2, 0, 3])
```

```
In [33]: plt.scatter(X[:,0], X[:,1])
plt.show()
```



```
In [61]: # k = 5로 설정해야지~!
```

```
from sklearn.cluster import KMeans
kmc = KMeans(n_clusters=5, init='random', max_iter=200, random_state=222)
kmc.fit(X)
label_kmc = kmc.labels_
```

```
In [63]: print(label_kmc)
```

```
[0 3 4 2 1 0 0 4 1 0 4 0 1 2 1 0 3 2 1 0 0 2 3 4 0 0 2 1 4 3 2 2 1 2 0 1 4
 2 4 3 2 2 2 1 4 4 0 1 3 1 3 1 0 4 1 1 2 3 2 4 1 3 3 2 0 3 1 3 1 4 4 0 3 1
 2 2 4 3 0 0 1 1 3 2 3 4 2 4 2 4 3 4 0 3 3 3 4 0 0 4]
```

```
In [65]: kmc_columns = ['kmc_comp1', 'kmc_comp2']
X_kmc_df = pd.DataFrame(X, columns=kmc_columns)
X_kmc_df['target'] = y
X_kmc_df['label_kmc'] = label_kmc
X_kmc_df.head()
```

```
Out[65]:
```

	kmc_comp1	kmc_comp2	target	label_kmc
0	-5.577854	5.872988	3	0
1	1.627832	4.178069	1	3
2	-6.950884	-9.024594	4	4
3	-0.952769	-5.034316	2	2
4	6.550104	-7.912339	0	1

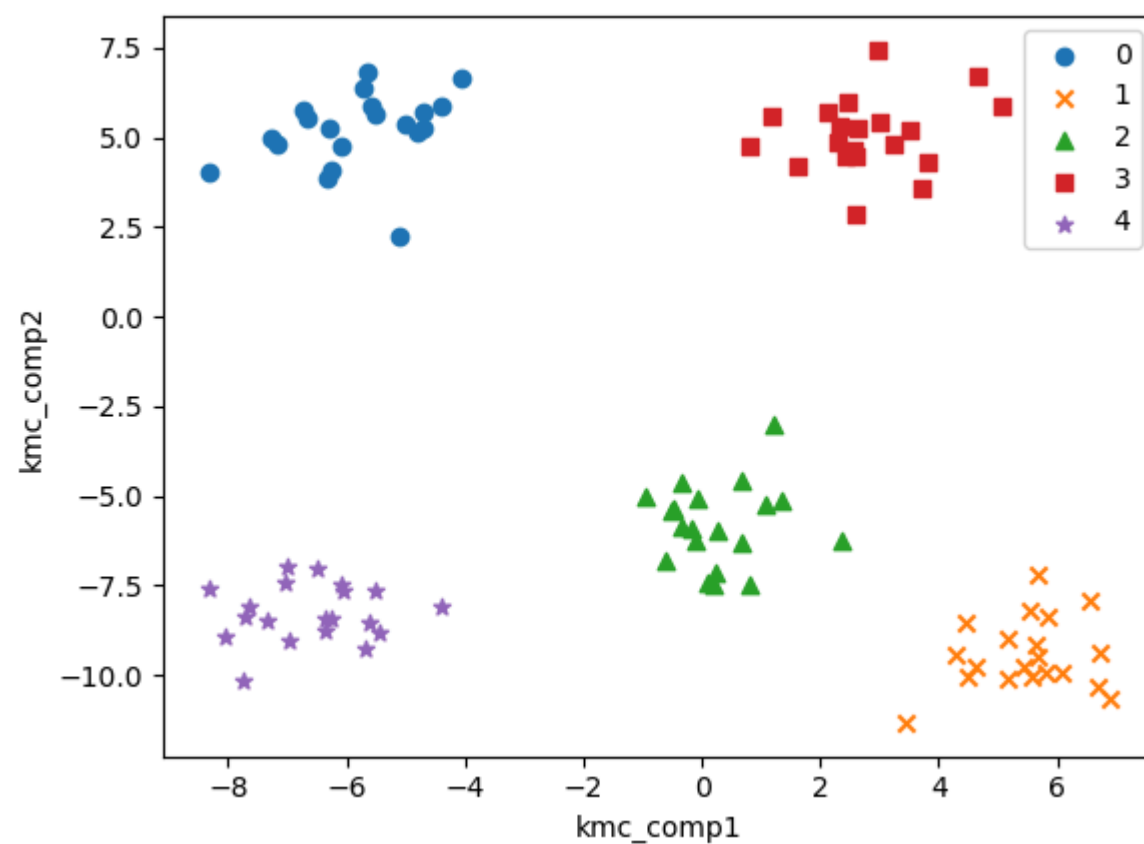
```
In [69]: print(set(X_kmc_df['target']))
print(set(X_kmc_df['label_kmc']))
```

```
{0, 1, 2, 3, 4}
{0, 1, 2, 3, 4}
```

```
In [73]: df = X_kmc_df
markers = ['o', 'x', '^', 's', '*']

for i, mark in enumerate(markers):
    df_i = df[df['label_kmc']==i]
    target_i = i
    X1 = df_i['kmc_comp1']
    X2 = df_i['kmc_comp2']
    plt.scatter(X1, X2, marker=mark, label=target_i)

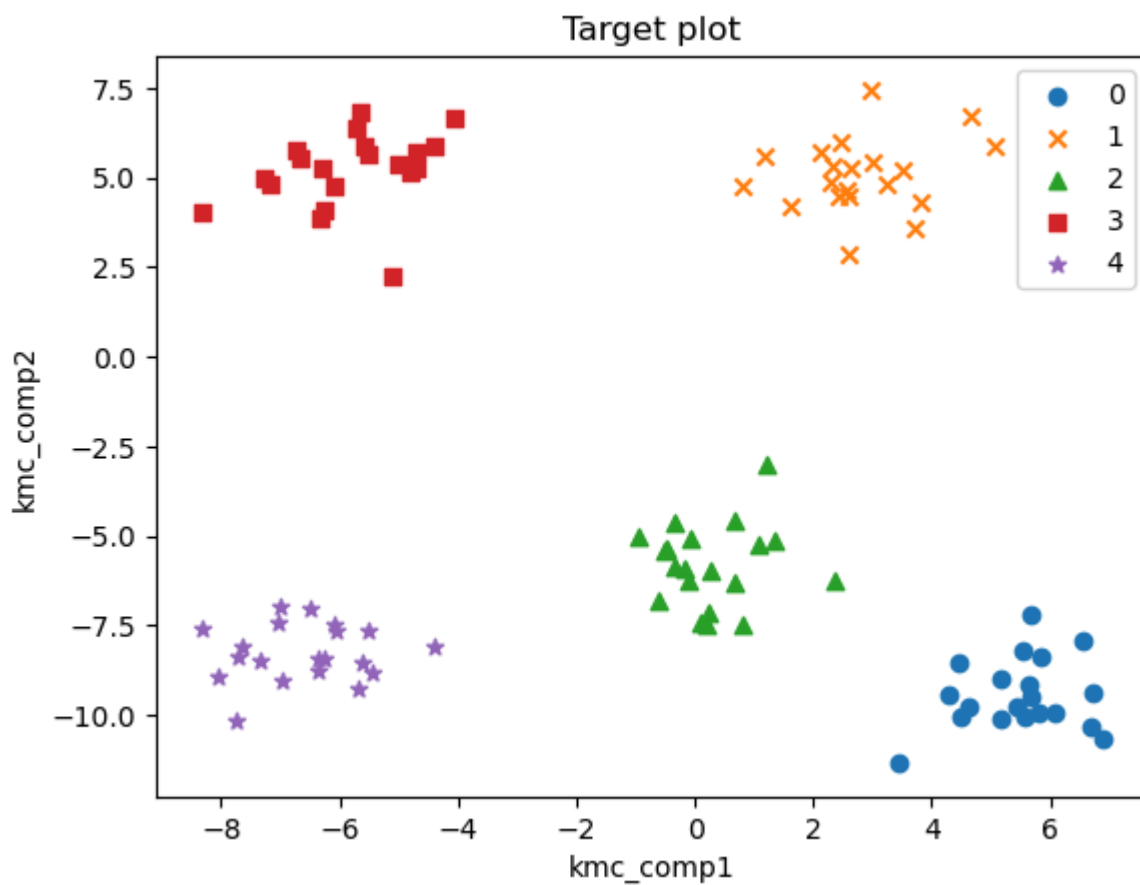
plt.xlabel('kmc_comp1')
plt.ylabel('kmc_comp2')
plt.legend()
plt.show()
```



```
In [75]: # 실제 target plot

for i, mark in enumerate(markers):
    df_i = df[df['target']==i]
    target_i = i
    X1 = df_i['kmc_comp1']
    X2 = df_i['kmc_comp2']
    plt.scatter(X1, X2, marker=mark, label=target_i)

plt.title('Target plot')
plt.xlabel('kmc_comp1')
plt.ylabel('kmc_comp2')
plt.legend()
plt.show()
```



```
In [77]: from sklearn.metrics import silhouette_score
sil_score = silhouette_score(X, label_kmc)
print(sil_score)
```

0.7598181300128782

계층 클러스터링

- 병합 계층 클러스터링 (Agglomerative) : 개별 데이터 포인트를 하나의 클러스터로 설정하고 시작, 이후 유사도에 따라 합침.
 - 연결방법 (Linkage Method) : 단일연결(Single Method), 가장 가까운 거리의 데이터를 비교 / 완전연결(Complete Method) 가장 먼거리의 데이터를 비교
- 분할 계층 클러스터링 (Divisive) : 전체 데이터 셋을 하나의 클러스터로 놓고 시작, 가장 멀리 떨어진 데이터를 다른 클러스터로 분리.

Dendrogram 으로 시각화 가능

병합계층클러스터링

- 전체 n 개 데이터로 구성된 데이터 셋을 n 개의 클러스터로 설정
- 각 데이터간 거리행렬 $D(n \times m)$ 계산. D 는 대칭행렬
- 거리행렬 D 에서 가장 가까운 클러스터 쌍을 찾아서 합침. ($u, v \rightarrow uv$)
- 거리 행렬에 새로운 클러스터(uv)를 설정하고 행, 열을 추가 및 기존 u, v 행, 열 은 삭제함.
- 단일연결의 경우 \min / 완전연결의 경우 \max 를 이용해 거리계산을 하여 3-4를 반복함.

Ward's 계층 클러스터링 정보의 손실을 최소화 하는 방향으로 클러스터링, 오차제곱합을 최소화하는 방법 이용
오차제곱합 > 각 데이터포인트가 클러스터 중심에서 얼마나 떨어져 있는 지를 의미함.

- 각 데이터포인트를 하나의 클러스터로 가정, 이 때 오차제곱합은 0이 됨.
- 모든 가능한 클러스터쌍을 고려하여 오차제곱합을 계산 후 가장 작은 오차 제곱합에 해당하는 클러스터를 만듦.
- 반복

```
In [105... X, y = make_blobs(n_samples =10, n_features = 2, random_state=1)
```

```
In [107... print(X.shape, y.shape)
```

(10, 2) (10,)

```
In [113... from sklearn.cluster import AgglomerativeClustering
aggc = AgglomerativeClustering(n_clusters = None, distance_threshold=0, linkage='complete')
label_aggc = aggc.fit_predict(X)
print(label_aggc)
```

[5 7 9 4 6 2 8 3 1 0]

```
In [123... aggc2 = AgglomerativeClustering(n_clusters = 2, linkage='complete')
label_aggc2 = aggc2.fit_predict(X)

print(label_aggc2)
```

```
[0 0 0 0 1 1 1 0 1 0]
```

```
In [121... agg3 = AgglomerativeClustering(n_clusters = 3, linkage='complete')
label_agg3 = agg3.fit_predict(X)

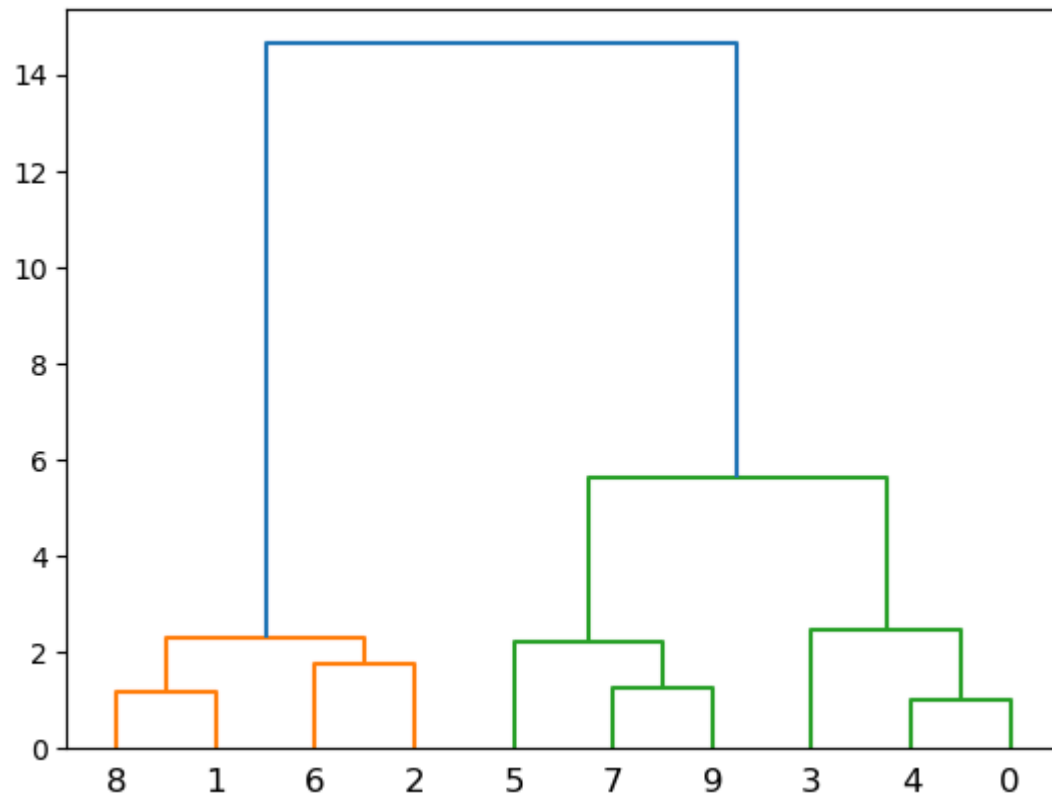
print(label_agg3)
```

```
[2 2 2 0 1 1 1 0 1 0]
```

```
In [129... from scipy.cluster.hierarchy import dendrogram
from scipy.cluster.hierarchy import linkage
import matplotlib.pyplot as plt

linked = linkage(X, 'complete')
labels = label_agg3
dendrogram(linked, orientation='top', labels=labels, show_leaf_counts=True)
plt.show
```

```
Out[129... <function matplotlib.pyplot.show(close=None, block=None)>
```



DBSCAN

밀집된 영역 : 클러스터 vs. 밀집 정도가 낮은 영역 : 클러스터 외부 영역 클러스터 개수를 미리 정하지 않음. 포인트간 거리 측정 -> 클러스터의 밀집 정도, 기본:Euclidean

** 반경 내에 외소한의 데이터 포인트 개수 이상이 존재한다. min_samples : 최소한의 데이터 포인트 개수 (hyperparameter)
eps : 데이터 포인트 개수를 측정할 반경

eps 내에 min_samples 개수 이상 존재하면 core point. eps 내 존재하는 데이터 포인트들 (border point)을 하나의 클러스터로 분류. 초기 핵심 데이터포인트는 무작위로 선정. eps 내 데이터포인트 개수가 min_samples 이하일 경우 noise로 labeling 함.
core point / border point / noise point

1. Eps-neighborhood of a point: Neps(x1)
2. Directly density-reachable: xn이 Neps(x1)에 속하고 Neps(x1)의 개수가 min_samples 이상. 항상 대칭적이지 않다.
3. Density-reachable
4. Density-connected

Cluster C: 데이터포인트 x1이 C에 속할 때 x1에 대해 xn이 density-reachable 하면 xn도 C 에 속하는 것. 이때 x1, xn 은 density connected 하다. Noise: 어떤 C에도 속하지 못한 포인트

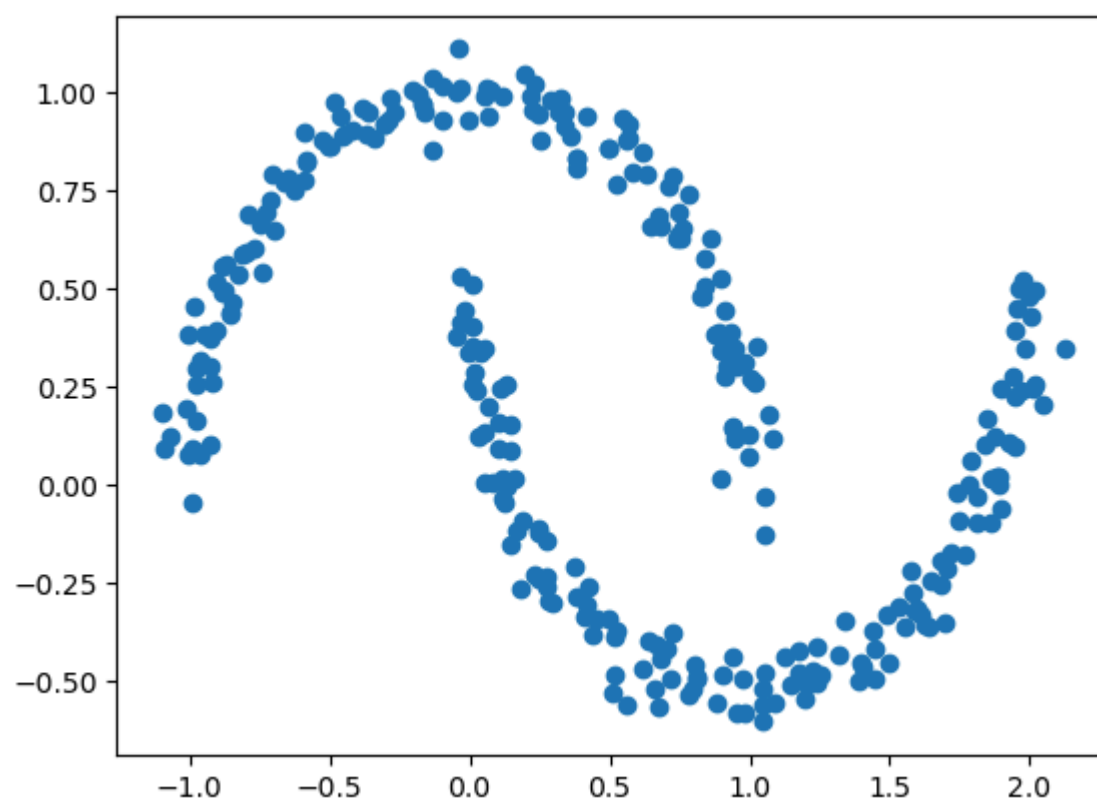
```
In [137... from sklearn.datasets import make_moons
X, y = make_moons(n_samples=300, noise=0.05, random_state=0)
```

```
In [139... print(X.shape)
print(y.shape)
```

```
(300, 2)
(300,)
```

```
In [143... plt.scatter(X[:,0], X[:,1])

plt.show()
```



```
In [145... from sklearn.cluster import DBSCAN
dbs = DBSCAN(eps=0.2)
dbs.fit(X)
label_dbs = dbs.labels_
print(label_dbs)
```

```
[0 0 1 0 0 1 0 0 1 1 0 1 0 0 1 1 0 1 0 0 0 1 1 1 0 1 0 0 0 0 1 1 1 1 0 0 0
0 0 1 0 1 1 1 1 1 0 1 1 1 1 0 0 1 1 0 0 1 0 0 1 1 1 0 0 0 0 1 1 1 0 0 0 1
1 0 1 1 0 1 1 0 0 0 0 1 0 0 0 0 0 1 0 0 0 0 1 1 0 1 0 0 1 0 1 0 0 0 0 0 0
0 1 1 0 1 0 0 1 1 1 1 1 1 1 1 0 0 0 1 1 0 1 1 1 0 0 0 1 0 1 1 0 1 1 1
1 0 0 1 0 0 0 1 1 1 0 1 0 1 1 1 0 1 1 1 0 0 1 0 0 1 0 0 1 1 1 0 0 1
1 0 1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 1 1 1 1 0 1 0 1 0 1 1 1 1 0 1 0 0 0 1
1 0 1 0 1 1 0 0 1 0 1 1 0 1 1 1 1 1 0 0 1 1 1 1 1 1 0 0 1 1 1 0 1
1 0 0 0 0 0 1 1 1 0 0 0 1 0 0 1 0 0 1 1 0 0 0 0 1 0 1 1 1 0 0 0 1 0 0
0 1 1 0]
```

```
In [147... dbs_columns = ['dbs_comp1', 'dbs_comp2']
X_dbs_df = pd.DataFrame(X, columns=dbs_columns)
X_dbs_df['target'] = y
X_dbs_df['label_dbs'] = label_dbs
X_dbs_df.head()
```

```
Out[147...   dbs_comp1  dbs_comp2  target  label_dbs
0    0.715413   -0.494089      1         0
1    0.246789   -0.240091      1         0
2    0.943261    0.346800      0         1
3    0.973742   -0.492901      1         0
4    1.239713   -0.411411      1         0
```

```
In [149... print(set(X_dbs_df['target']))
print(set(X_dbs_df['label_dbs']))
```

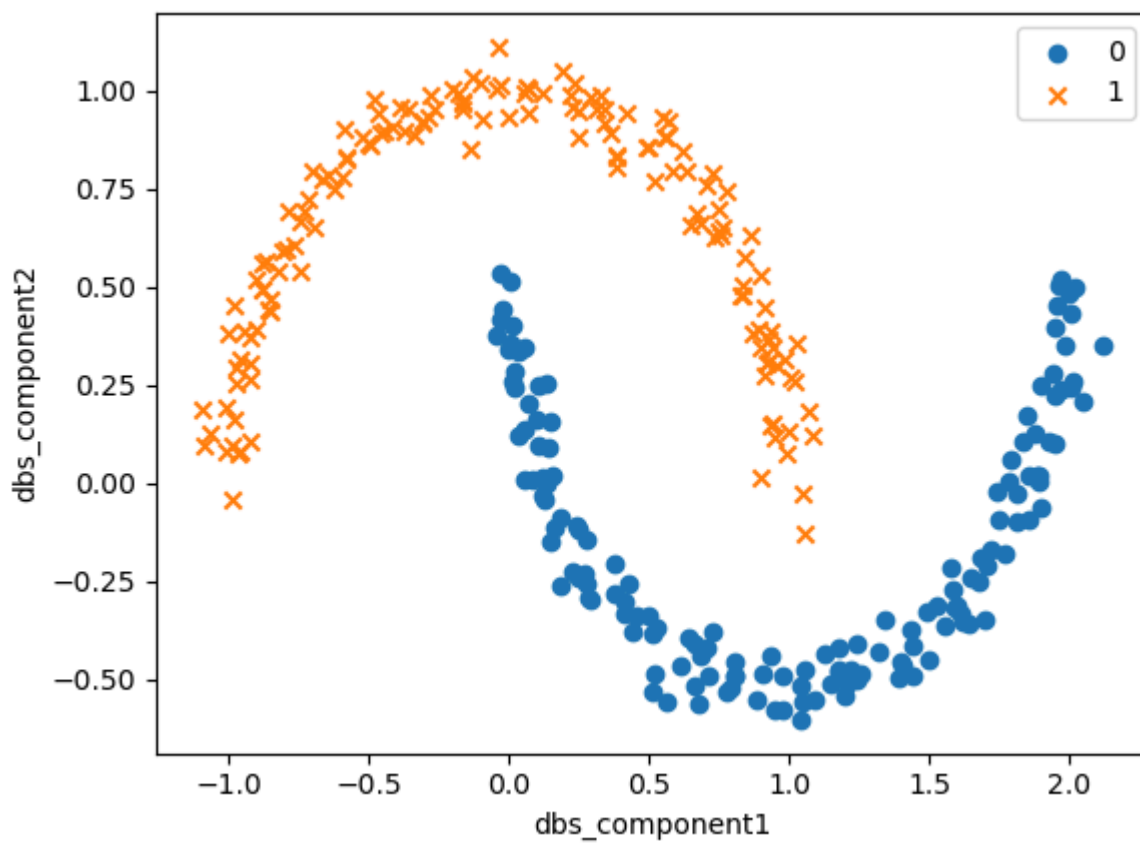
```
{0, 1}
{0, 1}
```

```
In [155... df = X_dbs_df
markers = ['o', 'x']

for i, mark in enumerate(markers):
    df_i = df[df['label_dbs']==i]
    target_i = i
    X1 = df_i['dbs_comp1']
    X2 = df_i['dbs_comp2']
    plt.scatter(X1, X2, marker=mark, label=target_i)

plt.xlabel('dbs_component1')
plt.ylabel('dbs_component2')

plt.legend()
plt.show()
```

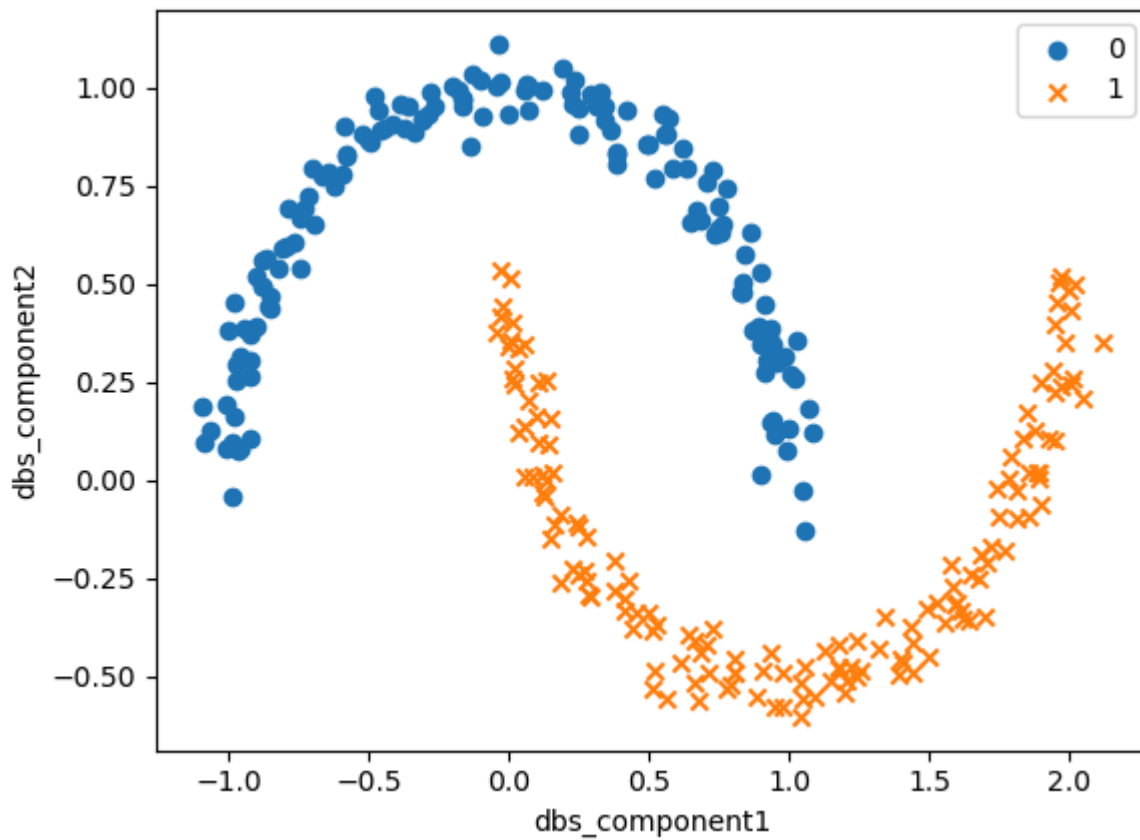


```
In [157... # 실제 타겟

for i, mark in enumerate (markers):
    df_i = df[df['target']==i]
    target_i = i
    X1 = df_i['dba_comp1']
    X2 = df_i['dba_comp2']
    plt.scatter(X1, X2, marker=mark, label=target_i)

plt.xlabel('dba_component1')
plt.ylabel('dba_component2')

plt.legend()
plt.show()
```



```
In [159... from sklearn.metrics import silhouette_score
sil_score = silhouette_score(X, label_dbs)
print(sil_score)
```

0.3284782012631504

가우시안 혼합 모형

전체 집단 내부에 속한 하위 집단의 존재를 가정한 확률 모델.

한 하위 집단 당 parameter = (평균 μ , 표준편차(다변량 Σ /단변량 σ), 전체분포에 대한 해당 하위분호의 비율 π) 데이터가 특정 집단에 속하는 경우 ~ 잠재변수(latent variable) z (unobservable)

Parameter를 추정해보자! EM 알고리즘 = E-step & M-step 을 반복하여 로그가능도함수를 증가시키는 방법.

1. Initialization - μ , σ , π
2. E-step: r_{ic} (i 번째 데이터가 그룹 c 에서 추출되었을 확률, responsibility) 구하기
3. M-setp: 구하고 싶었던 parameter 모두를 구함 (μ , σ , π) * 그룹개수, parameter update

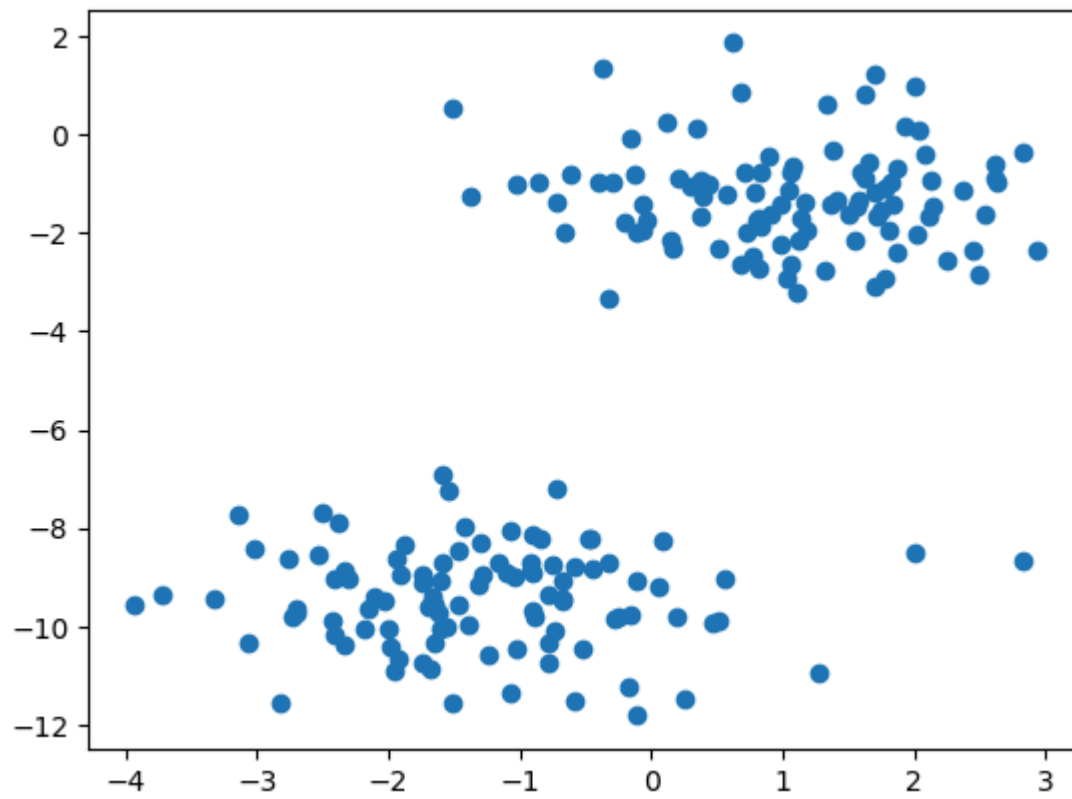
단점: 수렴속도가 느리고 local optimization 문제가 발생할 수 있음. K-nn과 마찬가지로 초기에 그룹개수를 정해줘야 함.

```
In [165... X, y = make_blobs(n_samples=200, n_features=2, centers=2, random_state=2)
```

```
In [167... print(X.shape, y.shape)
```

```
(200, 2) (200,)
```

```
In [173... plt.scatter(X[:,0], X[:,1])  
plt.show()
```



```
In [177... X
```

```
Out[177... array([[ 0.38115481, -1.64481461],
 [ -0.58390398, -8.78405909],
 [  1.83086535, -1.42523455],
 [  1.81313467, -1.92467083],
 [ -1.65577138, -9.55594613],
 [ -0.13265422, -0.80505548],
 [ -2.69891251, -9.73324948],
 [  0.18757605, -9.8171527 ],
 [  1.92513692,  0.17477999],
 [ -0.24707289, -9.8104778 ],
 [  0.80420551, -1.74288075],
 [ -1.39452325, -9.97964956],
 [ -1.60515159, -10.04170987],
 [  0.83352543, -0.74460559],
 [ -1.46957122, -9.55869403],
 [  1.55591864, -1.4580672 ],
 [  1.05937597, -0.7579938 ],
 [  2.13810493, -1.44566983],
 [  1.1848232 , -1.95576116],
 [ -0.37638912,  1.3767851 ],
 [ -0.6172497 , -0.79361238],
 [ -1.68399423, -10.86599403],
 [  0.42186795, -1.00112008],
 [  0.81825271, -2.73069558],
 [ -0.16344961, -0.05951747],
 [  0.67755635, -2.64355425],
 [ -0.90965742, -8.1218415 ],
 [ -0.65895073, -1.96921394],
 [  0.44030012, -0.99402533],
 [ -0.91504844, -8.70739333],
 [ -3.01806146, -8.44065141],
 [ -1.02353151, -10.47025441],
 [  1.59306999, -0.74416768],
 [ -0.66995787, -9.05797846],
 [ -2.50153112, -7.67699872],
 [  1.10320057, -3.20707537],
 [ -0.58498235, -11.51494191],
 [ -0.4075959 , -0.98602662],
 [  1.506501 , -1.62839627],
 [ -1.93335222, -8.63901908],
 [  0.20550002, -0.86879848],
 [ -2.41442044, -10.18889625],
 [  1.62504848, -0.87595942],
 [  0.29507856, -1.05360095],
 [ -1.95777753, -10.92091439],
 [ -1.46335853, -8.46162063],
 [ -1.42824915, -7.98003845],
 [ -0.84660563, -8.20309613],
 [ -0.45064353, -8.8508534 ],
 [  1.71860282, -1.65302661],
 [ -1.5841884 , -6.8961805 ],
 [ -0.72081785, -1.37019171],
 [ -2.76256743, -8.63516347],
 [ -1.55628145, -9.99835926],
 [  1.02581503, -2.93411237],
 [  0.33970811,  0.11528184],
 [  0.82608078, -1.87016308],
 [ -3.93955141, -9.57292799],
 [  2.12599563, -0.9232473 ],
 [ -1.2800922 , -8.93912279],
 [  1.36979547, -1.42903191],
 [ -1.06398595, -11.34008775],
 [  0.78454593, -1.15593416],
 [ -1.50834952, -11.55108763],
 [ -2.34090099, -8.88980884],
 [  0.88989739, -0.44520158],
 [ -1.9993558 , -10.06488996],
 [  1.99964344, -8.51061404],
 [  0.70973004, -0.75512788],
 [  1.70677401,  1.23618273],
 [  1.8230386 , -0.9574862 ],
 [ -1.66161844, -9.41498635],
 [ -2.30151669, -9.04907966],
 [  1.77939563, -1.09938345],
 [ -0.11858047, -9.09539732],
 [  1.86284776, -2.38064272],
 [  0.15873435, -2.29051183],
 [  1.57945366, -1.31393944],
 [ -0.32431771, -3.31914574],
 [ -1.91775697, -10.66908765],
 [  0.98564842, -2.22738281],
 [ -0.78216181, -9.35497119],
 [ -3.71486953, -9.36874886],
 [ -1.69941844, -9.61380426],
 [ -1.03866233, -8.98404971],
 [  0.82017839, -1.68889855],
 [  2.82419621, -0.35337615],
```


[-1.60368203, -9.05765066],
[0.62173043, 1.86741382],
[2.49020135, -2.82466326],
[0.55523077, -9.04078549],
[-0.45539895, -8.23326244],
[-0.74104364, -10.07763506],
[-1.29923245, -8.30647414],
[0.77192861, -2.46670777],
[-1.09969215, -8.92831109],
[0.91100418, -1.59821873],
[-0.06811619, -1.40206897],
[-0.10604775, -1.97508279],
[-0.77824475, -10.32568907],
[0.05546421, -9.17884603],
[1.86409032, -0.70074535],
[-0.75580553, -8.74619579],
[-1.97869191, -10.41036729],
[0.99104311, -1.43284403],
[-3.07353754, -10.32322273],
[-2.02797291, -9.47245011],
[-1.54915892, -7.25010857],
[-0.85715442, -0.96306408],
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```
[ -0.92096863, -8.85925495],
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[  0.72986148, -1.97091264],
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[ -2.3788409 , -7.89698831],
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[ -0.16221522, -9.75571745],
[  0.5124909 , -9.91048868],
[  1.32915795,  0.61082376],
[  0.25165836, -11.46732114]])
```

```
In [179... from sklearn.mixture import GaussianMixture
gmm = GaussianMixture(n_components=2, random_state=0)
gmm.fit(X)
label_gmm = gmm.predict(X)
print(label_gmm)
```

```
[1 0 1 1 0 1 0 0 1 0 1 0 0 1 0 1 1 1 1 1 0 1 1 1 1 0 1 1 0 0 0 1 0 0 1 0
 1 1 0 1 0 1 1 0 0 0 0 0 1 0 1 0 0 1 1 0 1 0 1 0 1 0 0 1 0 0 1 1 1 0 0 1
 0 1 1 1 1 0 1 0 0 0 0 1 1 0 1 1 0 0 0 0 1 0 1 1 1 0 0 1 0 0 1 0 0 0 1 0 0
 1 1 1 1 0 1 1 1 1 1 1 0 0 0 1 0 0 1 1 1 0 0 1 0 0 0 0 1 1 0 1 1 0 0 0 0 1
 1 0 1 0 1 1 0 0 1 1 0 0 1 1 1 0 0 1 1 0 0 0 0 0 1 1 0 1 0 1 0 1 0 1 1
 0 0 1 0 0 1 1 0 1 1 0 0 0 1 0]
```

```
In [181... gmm_columns = ['gmm_comp1', 'gmm_comp2']
X_gmm_df = pd.DataFrame(X, columns=gmm_columns)
X_gmm_df['target'] = y
X_gmm_df['label_gmm'] = label_gmm
X_gmm_df.head()
```

```
Out[181...      gmm_comp1  gmm_comp2  target  label_gmm
0      0.381155   -1.644815      1          1
1     -0.583904   -8.784059      0          0
2      1.830865   -1.425235      1          1
3      1.813135   -1.924671      1          1
4     -1.655771   -9.555946      0          0
```

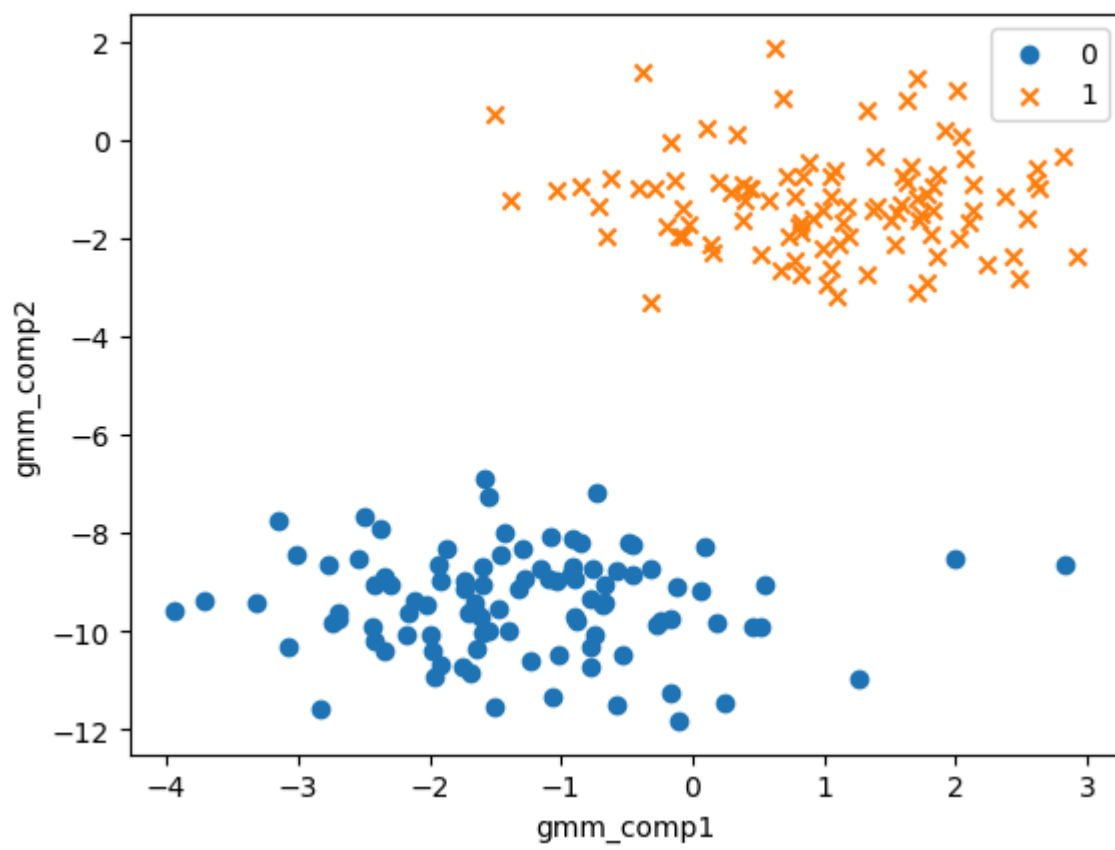
```
In [183... print(set(X_gmm_df['target']))
print(set(X_gmm_df['label_gmm']))
```

```
{0, 1}
{0, 1}
```

```
In [187... df = X_gmm_df
markers = ['o', 'x']

for i, mark in enumerate(markers):
    df_i = df[df['label_gmm']==i]
    target_i = i
    X1 = df_i['gmm_comp1']
    X2 = df_i['gmm_comp2']
    plt.scatter(X1, X2, marker = mark, label = target_i)

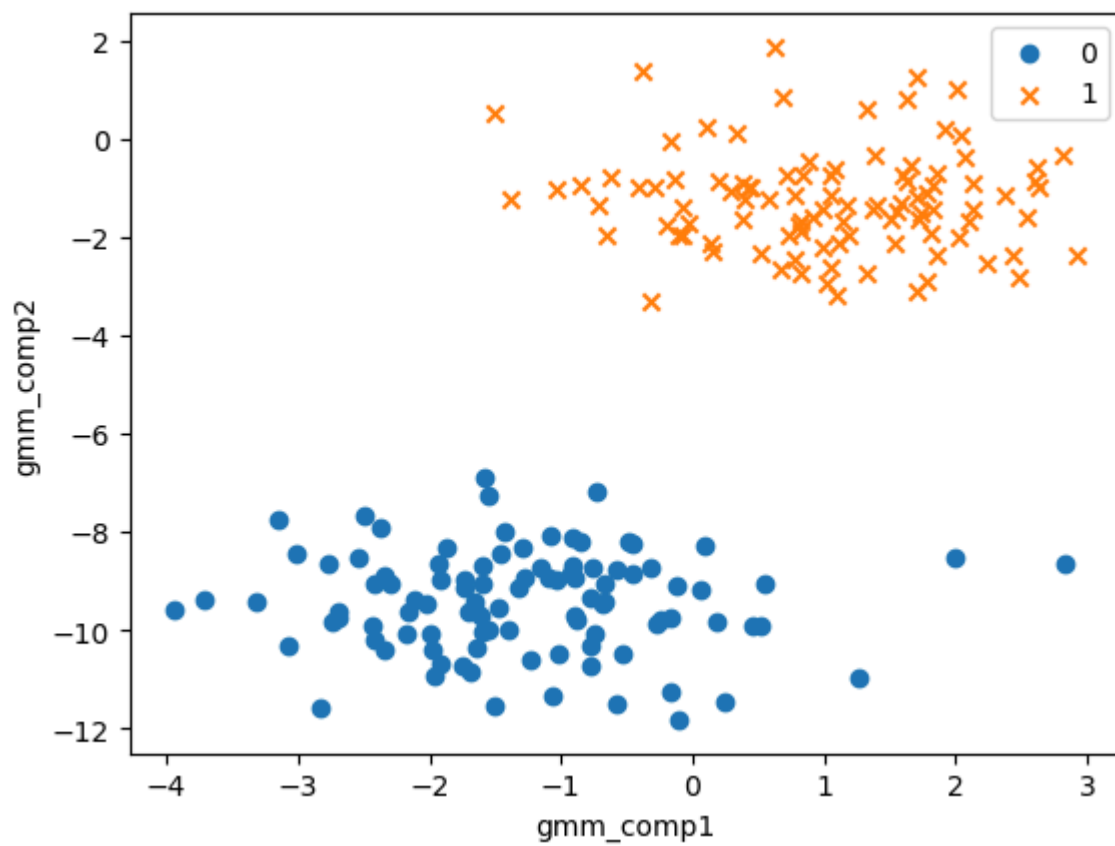
plt.xlabel('gmm_comp1')
plt.ylabel('gmm_comp2')
plt.legend()
plt.show()
```



```
In [189... # 실제 target plot

for i, mark in enumerate(markers):
    df_i = df[df['target']==i]
    target_i = i
    X1 = df_i['gmm_comp1']
    X2 = df_i['gmm_comp2']
    plt.scatter(X1, X2, marker = mark, label = target_i)

plt.xlabel('gmm_comp1')
plt.ylabel('gmm_comp2')
plt.legend()
plt.show()
```



```
In [193... from sklearn.metrics import silhouette_score
sil_score = silhouette_score(X, label_gmm)
print(sil_score)
```

0.7842908753561848

In []: