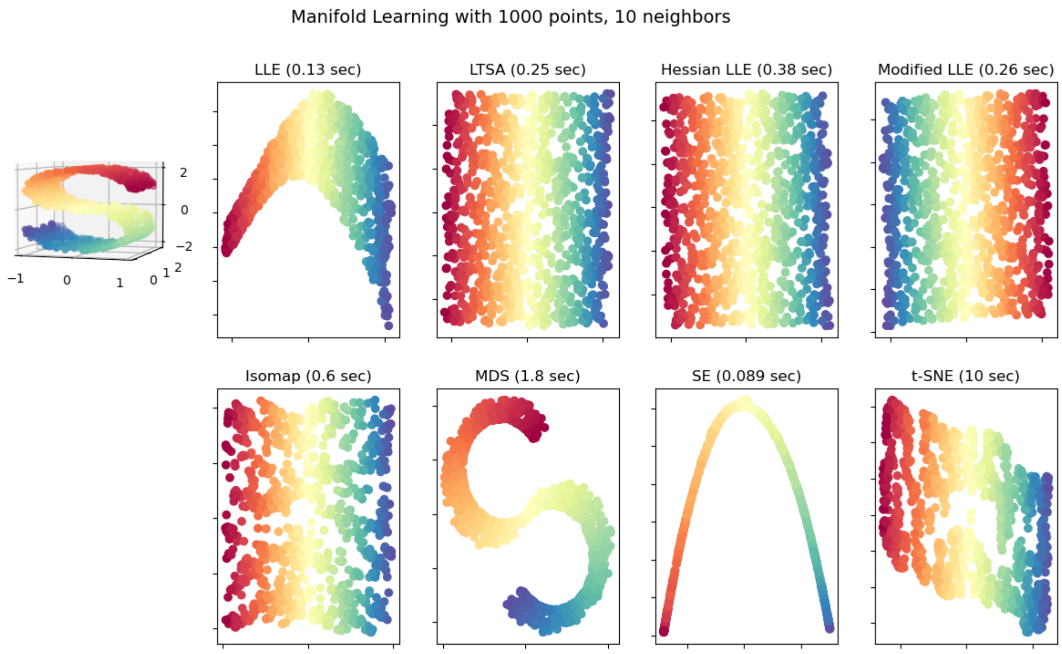
다양체 학습 (Manifold Learning)

- 높은 차원의 데이터를 저차원으로 축소하는 방법



- 고차원 데이터를 2차원 또는 3차원으로 축소해 시각화에 활용할 수 있음
- 차원 축소 과정에서 중요하지 않은 정보는 버려지고 중요한 정보만 남기 때문에 데이터 정제에 활용 가능

데이터 생성 및 시각화 함수

```
import numpy as np
import matplotlib.pyplot as plt
plt.style.use(['seaborn-whitegrid'])

from sklearn import manifold
from sklearn import random_projection
from sklearn import datasets
```

```
s_curve, color = datasets.make_s_curve(1000, random_state=0)
```

```
digits, labels = datasets.load_digits(return_X_y=True)
rand_proj = random_projection.SparseRandomProjection(n_components=3, random_state=0)
projected_digits = rand_proj.fit_transform(digits)
```

```
def min_max_scale(x):
  min_value, max_value = np.min(x, 0), np.max(x, 0)
  x = (x - min_value) / (max_value - min_value)
```

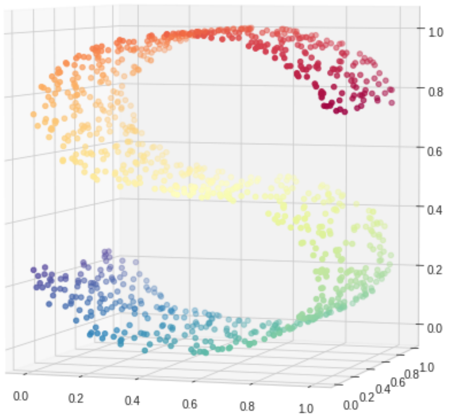
```
  return x
```

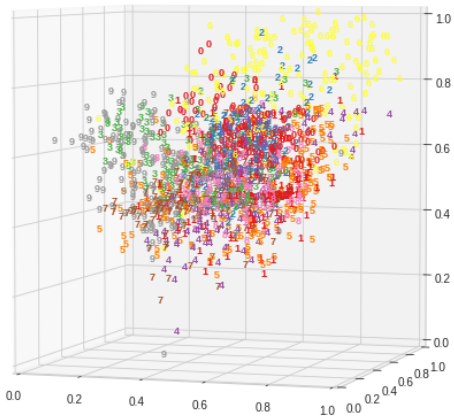
```
def plot_s_curve(s_curve, color, position, projection):
  s_curve = min_max_scale(s_curve)
  if projection == '3d':
    ax = plt.subplot(position, projection=projection)
    ax.scatter(s_curve[:, 0], s_curve[:, 1], s_curve[:, 2], c=color, cmap=plt.cm.Spectral)
    ax.view_init(4, -72)
  elif projection == '2d':
    ax = plt.subplot(position)
    ax.scatter(s_curve[:, 0], s_curve[:, 1], c=color, cmap=plt.cm.Spectral)
```

```
def plot_digits(digits, labels, position, projection):
  digits = min_max_scale(digits)
  if projection == '3d':
    ax = plt.subplot(position, projection=projection)
    for i in range(digits.shape[0]):
      ax.text(digits[i, 0], digits[i, 1], digits[i, 2], str(labels[i]),
              color=plt.cm.Set1(labels[i] / 10.), fontdict={'weight':'bold', 'size': 9})
    ax.view_init(4, -72)
  elif projection == '2d':
    ax = plt.subplot(position)
    for i in range(digits.shape[0]):
      ax.text(digits[i, 0], digits[i, 1], str(labels[i]),
              color=plt.cm.Set1(labels[i] / 10.), fontdict={'weight':'bold', 'size': 9})
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve, color, 121, '2d')
plot_digits(projected_digits, labels, 122, '2d')
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve, color, 121, '3d')
plot_digits(projected_digits, labels, 122, '3d')
```



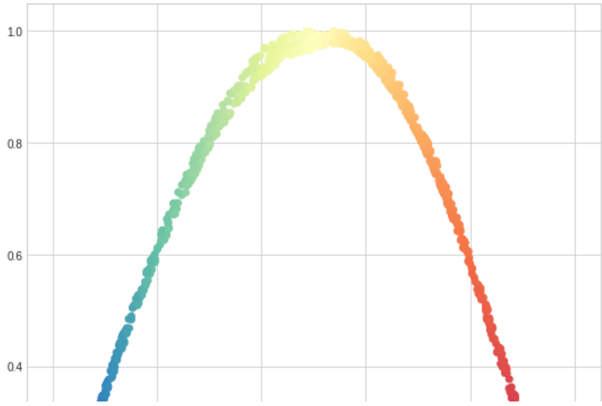


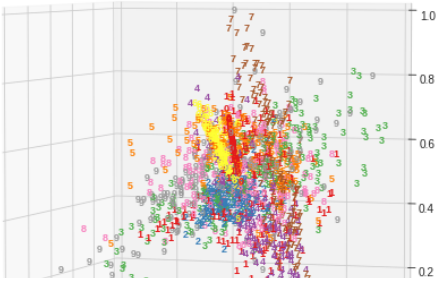
Locally Linear Embedding (LLE)

- 국소 이웃 거리를 보존하는 저차원 임베딩을 찾음

```
s_curve_lle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=2,
                                              method='standard', random_state=0).fit_transform(s_cu
digits_lle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=3,
                                             method='standard', random_state=0).fit_transform(digit
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_lle, color, 121, '2d')
plot_digits(digits_lle, labels, 122, '3d')
```





Local Tangent Space Alignment (LTSA)

- 탄젠트 공간을 통해 각 이웃의 국소 성질을 특성화
- 국소 탄젠트 공간을 정렬

```
s_curve_ltsa = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=2,
                                               method='ltsa', random_state=0).fit_transform(s_curve)
digits_ltsa = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=3,
                                              method='ltsa', random_state=0).fit_transform(digits)
```

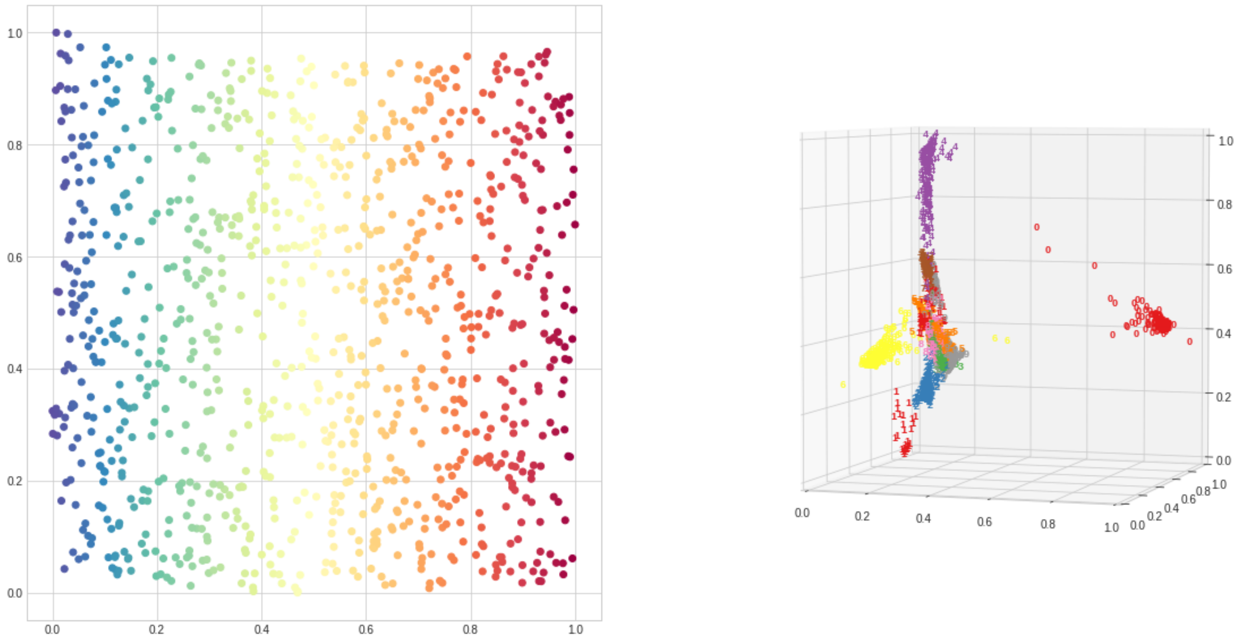
```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_ltsa, color, 121, '2d')
plot_digits(digits_ltsa, labels, 122, '3d')
```

Hessian Eigenmapping

- LLE의 문제를 해결한 다른 방법
- 국소 선형 구조를 복원하기 위해 각 이웃에서 hessian 기반의 이차 형태를 중심으로 회전

```
s_curve_hlle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=2,
                                                method='hessian', random_state=0).fit_transform(s_cur
digits_hlle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=3,
                                               method='hessian', random_state=0).fit_transform(digits
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_hlle, color, 121, '2d')
plot_digits(digits_hlle, labels, 122, '3d')
```

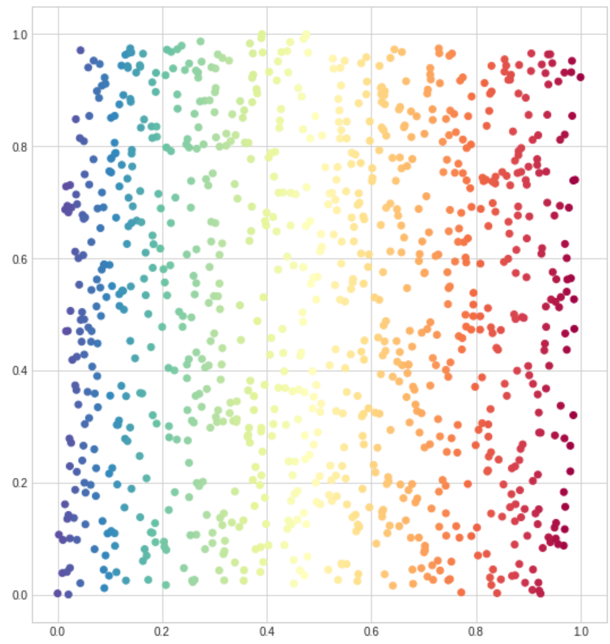


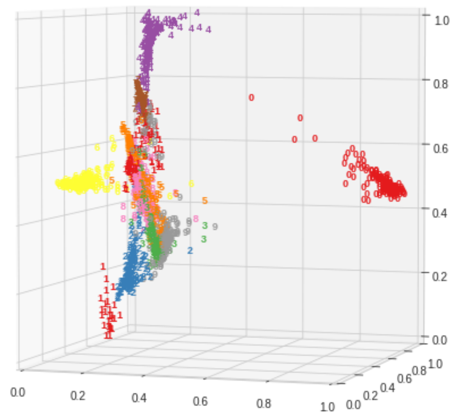
Modified Locally Linear Embedding

- 각 이웃에 여러 가중치 벡터를 사용
- n_neighbors > n_components를 만족해야 함

```
s_curve_mlle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=2,
                                                method='modified', random_state=0).fit_transform(s_cu
digits_mlle = manifold.LocallyLinearEmbedding(n_neighbors=30, n_components=3,
                                               method='modified', random_state=0).fit_transform(digit
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_mlle, color, 121, '2d')
plot_digits(digits_mlle, labels, 122, '3d')
```



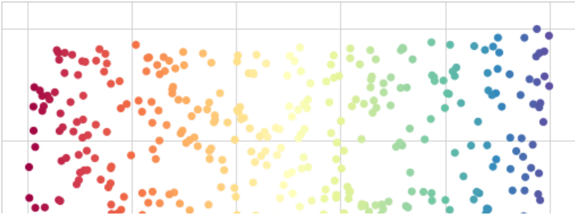


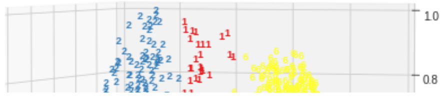
Isomap

- 초기의 다양체 학습 알고리즘
- MDS와 커널 PCA의 확장으로 볼 수 있음
- 모든 점들 사이의 측지 거리를 유지하는 저차원 임베딩을 찾음

```
s_curve_isomap = manifold.Isomap(n_neighbors=30, n_components=2).fit_transform(s_curve)
digits_isomap = manifold.Isomap(n_neighbors=30, n_components=3).fit_transform(digits)
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_isomap, color, 121, '2d')
plot_digits(digits_isomap, labels, 122, '3d')
```



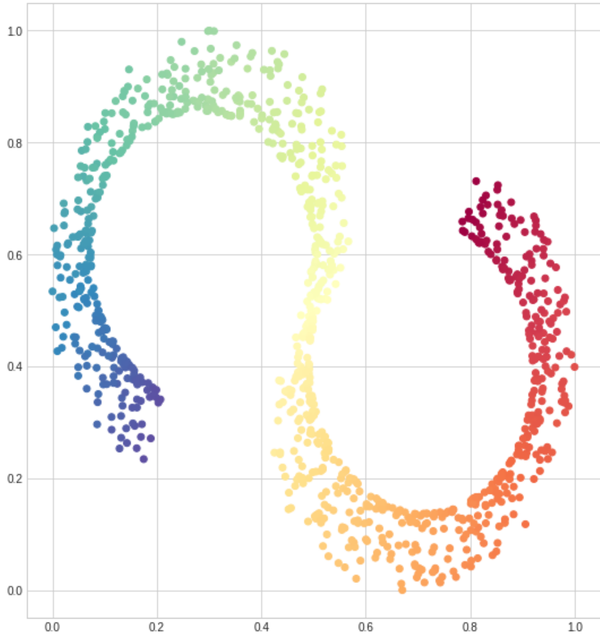


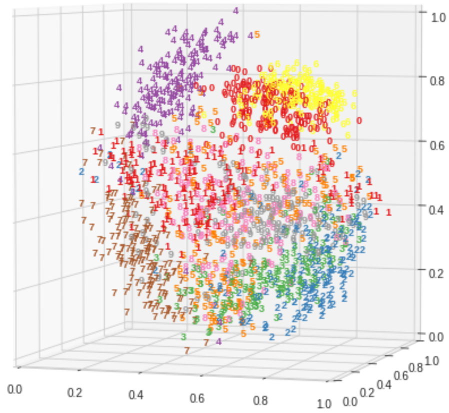
Multi-Dimensional Scaling (MDS)

- 고차원 공간에서의 거리를 고려하는 저차원 공간을 찾음

```
s_curve_mds = manifold.MDS(n_components=2, random_state=0).fit_transform(s_curve)
digits_mds = manifold.MDS(n_components=3, random_state=0).fit_transform(digits)
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_mds, color, 121, '2d')
plot_digits(digits_mds, labels, 122, '3d')
```





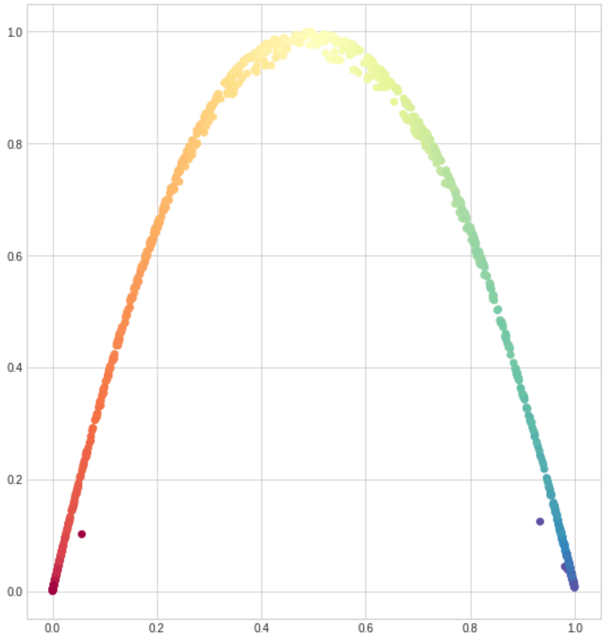
Spectral Embedding

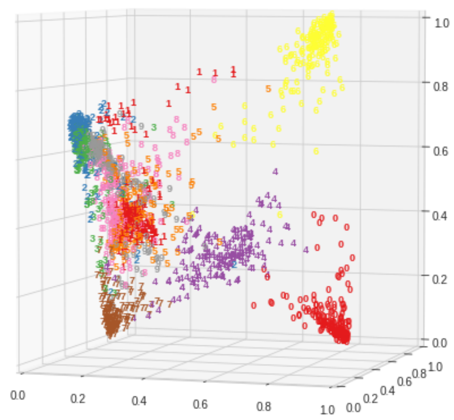
- 스펙트럼 분해를 통해 데이터의 저차원 표현을 찾음
- 데이터의 점이 저차원 공간에서도 서로 가깝게 유지되도록 함

```
s_curve_se = manifold.SpectralEmbedding(n_components=2, random_state=0).fit_transform(s_curve)
digits_se = manifold.SpectralEmbedding(n_components=3, random_state=0).fit_transform(digits)
```

```
fig = plt.figure(figsize=(20, 10))
```

```
plot_s_curve(s_curve_se, color, 121, '2d')
plot_digits(digits_se, labels, 122, '3d')
```



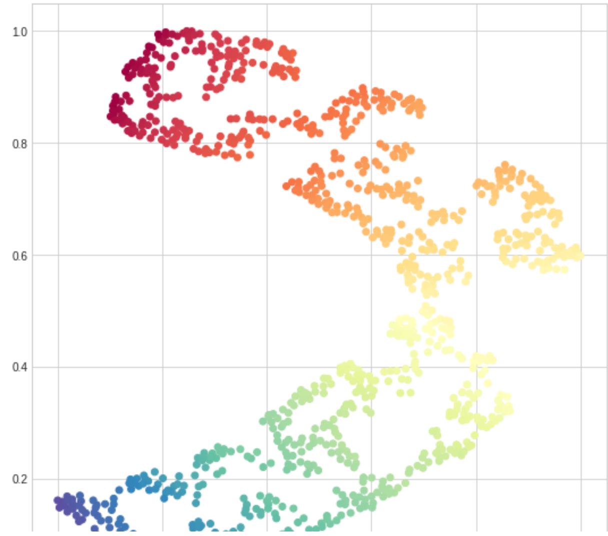


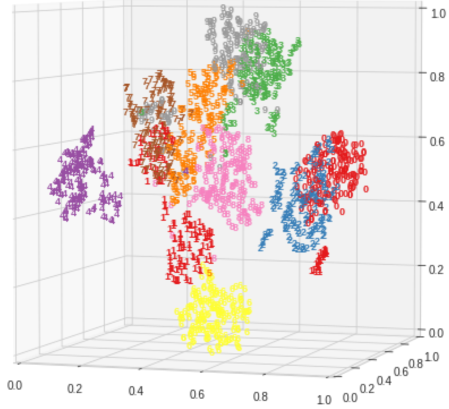
t-distributed Stochastic Neighbor Embedding (t-SNE)

- 데이터 포인트의 유사성을 확률로 변환
- 국소 구조에 민감
- 국소 구조를 기반으로 샘플 그룹을 추출하는데 강함
- 항상 KL발산의 국소 최소값에서 끝남
- 계산 비용이 많이 듬
- 전역 구조를 보존하지 않음

```
s_curve_tsne = manifold.TSNE(n_components=2, random_state=0).fit_transform(s_curve)
digits_tsne = manifold.TSNE(n_components=3, random_state=0).fit_transform(digits)
```

```
fig = plt.figure(figsize=(20, 10))
plot_s_curve(s_curve_tsne, color, 121, '2d')
plot_digits(digits_tsne, labels, 122, '3d')
```





정제된 표현을 이용한 학습

- 다양체 학습의 결과를 정제된 데이터로 생각할 수 있음
- 정제된 표현이기 때문에 분석에 비교적 용이함
- 기계학습 모델의 입력으로 사용했을때 성능향상을 기대할 수 있음

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import cross_val_score
```

```
raw_digits, target = datasets.load_digits(return_X_y=True)
```

```
knn = KNeighborsClassifier()
svm = SVC()
decision_tree = DecisionTreeClassifier()
random_forest = RandomForestClassifier()
```

원본 데이터를 사용할 때

KNN

```
score = cross_val_score(
    estimator=knn,
    X=raw_digits, y=target,
    cv=5
)
score
```

```
array([0.94722222, 0.95555556, 0.96657382, 0.98050139, 0.9637883 ])
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

    mean cross val score: 0.9627282575054161 (+/- 0.011168537355954218)

SVM

```
score = cross_val_score(
    estimator=svm,
    X=raw_digits, y=target,
    cv=5
)
score
```

    array([0.96111111, 0.94444444, 0.98328691, 0.98885794, 0.93871866])

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

    mean cross val score: 0.9632838130609718 (+/- 0.020086058632225686)

Decision Tree

```
score = cross_val_score(
    estimator=decision_tree,
    X=raw_digits, y=target,
    cv=5
)
score
```

    array([0.79166667, 0.71111111, 0.78830084, 0.8356546 , 0.80779944])

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

    mean cross val score: 0.7869065304859177 (+/- 0.04143051115234278)

Random Forest

```
score = cross_val_score(
    estimator=random_forest,
    X=raw_digits, y=target,
    cv=5
)
score
```

    array([0.93333333, 0.91388889, 0.96100279, 0.96935933, 0.9275766])

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

    mean cross val score: 0.941032188177035 (+/- 0.020872640829131657)

정제된 데이터를 사용할 때

KNN

```
score = cross_val_score(
    estimator=knn,
    X=digits_tsne, y=target,
    cv=5
)
score
```

```
array([0.96111111, 0.96944444, 0.98885794, 0.99164345, 0.97214485])
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

```
mean cross val score: 0.9766403590219745 (+/- 0.011726128697800348)
```

SVM

```
score = cross_val_score(
    estimator=svm,
    X=digits_tsne, y=target,
    cv=5
)
score
```

```
array([0.94722222, 0.94722222, 0.98607242, 0.99164345, 0.96935933])
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

```
mean cross val score: 0.9683039306716186 (+/- 0.018710656952361866)
```

Decision Tree

```
score = cross_val_score(
    estimator=decision_tree,
    X=digits_tsne, y=target,
    cv=5
)
score
```

```
array([0.91666667, 0.90555556, 0.96657382, 0.96657382, 0.93314763])
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

```
mean cross val score: 0.9377034973692355 (+/- 0.025154661313489233)
```

Random Forest

```
score = cross_val_score(
    estimator=random_forest,
    X=digits_tsne, y=target,
    cv=5
)
score
```

```
array([0.93055556, 0.925     , 0.98885794, 0.98607242, 0.95543175])
```

```
print('mean cross val score: {} (+/- {})'.format(score.mean(), score.std()))
```

```
mean cross val score: 0.9571835345094397 (+/- 0.026779595485449274)
```