TP2_SUTTER

October 8, 2024

[429]:
```
%matplotlib inline
%config InlineBackend.figure_format ='retina'
import seaborn as sns
import matplotlib.pyplot as plt

sns.set()
```

[430]:
```
import numpy as np
from sklearn.decomposition import PCA
from tqdm.autonotebook import trange
```

slide N18 from lecture about PCA algorithm:

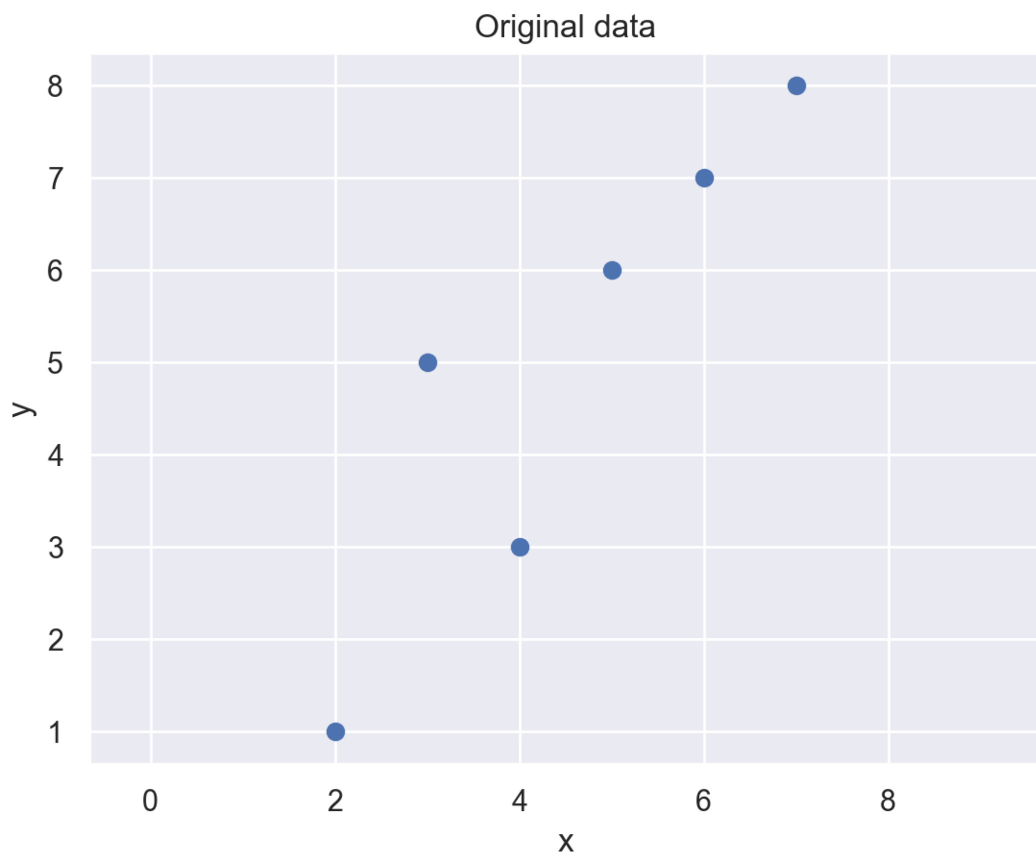
1 Part 1: PCA calculation step by step

Step 1: Get your data

[431]:
```
X = np.array([(2, 1), (3, 5), (4, 3),
              (5, 6), (6, 7), (7, 8)])
X, X.shape
```

[431]:
```
(array([[2, 1],
        [3, 5],
        [4, 3],
        [5, 6],
        [6, 7],
        [7, 8]]),
 (6, 2))
```

[432]:
```
plt.scatter(X[:, 0], X[:, 1])
plt.title("Original data")
plt.xlabel('x')
plt.ylabel('y')
plt.axis('equal');
```



Step 2: Center your data

[433]:
```
mu = np.mean(X, axis=0)  # compute mean
mu
```

[433]:
```
array([4.5, 5. ])
```

[434]:
```
assert mu[1] == (1 + 5 + 3 + 6 + 7 + 8) / 6
```

[435]:
```
A = X - mu # substract mean from data
A
```

[435]:
```
array([[-2.5, -4. ],
       [-1.5,  0. ],
       [-0.5, -2. ],
       [ 0.5,  1. ],
       [ 1.5,  2. ],
       [ 2.5,  3. ]])
```

[436]:
```
np.mean(A, axis=0)
```

[436]: array([0., 0.])

[437]:
```
assert np.allclose(np.mean(A, axis=0), 0)
```

Step 3: Get Covariance of A

[438]:
```
cov = np.cov(X, rowvar=False) # compute covariance
cov
```

[438]:
```
array([[3.5, 4.4],
       [4.4, 6.8]])
```

[439]:
```
assert cov.shape == (2, 2), 'covariance of two features should by 2x2 matrix'
assert np.all(np.linalg.eigvals(cov) >= 0) and np.array_equal(cov,
                                                               cov.T),␣
 ↪'covariance should b positive semidefinite matrix'
```

Step 4: Calculate Eigen Vectors and Eigen Values

[440]:
```
values, vectors = np.linalg.eigh(cov) # find values and vectors
```

[441]:
```
values, vectors
```

[441]:
```
(array([0.45079794, 9.84920206]),
 array([[-0.82192562,  0.56959484],
        [ 0.56959484,  0.82192562]]))
```

The second one should be much more important.

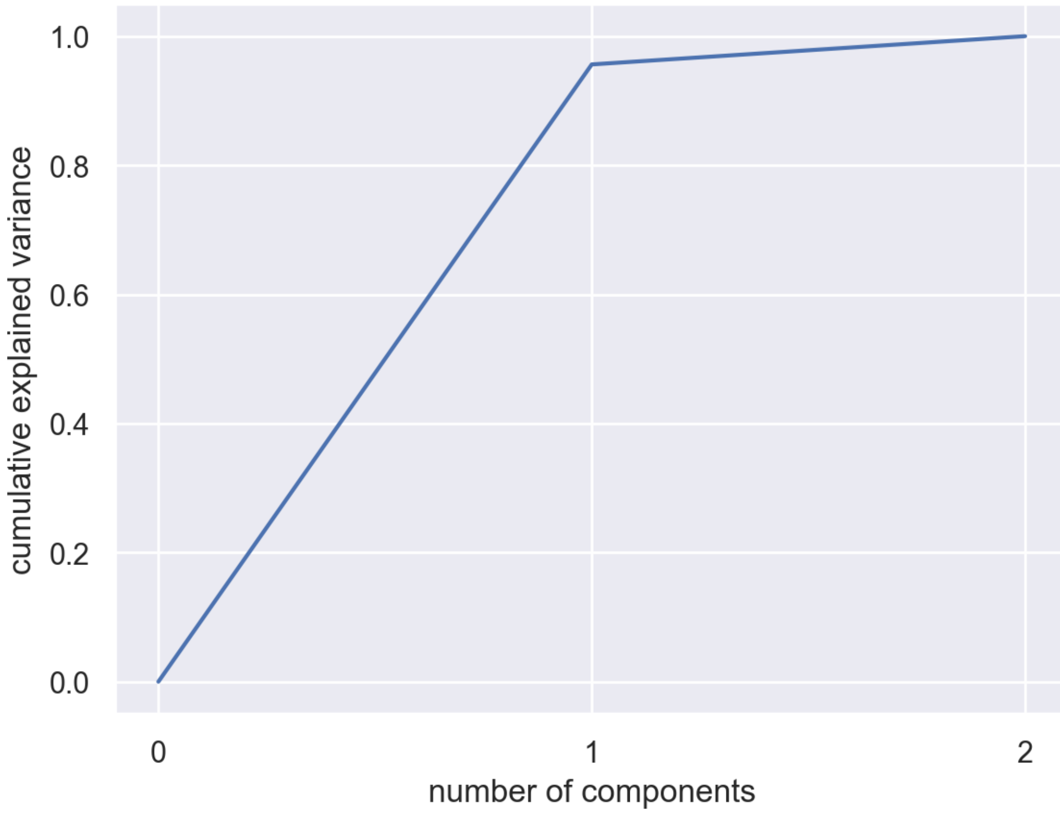
Step 5: Sort values and vectors descending

[442]:
```
index = np.argsort(values)[::-1]
values, vectors = values[index], vectors[:, index] # sort by importance
values, vectors
```

[442]:
```
(array([9.84920206, 0.45079794]),
 array([[ 0.56959484, -0.82192562],
        [ 0.82192562,  0.56959484]]))
```

Plot Explained Variance

[443]:
```
plt.plot(np.concatenate([[0], np.cumsum(values / values.sum())]))
plt.gca().xaxis.get_major_locator().set_params(integer=True)
plt.xlabel('number of components')
plt.ylabel('cumulative explained variance');
```

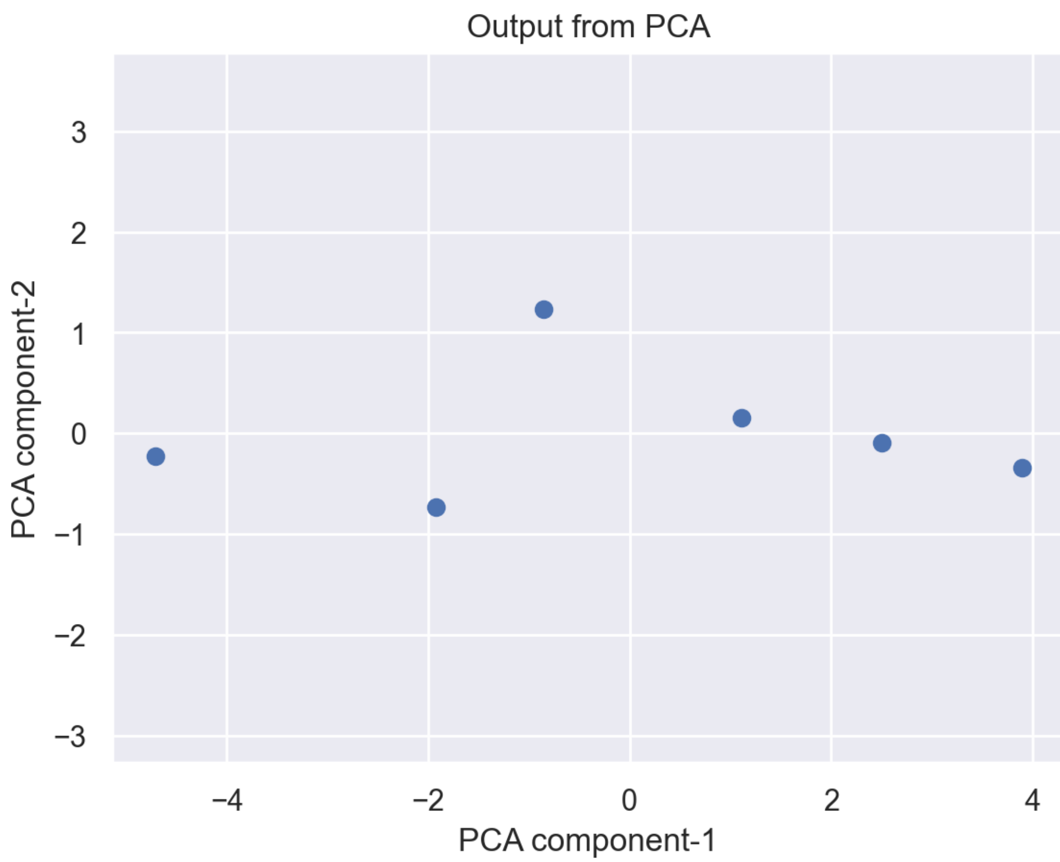


Step 6: Calculate the transformation using all vectors initially

[444]:
```
P = np.dot(A, vectors)
P
```

[444]:
```
array([[-4.71168956, -0.22356531],
       [-0.85439226,  1.23288843],
       [-1.92864865, -0.72822687],
       [ 1.10672304,  0.15863203],
       [ 2.49824349, -0.09369875],
       [ 3.88976395, -0.34602953]])
```

[445]:
```
plt.scatter(P[:, 0], P[:, 1])
plt.title("Output from PCA")
plt.xlabel('PCA component-1')
plt.ylabel('PCA component-2')
plt.axis('equal');
```

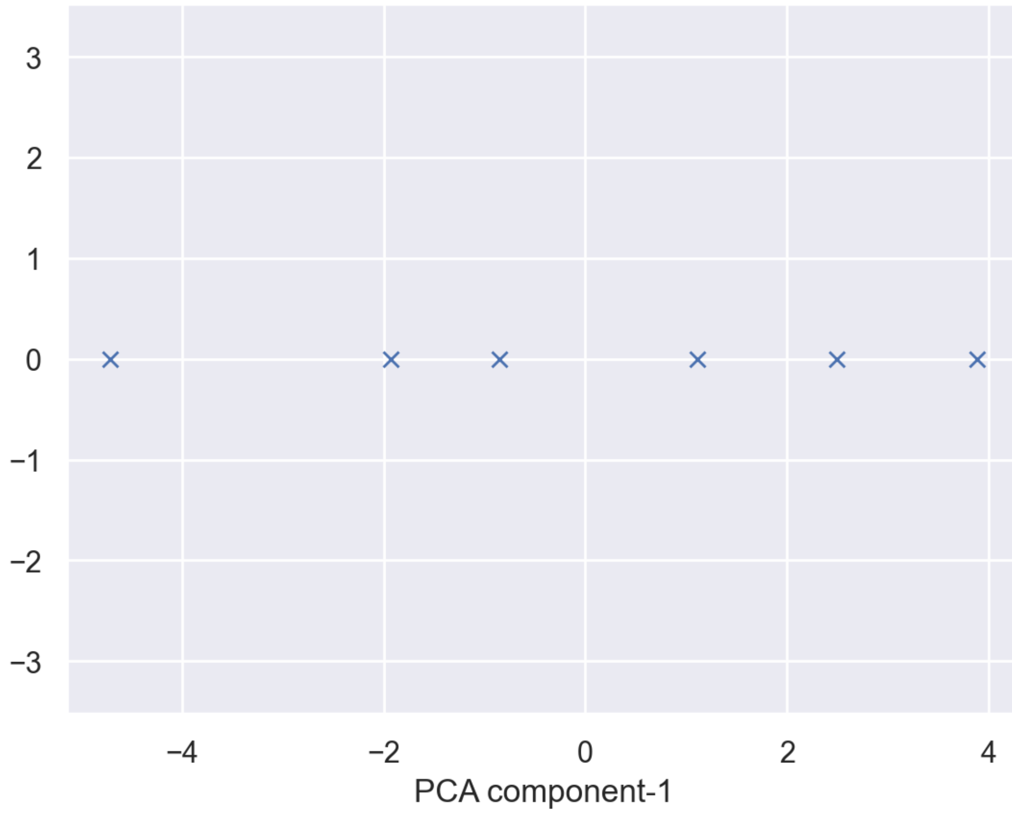


Step 7: select only from the biggest eigen value

[446]:
```
component_1 = P[:, 0]
component_1
```

[446]:
```
array([-4.71168956, -0.85439226, -1.92864865,  1.10672304,  2.49824349,
        3.88976395])
```

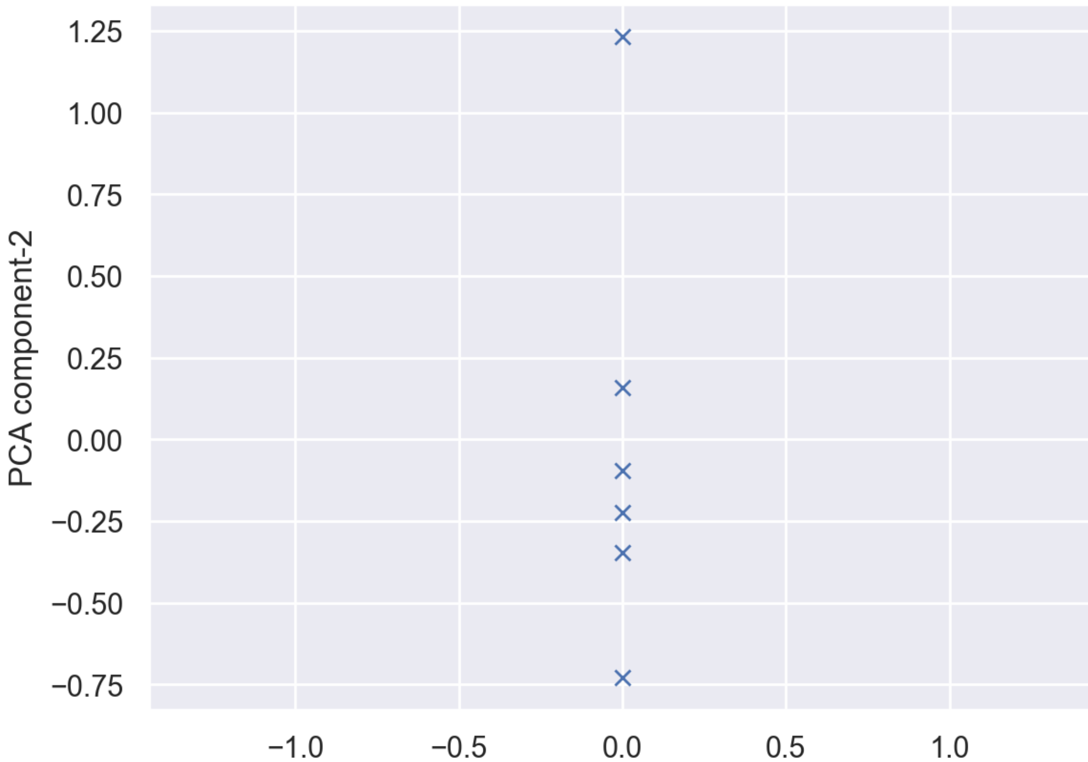
[447]:
```
plt.plot(component_1, np.zeros_like(component_1), 'x')
plt.xlabel('PCA component-1')
plt.axis('equal');
```



Step 8: select only from the smallest eigen value (for debug only)

[448]:
```
component_2 = P[:, 1]
```

[449]:
```
plt.plot(np.zeros_like(component_2), component_2, 'x')
plt.ylabel('PCA component-2')
plt.axis('equal');
```



1.0.1 Compare with sklearn

[450]:
```
from sklearn.decomposition import PCA

pca = PCA(n_components=1, svd_solver='full')
```

[451]:
```
pca.fit(X)
```

[451]:
```
PCA(n_components=1, svd_solver='full')
```

[452]:
```
pca.mean_
```

[452]:
```
array([4.5, 5. ])
```

[453]:
```
assert np.allclose(pca.mean_, mu)
```

[454]:
```
pca.get_covariance()
```

[454]:
```
array([[3.5, 4.4],
       [4.4, 6.8]])
```

[455]:
```
assert np.allclose(pca.get_covariance(), cov)
```

[456]:
```
R = pca.transform(X)
R
```

[456]:
```
array([[-4.71168956],
       [-0.85439226],
       [-1.92864865],
       [ 1.10672304],
       [ 2.49824349],
       [ 3.88976395]])
```

[457]:
```
L = component_1.reshape(-1, 1)
assert np.allclose(R, L)
```

They are the same!

[458]:
```
pca.inverse_transform(pca.transform(X))
```

[458]:
```
array([[1.81624595, 1.12734164],
       [4.01334258, 4.29775312],
       [3.40145168, 3.41479426],
       [5.13038373, 5.90964402],
       [5.9229866 , 7.05337032],
       [6.71558946, 8.19709663]])
```

1.0.2 Conclusion of the first part

To compute PCA you need to do the following: * Compute the mean for every dimension of the whole dataset. * Compute the covariance matrix of the whole dataset. * Compute eigenvectors and the corresponding eigenvalues. * Sort the eigenvectors by decreasing eigenvalues and choose k eigenvectors with the largest eigenvalues to form a d × k dimensional matrix W. * Use this d × k eigenvector matrix to transform the samples onto the new subspace.

source

Steps from here

Or you can just use `sklearn` library (much cleaner, faster, …)

2 Part 2: PCA calculation via single class

You've successfully implemented PCA calculation step-by-step. Congratulations!

Now you need to combine your solution in a single class, based on `sklearn` interface. To know more about the interface refer to the documentation.

In this section you need to implement `__init__`, `fit`, `transform` and `inverse_transform` methods.

Then you need to launch the next cell to test correctness of your class.

[459]:
```
from sklearn.base import TransformerMixin, BaseEstimator
```

[460]:
```
class CustomPCA(TransformerMixin, BaseEstimator):
    def __init__(self, n_components):
        self.n_components = n_components

    def fit(self, X):
        """
        Fit the model with X.
        """
        self.mean_ = np.mean(X, axis=0)
        A = X - self.mean_

        # Compute covariance matrix
        cov = np.cov(A, rowvar=False)

        # Compute eigenvalues and eigenvectors
        eig_values, eig_vectors = np.linalg.eigh(cov)

        # Sort eigenvalues and eigenvectors
        sorted_indices = np.argsort(eig_values)[::-1]
        self.eig_values_ = eig_values[sorted_indices]
        self.eig_vectors_ = eig_vectors[:, sorted_indices]

        # Select a subset of the eigenvectors (principal components)
        self.eig_vectors_ = self.eig_vectors_[:, :self.n_components]

        return self

    def transform(self, X):
        """
        Apply dimensionality reduction to X.
        """
        A = X - self.mean_
        return np.dot(A, self.eig_vectors_)


    def inverse_transform(self, X):
        """
        Transform data back to its original space.
        """
        return np.dot(X, self.eig_vectors_.T) + self.mean_
```

[461]:
```
### some utility code ###

SAMPLES_MIN, SAMPLES_MAX = 5, 10000
FEATURES_MIN, FEATURES_MAX = 2, 300
```

```python
def generate_random_matrix(rng, n_samples=None, n_features=None):
    if n_samples is None:
        n_samples = rng.randint(SAMPLES_MIN, SAMPLES_MAX + 1)
    if n_features is None:
        n_features = rng.randint(FEATURES_MIN, FEATURES_MAX + 1)
    random_type = rng.randint(2)
    if random_type == 0:
        # uniform distribution
        low, high = rng.rand(2) * 100
        low, high = min(low, high), max(low, high)
        return rng.uniform(low, high, (n_samples, n_features)).astype(np.
 ↪float64)
    # normal distribution
    loc, scale = rng.rand(2) * 100
    return rng.normal(loc, scale, (n_samples, n_features)).astype(np.float64)


def check_pca(X, custom_pca, sklearn_pca, matrix_name=''):
    custom_transform = custom_pca.transform(X)
    sklearn_transform = sklearn_pca.transform(X)
    assert np.all(np.isclose(custom_transform - sklearn_transform, 0) | np.
 ↪isclose(custom_transform + sklearn_transform,
                                                                              ␣
 ↪   0)), f'pca transform does not equal with sklearn for {matrix_name} matrix'

    custom_inverse_transform = custom_pca.inverse_transform(custom_transform)
    sklearn_inverse_transform = sklearn_pca.inverse_transform(sklearn_transform)

    assert np.allclose(custom_inverse_transform,
                       sklearn_inverse_transform), f'pca inverse transform does␣
 ↪not equal with sklearn for {matrix_name} matrix'
```

[462]:
```python
%%time
rng = np.random.RandomState(42)
N_RETRIES = 20
N_DIFFERENT_COMPONENTS = 2
N_DIFFERENT_MATRICIES = 2

for _ in trange(N_RETRIES):
    X = generate_random_matrix(rng)
    n_samples, n_features = X.shape

    for n_components in rng.choice(range(1, n_features + 1),␣
 ↪min(N_DIFFERENT_COMPONENTS, n_features), replace=False):
        custom_pca = CustomPCA(n_components=n_components).fit(X)
        sklearn_pca = PCA(n_components=n_components, svd_solver='full').fit(X)
```

```
    check_pca(X, custom_pca, sklearn_pca, 'original')

    for _ in range(N_DIFFERENT_MATRICIES):
        Y = generate_random_matrix(rng, n_features=n_features)
        check_pca(Y, custom_pca, sklearn_pca, 'different')
```

```
100%|      | 20/20 [00:14<00:00,  1.36it/s]
```

```
CPU times: user 23.7 s, sys: 6.28 s, total: 29.9 s
Wall time: 14.7 s
```