Sheet#01 Proposed Solution MLPH_W24

J. Schubert, M. Schümann

October 26, 2024

1 Sheet 1

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import pyplot as plt
%matplotlib inline
```

1.1 1 Principal Component Analysis

1.1.1 (a)

[2]:
```
# TODO: implement PCA (fill in the blanks in the function below)

def pca(data, n_components=None):
    """
    Principal Component Analysis on a p x N data matrix.

    Parameters
    ----------
    data : np.ndarray
        Data matrix of shape (p, N).
    n_components : int, optional
        Number of requested components. By default returns all components.

    Returns
    -------
    np.ndarray, np.ndarray
        the pca components (shape (n_components, p)) and the projection (shape␣
 ↪(n_components, N))

    """
    # set n_components to p by default
    n_components = data.shape[0] if n_components is None else n_components
    assert n_components <= data.shape[0], f"Got n_components larger than␣
 ↪dimensionality of data!"

    # center the data
    X_c = data - np.expand_dims(np.mean(data, axis=1), axis=-1)

    # compute X times X transpose
    XXT = X_c @ X_c.T
    assert XXT.shape == (data.shape[0], data.shape[0])

    # compute the eigenvectors and eigenvalues
    from numpy.linalg import eig
    evalues, evectors = eig(XXT)

    # sort the eigenvectors by eigenvalue and take the n_components largest ones

    evalues, evectors = zip(*sorted(zip(evalues, evectors), key=lambda x: x[0],␣
 ↪reverse=True))

    # verify that the sorting went well / indeed all eigenvectos are shape (p,)
    assert all(map(lambda x: x.shape == (data.shape[0],), evectors))

    # compute X_projected, the projection of the data to the components
    basis = np.array(evectors[:n_components])
    X_projected = basis @ X_c


    return basis, X_projected  # return the n_components first components and␣
 ↪the pca projection of the data

# test
_, _ = pca(np.random.random(size=(100, 1000)));
```

[3]:
```
# Example data to test your implementation
# All the asserts on the bottom should go through if your implementation is␣
 ↪correct

data = np.array([
    [ 1,  0,  0, -1,  0,  0],
    [ 0,  3,  0,  0, -3,  0],
    [ 0,  0,  5,  0,  0, -5]
], dtype=np.float32)

# add a random offset to all samples. it should not affect the results
data += np.random.randn(data.shape[0], 1)

n_components = 2
components, projection = pca(data, n_components=n_components)  # apply your␣
 ↪implementation

# the correct results are known (up to some signs)
```

```
true_components = np.array([[0, 0, 1], [0, 1, 0]], dtype=np.float32)
true_projection = np.array([
    [ 0,  0,  5,  0,  0, -5],
    [ 0,  3,  0,  0, -3,  0]
], dtype=np.float32)

# check that components match, up to sign
assert isinstance(components, np.ndarray), f'Expected components to be numpy␣
  ↪array but got {type(components)}'
assert components.shape == true_components.shape, f'{components.shape}!
  ↪={true_components.shape}'
assert np.allclose(np.abs(components * true_components).sum(1), np.
  ↪ones(n_components)), f'Components not matching'

# check that projections agree, taking into account potentially flipped␣
  ↪components
assert isinstance(projection, np.ndarray), f'Expected projection to be numpy␣
  ↪array but got {type(projection)}'
assert projection.shape == (n_components, data.shape[1]), f'Incorrect shape of␣
  ↪projection: Expected {(n_components, data.shape[1])}, got {projection.shape}'
assert np.allclose(projection, true_projection * (components * true_components).
  ↪sum(1, keepdims=True), atol=1e-6), f'Projections not matching'

print('Test successful!')
```

```
Test successful!
```

1.1.2 (b)

Load the data (it is a subset of the data at https://opendata.cern.ch/record/4910#)

[4]:
```
features = np.load('data/dijet_features.npy')
labels = np.load('data/dijet_labels.npy')
label_names = ['b', 'c', 'q']  # bottom, charm or light quarks

print(f'{features.shape=}, {labels.shape=}')  # print the shapes

# TODO: print how many samples of each class are present in the data (hint:␣
  ↪numpy.unique)
for label in np.unique(labels).astype(int):
    print(f"Label \"{label_names[label]}\": {(labels == label).sum()} total␣
  ↪samples.")
```

```
features.shape=(116, 2233), labels.shape=(2233,)
Label "b": 999 total samples.
Label "c": 864 total samples.
Label "q": 370 total samples.
```

Normalize the data

```
[5]: # TODO: report range of features and normalize the data to zero mean and unit␣
     ↪variance
     features = features / np.expand_dims(np.std(features, axis=1), axis=-1)
```

1.1.3 (c)

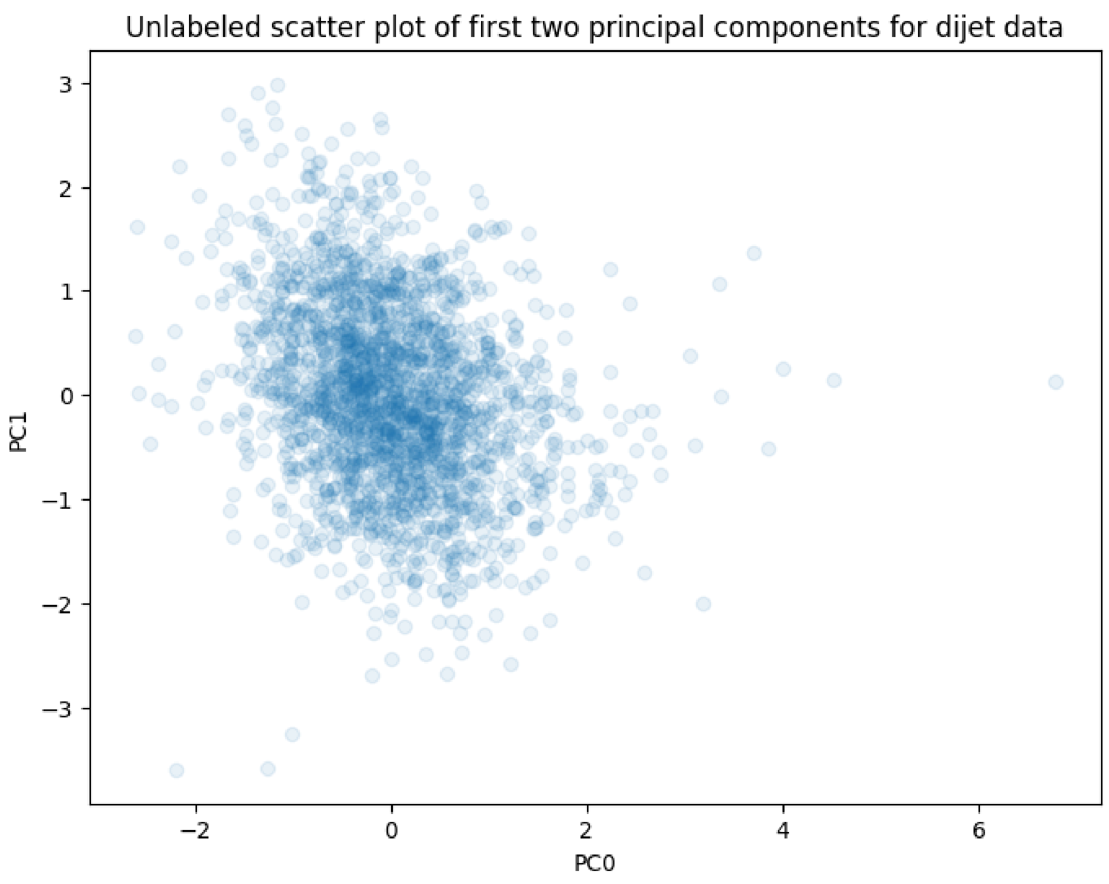
Compute a 2D PCA projection and make a scatterplot of the result, once without color, once coloring the dots by label. Interpret your results.

```
[6]: # TODO: apply PCA as implemented in (a)
     components, projection = pca(features, n_components=2)
```

```
[7]: # TODO: make a scatterplot of the PCA projection
     plt.rcParams["figure.figsize"] = 8,6
     plt.scatter(*projection, alpha=0.1)
     plt.xlabel("PC0")
     plt.ylabel("PC1")
     plt.title("Unlabeled scatter plot of first two principal components for dijet␣
     ↪data")
```

```
/home/jona/.local/lib/python3.10/site-packages/matplotlib/cbook.py:1699:
ComplexWarning: Casting complex values to real discards the imaginary part
  return math.isfinite(val)
/home/jona/.local/lib/python3.10/site-packages/matplotlib/collections.py:194:
ComplexWarning: Casting complex values to real discards the imaginary part
  offsets = np.asanyarray(offsets, float)
```

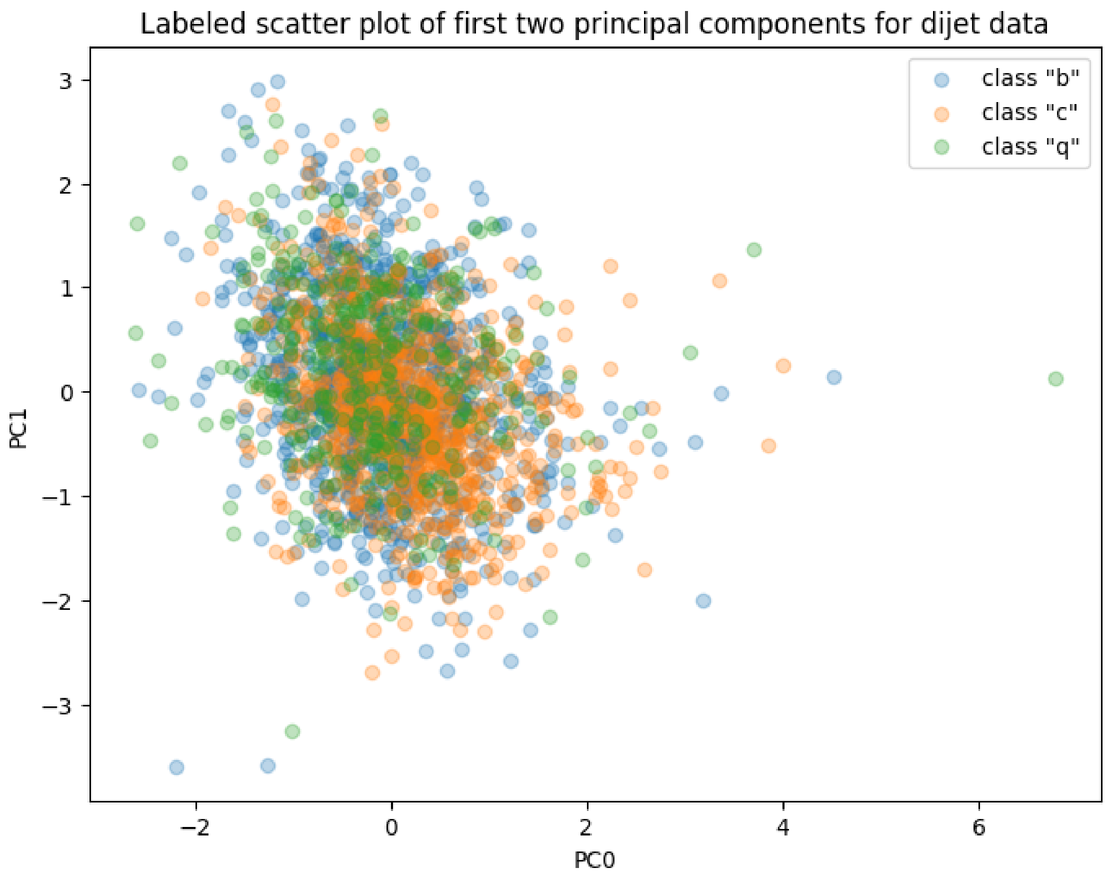
```
[7]: Text(0.5, 1.0, 'Unlabeled scatter plot of first two principal components for
     dijet data')
```



From this plot one can not tell wether the diffrent classes are seperated or not.

[8]:
```
# TODO: make a scatterplot, coloring the dots by their label and including a␣
 ↪legend with the label names
# (hint: one way is to call plt.scatter once for each of the three possible␣
 ↪labels. Why could it be problematic to scatter the data sorted by labels␣
 ↪though?)
for label in np.unique(labels).astype(int):
    mask = labels == label
    relevant_projection = projection[:, mask]
    plt.scatter(*relevant_projection, alpha=0.3, label=f"class␣
 ↪\"{label_names[label]}\"")

plt.legend()
plt.xlabel("PC0")
plt.ylabel("PC1")
plt.title("Labeled scatter plot of first two principal components for dijet␣
 ↪data")
```

[8]:
```
Text(0.5, 1.0, 'Labeled scatter plot of first two principal components for dijet
data')
```



In this plot one can see that the diffrent classes are not well seperated within the plane. This shows that PCA is a solid first step, but as seen in the lecture has rather lackluster results. In order to improve one has to use diffrent (non-linear) methods.

1.2 2 Nonlinear Dimension Reduction

[9]:
```python
import umap  # import umap-learn, see https://umap-learn.readthedocs.io/
```

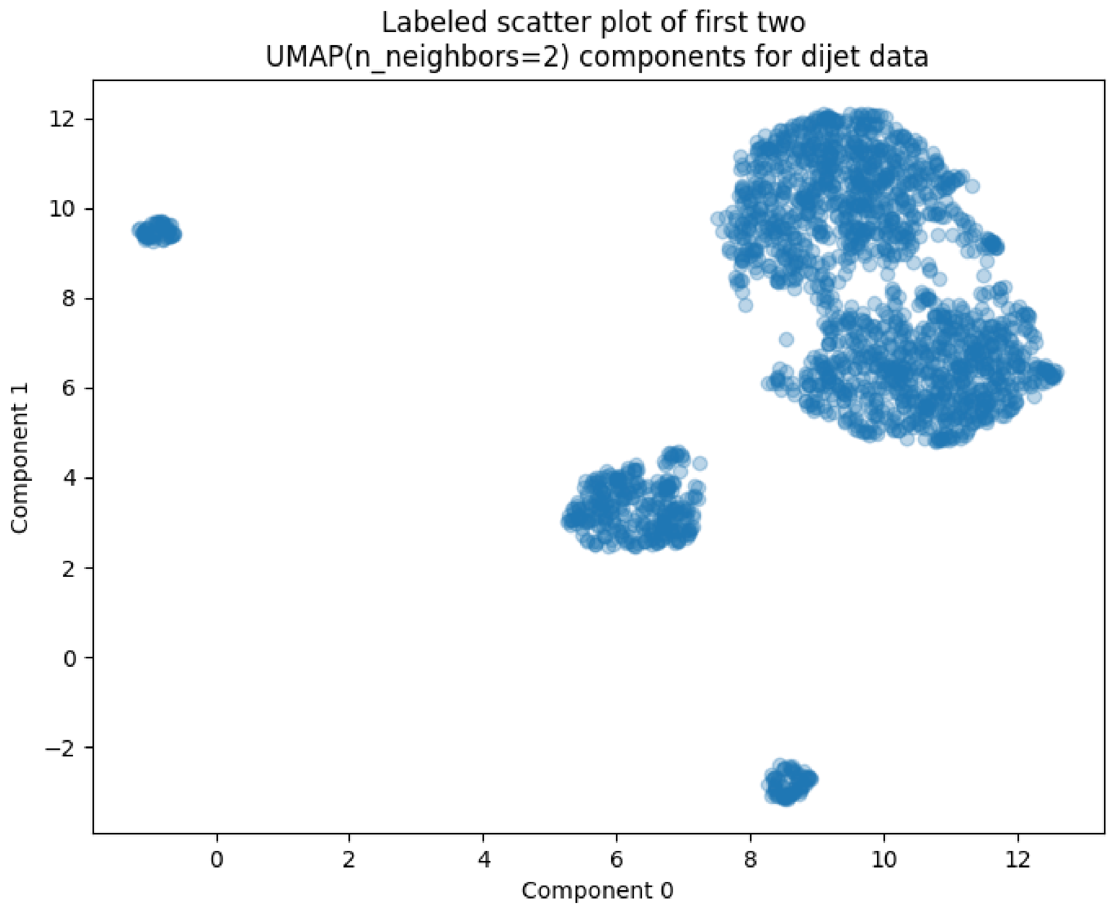
```
/home/jona/.local/lib/python3.10/site-packages/tqdm/auto.py:21: TqdmWarning:
IProgress not found. Please update jupyter and ipywidgets. See
https://ipywidgets.readthedocs.io/en/stable/user_install.html
  from .autonotebook import tqdm as notebook_tqdm
```

[10]:
```python
# if you have not done 1(b) yet, you can load the normalized features directly:
features = np.load('data/dijet_features_normalized.npy')
labels = np.load('data/dijet_labels.npy')
label_names = ['b', 'c', 'q']  # bottom, charm or light quarks
```

1.2.1 (a)

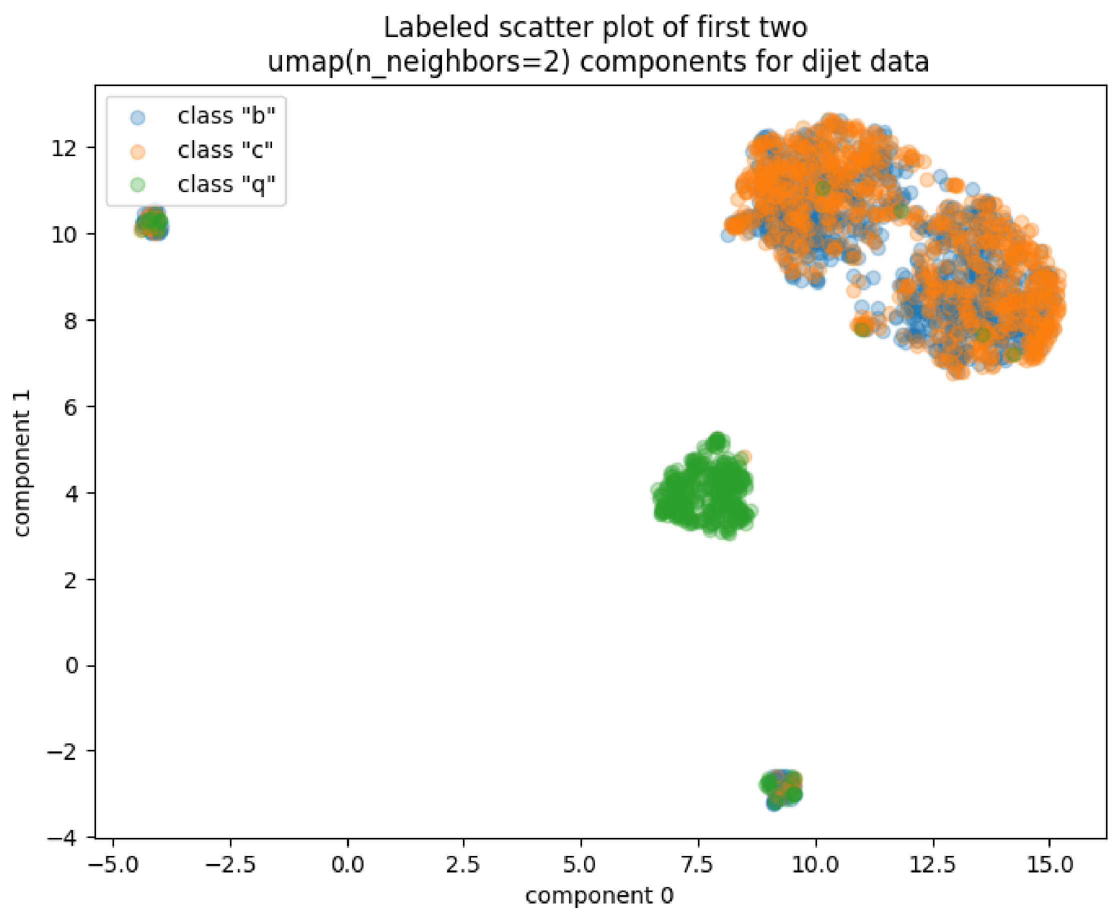
[11]:
```python
# TODO: Apply umap on the normalized jet features from excercise 1. It will␣
↪take a couple of seconds.
# note: umap uses a different convention regarding the feature- and sample␣
↪dimension, N x p instead of p x N!

n_neighbors = 2
reducer = umap.UMAP(n_components=n_neighbors)
```

[15]:
```python
# TODO: make a scatterplot of the UMAP projection
def create_scatter_plot(transformed_features, title=None):
    # Combine all data points into a single scatter plot
    plt.scatter(*transformed_features, alpha=0.3)  # Set color for all points
    plt.xlabel("Component 0")
    plt.ylabel("Component 1")
    plt.title(title if title else "")

# Assuming `reducer` and `features` are already defined and initialized
projection = reducer.fit_transform(features.T).T
create_scatter_plot(projection, title=f"Labeled scatter plot of first two␣
↪\nUMAP(n_neighbors={n_neighbors}) components for dijet data")
```



Looking at this plot it seems that the three classes are well seperated as we have four seperate areas in the plane.

[12]:
```
def create_scatter_plot(transformed_features, title=None):
    for label in np.unique(labels).astype(int):
        mask = labels == label
        relevant_projection = projection[:, mask]
        plt.scatter(*relevant_projection, alpha=0.3, label=f"class␣
 ↪\"{label_names[label]}\"")
    plt.legend()
    plt.xlabel("component 0")
    plt.ylabel("component 1")
    plt.title(title if title else "")
projection = reducer.fit_transform(features.T, ).T
create_scatter_plot(projection, title=f"Labeled scatter plot of first two␣
 ↪\numap(n_neighbors={n_neighbors}) components for dijet data")
```



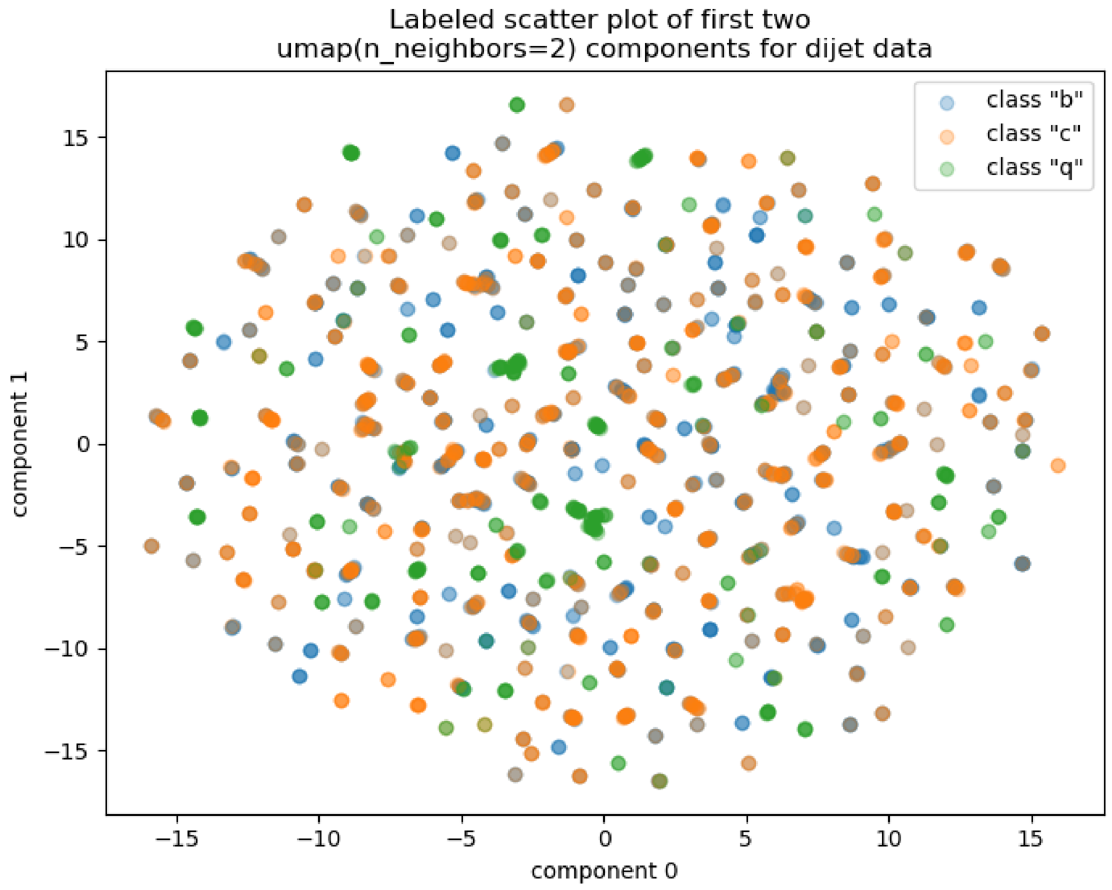
Looking at the colored in version we can see that b and c are not wwell seperated from each other but only have a small overlap with q.

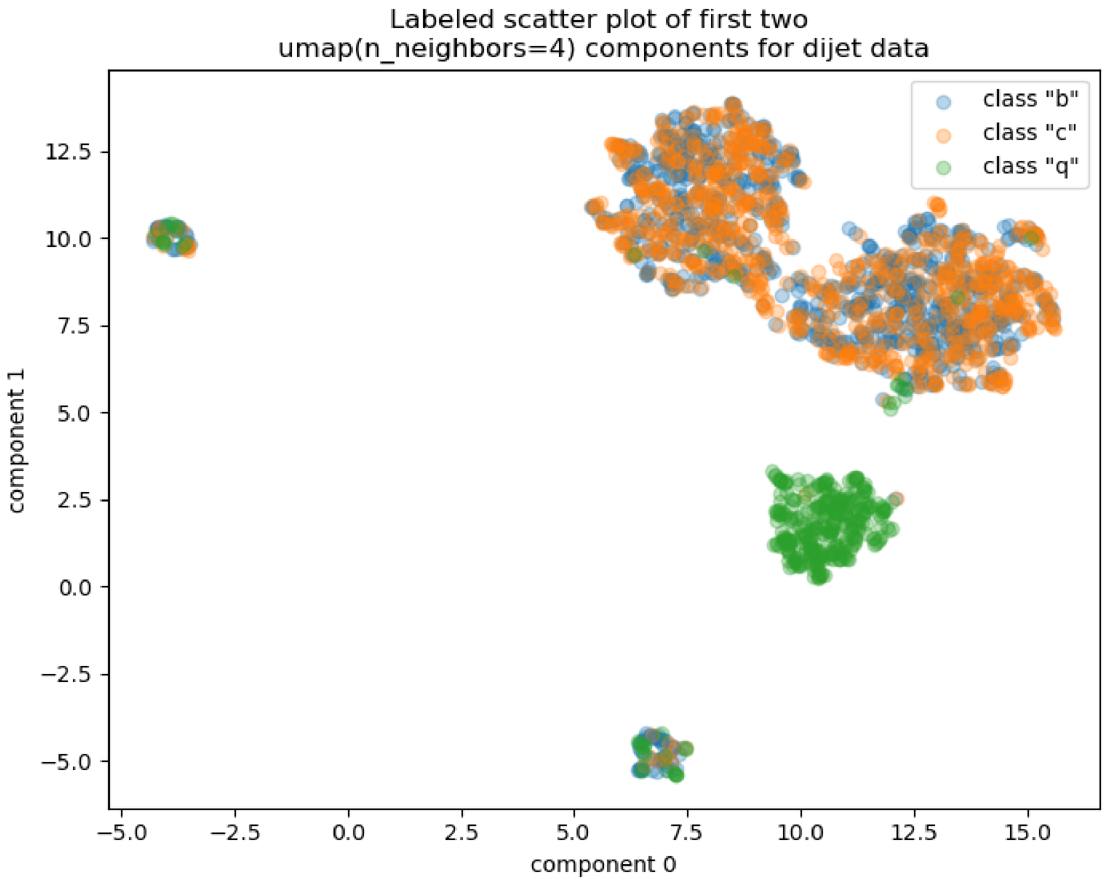
1.2.2 (b)

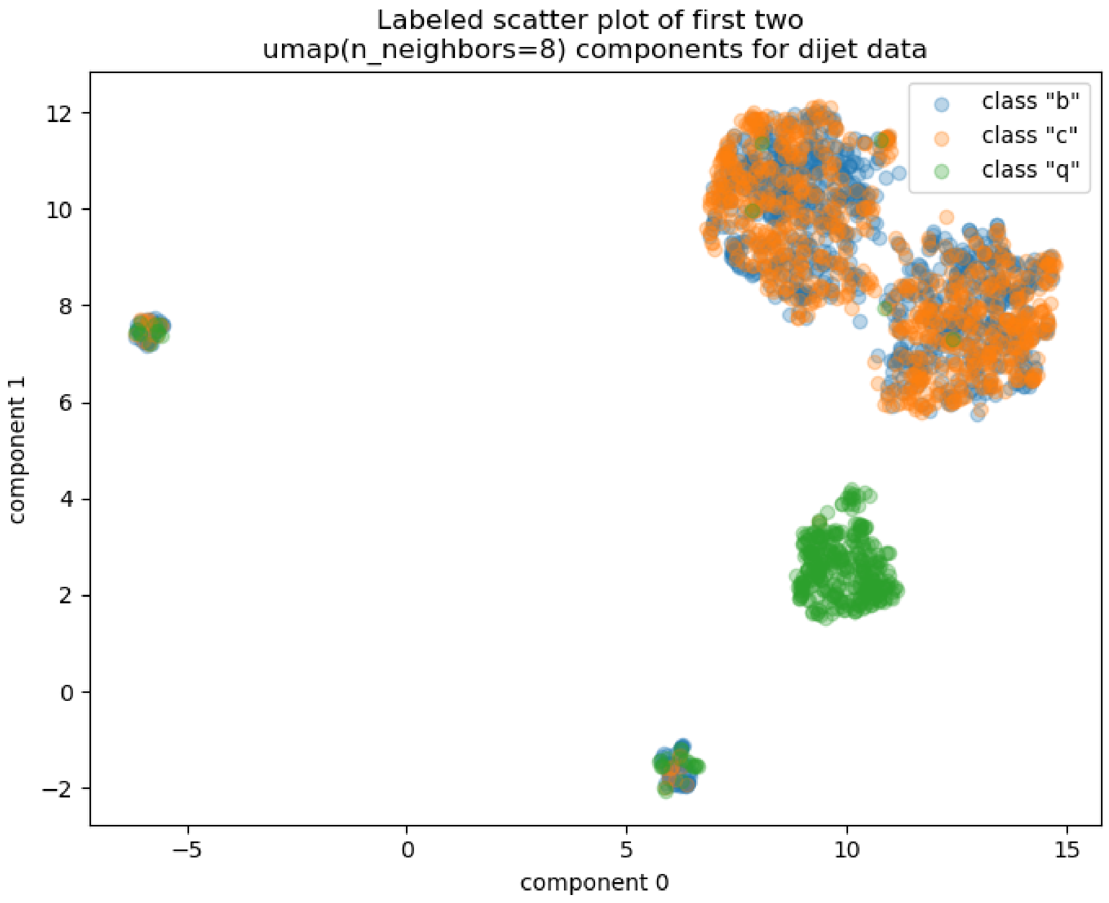
```
[21]: for n_neighbors in (2, 4, 8, 15, 30, 60, 100):
          # TODO: repeat the above, varying the n_neighbors parameter of UMAP
          reducer = umap.UMAP(n_neighbors=n_neighbors)
          projection = reducer.fit_transform(features.T, ).T
          create_scatter_plot(projection, title=f"Labeled scatter plot of first two␣
       ↪\numap(n_neighbors={n_neighbors}) components for dijet data")
          plt.show()
```

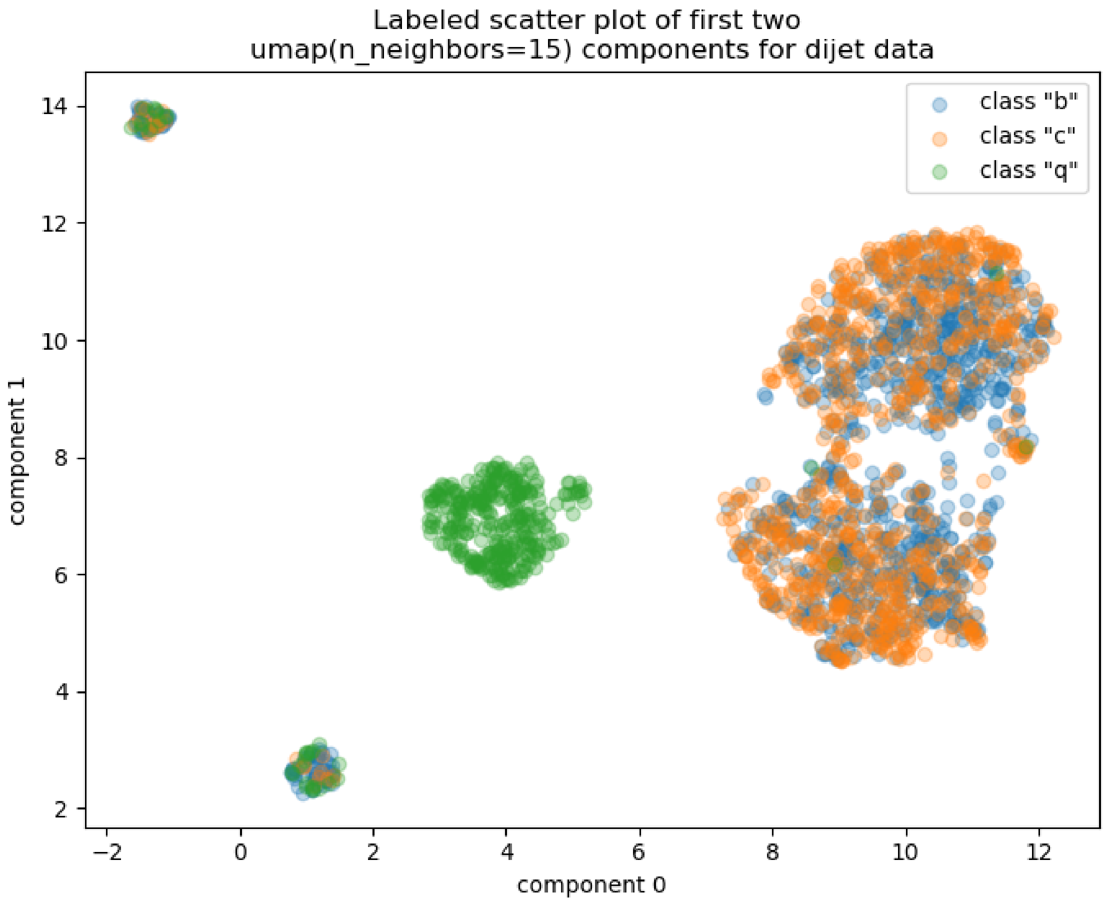
```
/root/miniconda3/envs/mlph/lib/python3.9/site-
packages/sklearn/manifold/_spectral_embedding.py:455: UserWarning: Exited at
iteration 2000 with accuracies
[2.93465312e-15 2.05340802e-06 3.17304847e-06 9.69502793e-06]
not reaching the requested tolerance 4.664063453674316e-06.
Use iteration 1955 instead with accuracy
```

```
2.2299514031715795e-06.

  _, diffusion_map = lobpcg(
/root/miniconda3/envs/mlph/lib/python3.9/site-
packages/sklearn/manifold/_spectral_embedding.py:455: UserWarning: Exited
postprocessing with accuracies
[4.95009064e-15 1.32157027e-06 2.49654518e-06 5.10660318e-06]
not reaching the requested tolerance 4.664063453674316e-06.
  _, diffusion_map = lobpcg(
/root/miniconda3/envs/mlph/lib/python3.9/site-packages/umap/spectral.py:550:
UserWarning: Spectral initialisation failed! The eigenvector solver
failed. This is likely due to too small an eigengap. Consider
adding some noise or jitter to your data.

Falling back to random initialisation!
  warn(
/root/miniconda3/envs/mlph/lib/python3.9/site-packages/umap/spectral.py:550:
UserWarning: Spectral initialisation failed! The eigenvector solver
failed. This is likely due to too small an eigengap. Consider
adding some noise or jitter to your data.

Falling back to random initialisation!
  warn(
```

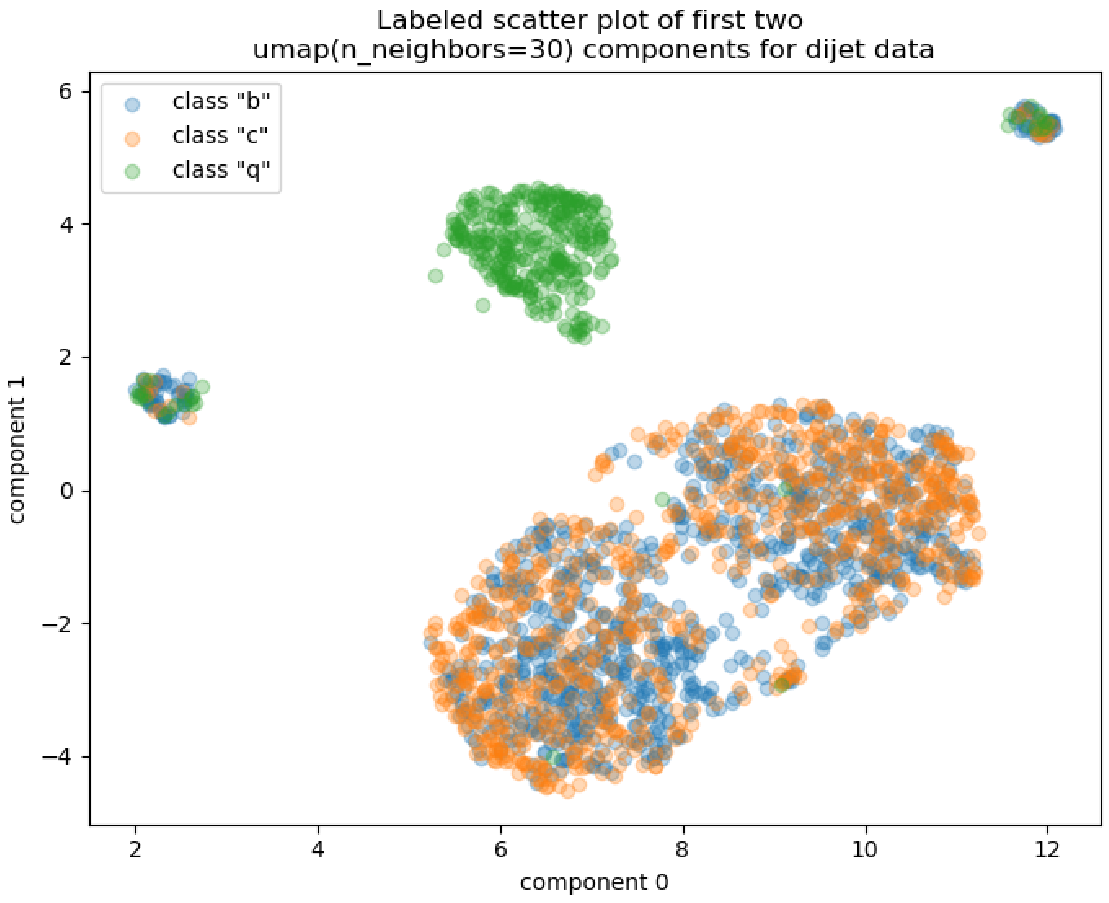

Labeled scatter plot of first two
umap(n_neighbors=2) components for dijet data
class "b"
class "c"
class "q"
component 1
component 0
15
10
5
0
−5
−10
−15
−15
−10
−5
0
5
10
15

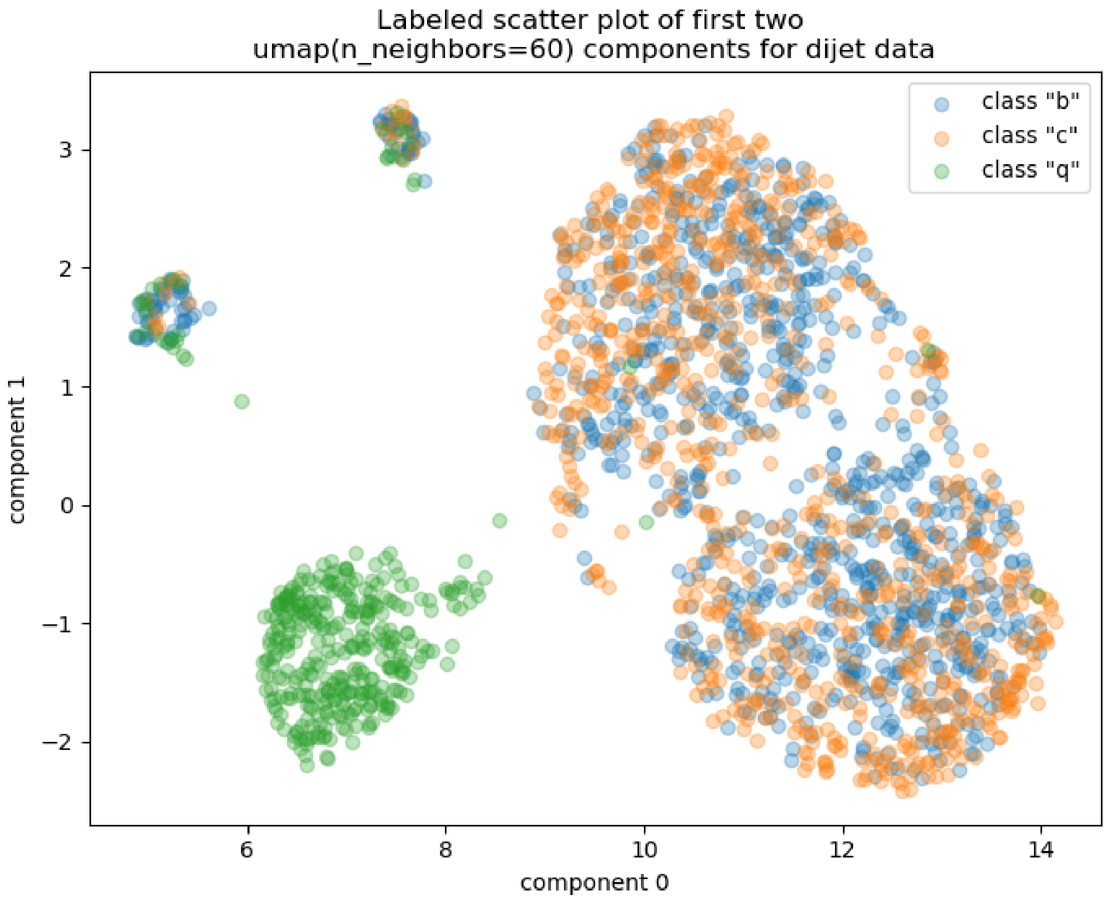

Labeled scatter plot of first two
umap(n_neighbors=4) components for dijet data
class "b"
class "c"
class "q"
component 1
component 0
12.5
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0

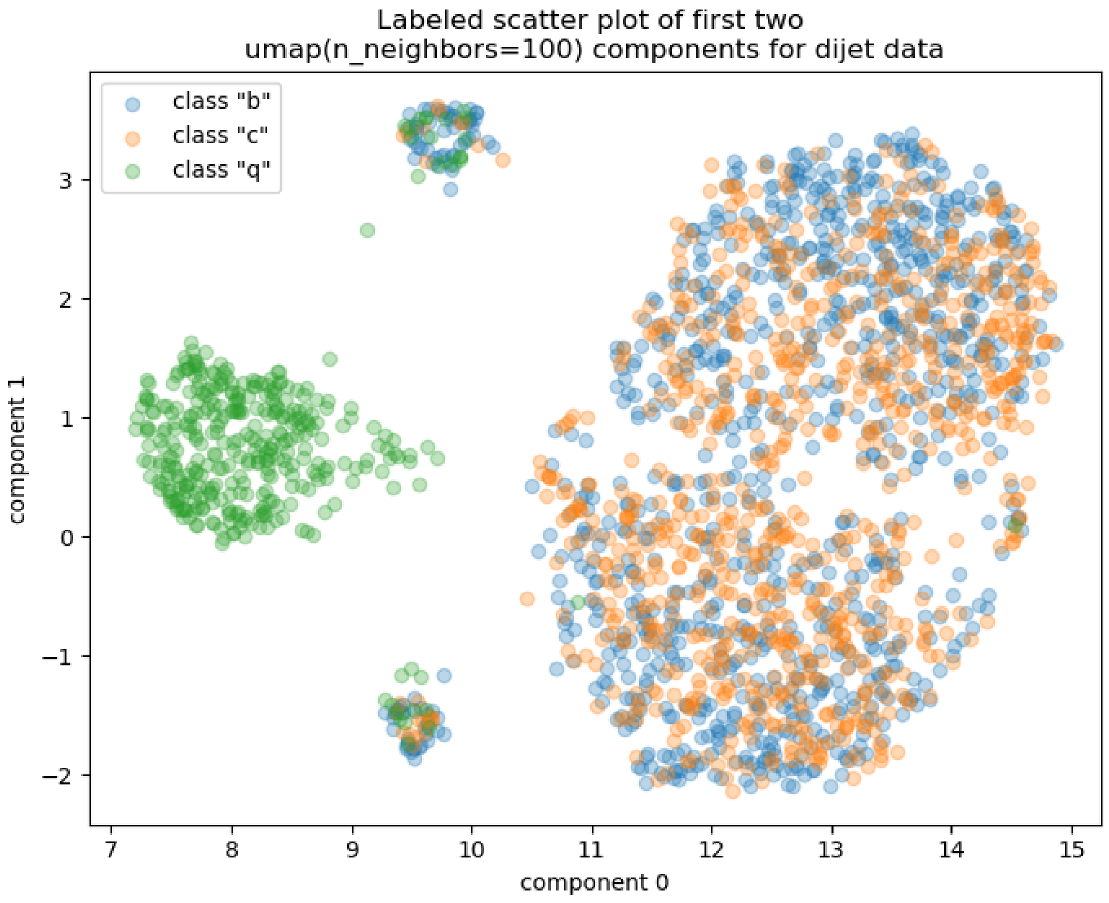

Labeled scatter plot of first two
umap(n_neighbors=8) components for dijet data
class "b"
class "c"
class "q"
component 0
component 1
12
10
8
6
4
2
0
−2
−5
0
5
10
15



Labeled scatter plot of first two
umap(n_neighbors=15) components for dijet data
class "b"
class "c"
class "q"
component 0
component 1


Labeled scatter plot of first two
umap(n_neighbors=30) components for dijet data
class "b"
class "c"
class "q"
component 1
component 0
6
4
2
0
−2
−4
2
4
6
8
10
12


Labeled scatter plot of first two
umap(n_neighbors=60) components for dijet data
class "b"
class "c"
class "q"
component 1
component 0
3
2
1
0
−1
−2
6
8
10
12
14



From these plots one can observe that the clustersizes increase with n. And the single points in a cluster are further appart. This allows us to chose n according to the task; if the goal is to visualize small, tight clusters, lower values are preferred, whereas understanding broader relationships benefits from higher values.

1.3 3 RANSAC

- p: Probability of an inlier
- $1-p$: Probability of an outlier
- m: Number of data points (small sample for outliers)
- With this we get:
  - P(inlier-free subset) $= p^m$
  - P(not inlier-free subset) $= (1-p_m)$
  - P(not inlier-free subset in r runs) $= (1-p_m)^r$
  - P(at least one inlier-free subset) $= 1-(1-p_m)^r$

So, we get:

$$1-(1-p^m)^r \geq 0.99 \tag{1}$$

$$(1 - p^m)^r \leq 0.01 \tag{2}$$

$$\ln((1 - p^m)^r) \leq \ln(0.01) \tag{3}$$

Simplifying further:

$$r \geq \frac{ln(0.01)}{ln(1 - p^m)} = -\frac{2ln(10)}{ln(1 - p^m)} \tag{4}$$