

# Basics of hierarchical clustering

CLUSTER ANALYSIS IN PYTHON



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# Creating a distance matrix using linkage

```
scipy.cluster.hierarchy.linkage(observations,  
                                method='single',  
                                metric='euclidean',  
                                optimal_ordering=False  
)
```

- `method` : how to calculate the proximity of clusters
- `metric` : distance metric
- `optimal_ordering` : order data points

# Which method should use?

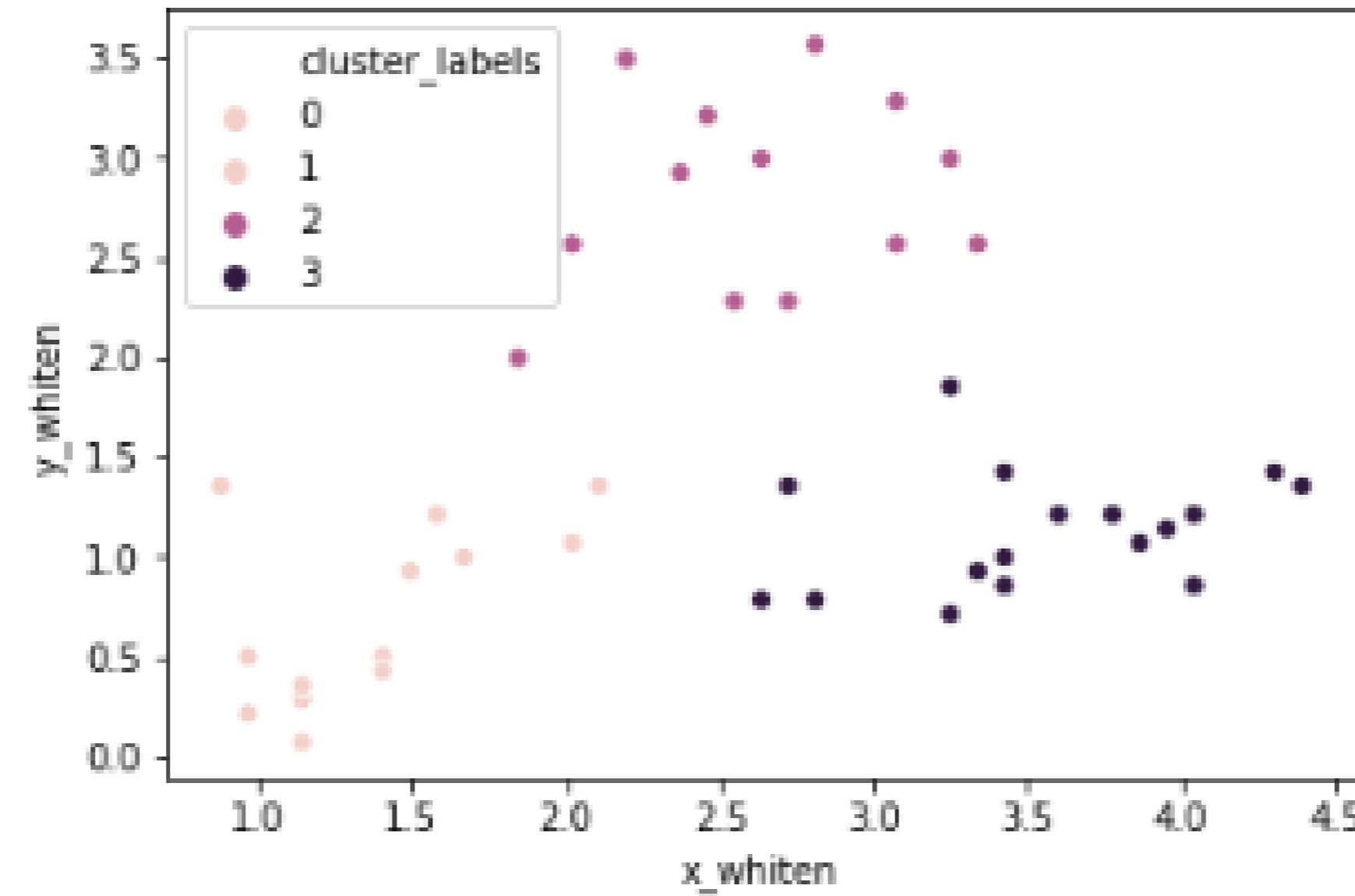
- single: based on two closest objects
- complete: based on two farthest objects
- average: based on the arithmetic mean of all objects
- centroid: based on the geometric mean of all objects
- median: based on the median of all objects
- ward: based on the sum of squares

# Create cluster labels with fcluster

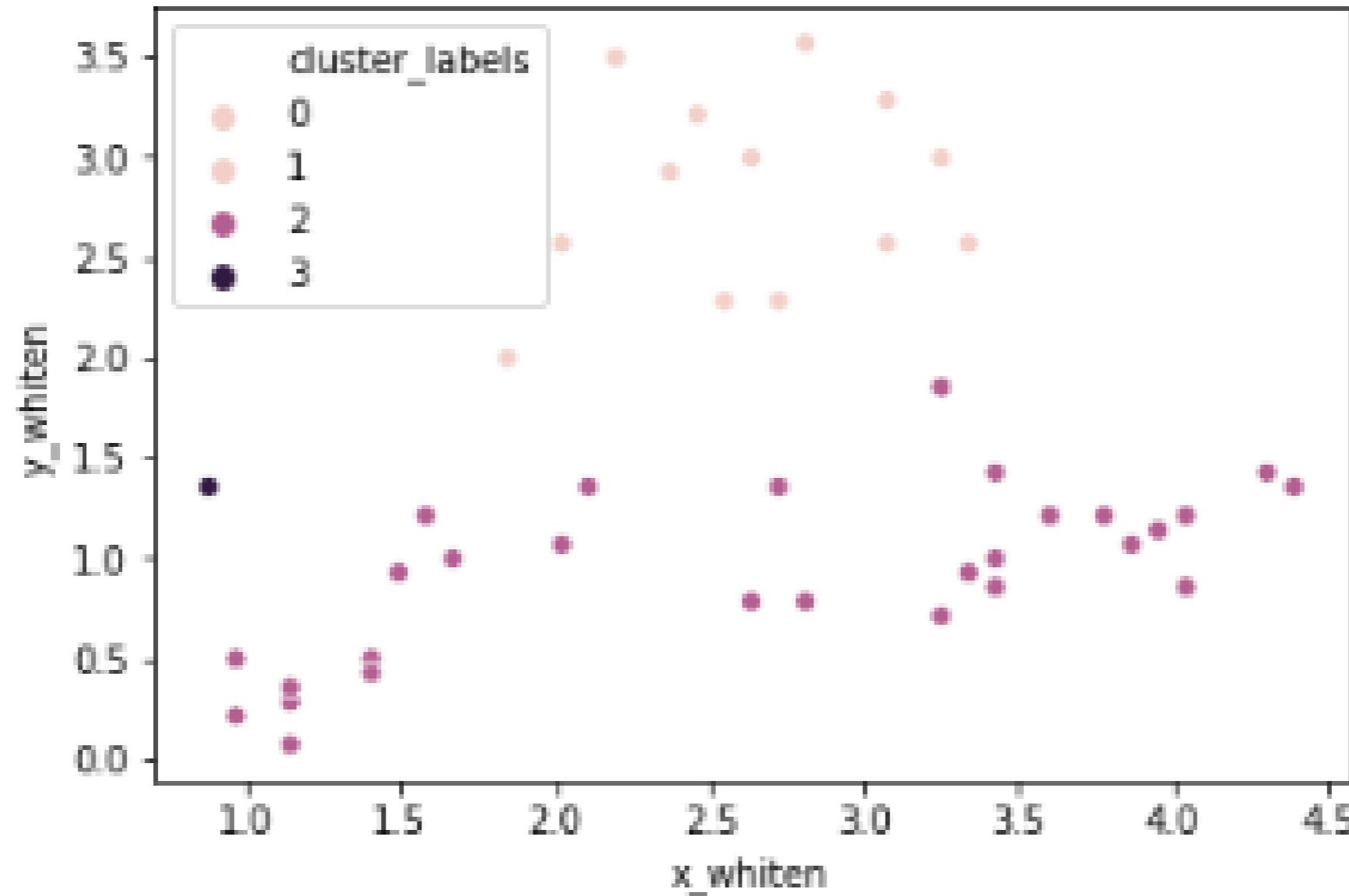
```
scipy.cluster.hierarchy.fcluster(distance_matrix,  
                                 num_clusters,  
                                 criterion  
)
```

- `distance_matrix` : output of `linkage()` method
- `num_clusters` : number of clusters
- `criterion` : how to decide thresholds to form clusters

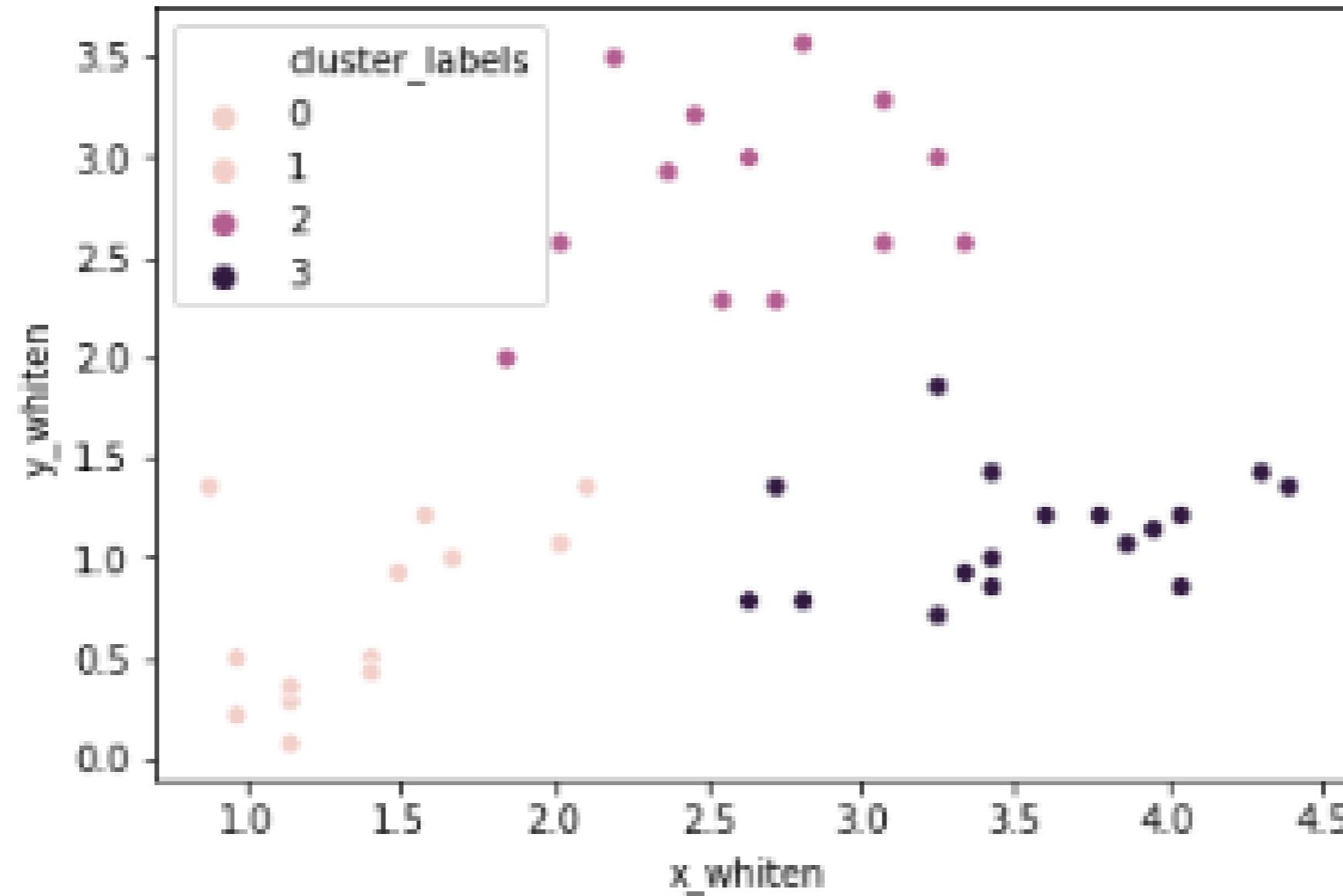
# Hierarchical clustering with ward method



# Hierarchical clustering with single method



# Hierarchical clustering with complete method



# Final thoughts on selecting a method

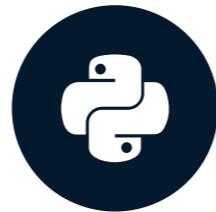
- No one right method for all
- Need to carefully understand the distribution of data

# **Let's try some exercises**

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# Visualize clusters

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# Why visualize clusters?

- Try to make sense of the clusters formed
- An additional step in validation of clusters
- Spot trends in data

# An introduction to seaborn

- `seaborn` : a Python data visualization library based on `matplotlib`
- Has better, easily modifiable aesthetics than `matplotlib`!
- Contains functions that make data visualization tasks easy in the context of data analytics
- Use case for clustering: `hue` parameter for plots

# Visualize clusters with matplotlib

```
from matplotlib import pyplot as plt

df = pd.DataFrame({'x': [2, 3, 5, 6, 2],
                    'y': [1, 1, 5, 5, 2],
                    'labels': ['A', 'A', 'B', 'B', 'A']})
colors = {'A':'red', 'B':'blue'}
df.plot.scatter(x='x',
                 y='y',
                 c=df['labels'].apply(lambda x: colors[x]))
plt.show()
```

# Visualize clusters with seaborn

```
from matplotlib import pyplot as plt
import seaborn as sns

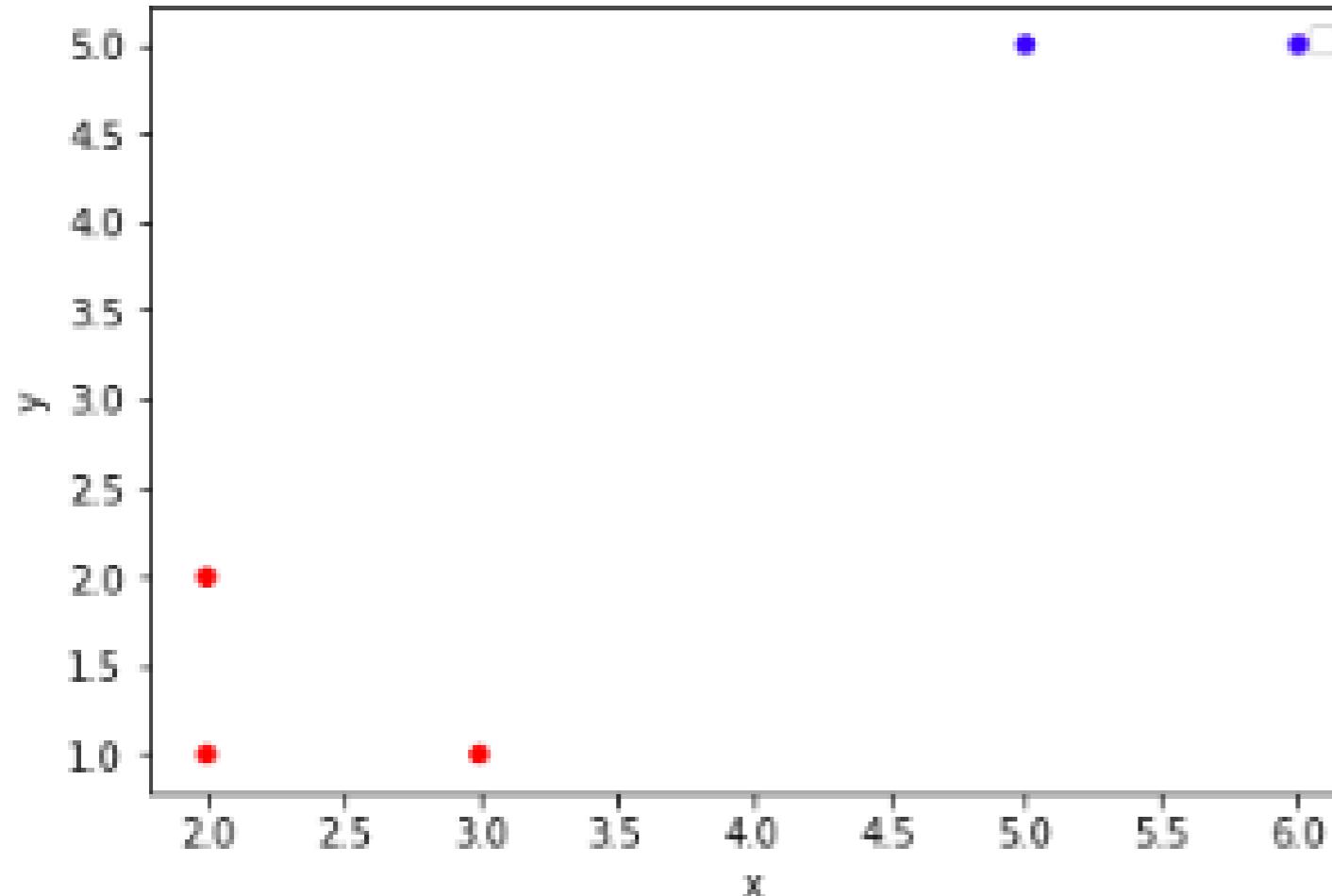
df = pd.DataFrame({'x': [2, 3, 5, 6, 2],
                   'y': [1, 1, 5, 5, 2],
                   'Labels': ['A', 'A', 'B', 'B', 'A']})

sns.scatterplot(x='x',
                 y='y',
                 hue='Labels',
                 data=df)

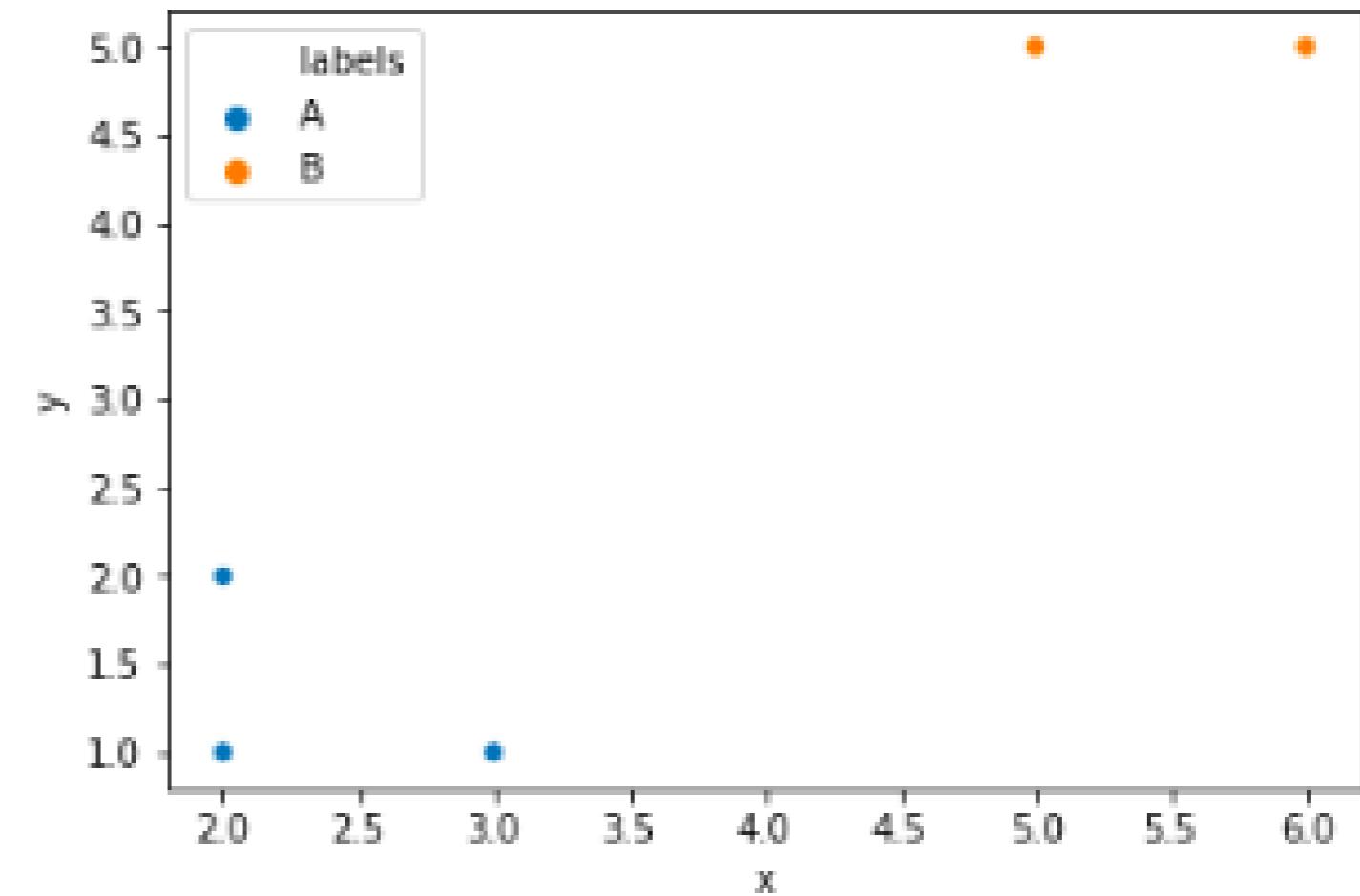
plt.show()
```

# Comparison of both methods of visualization

MATPLOTLIB PLOT



SEABORN PLOT

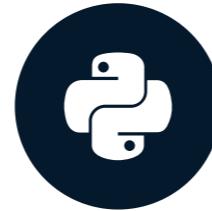


# **Next up: Try some visualizations**

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# How many clusters?

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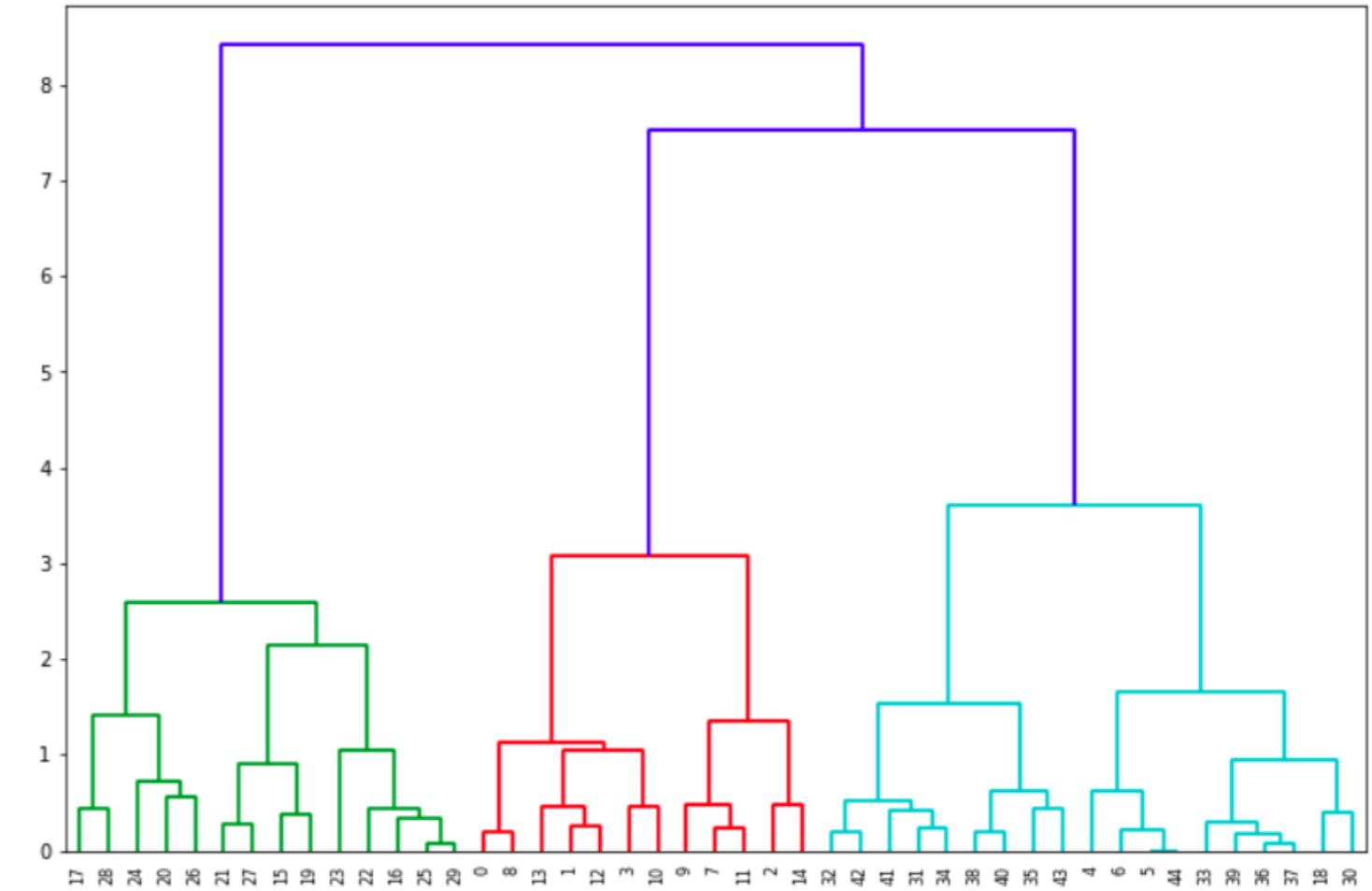


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# Introduction to dendograms

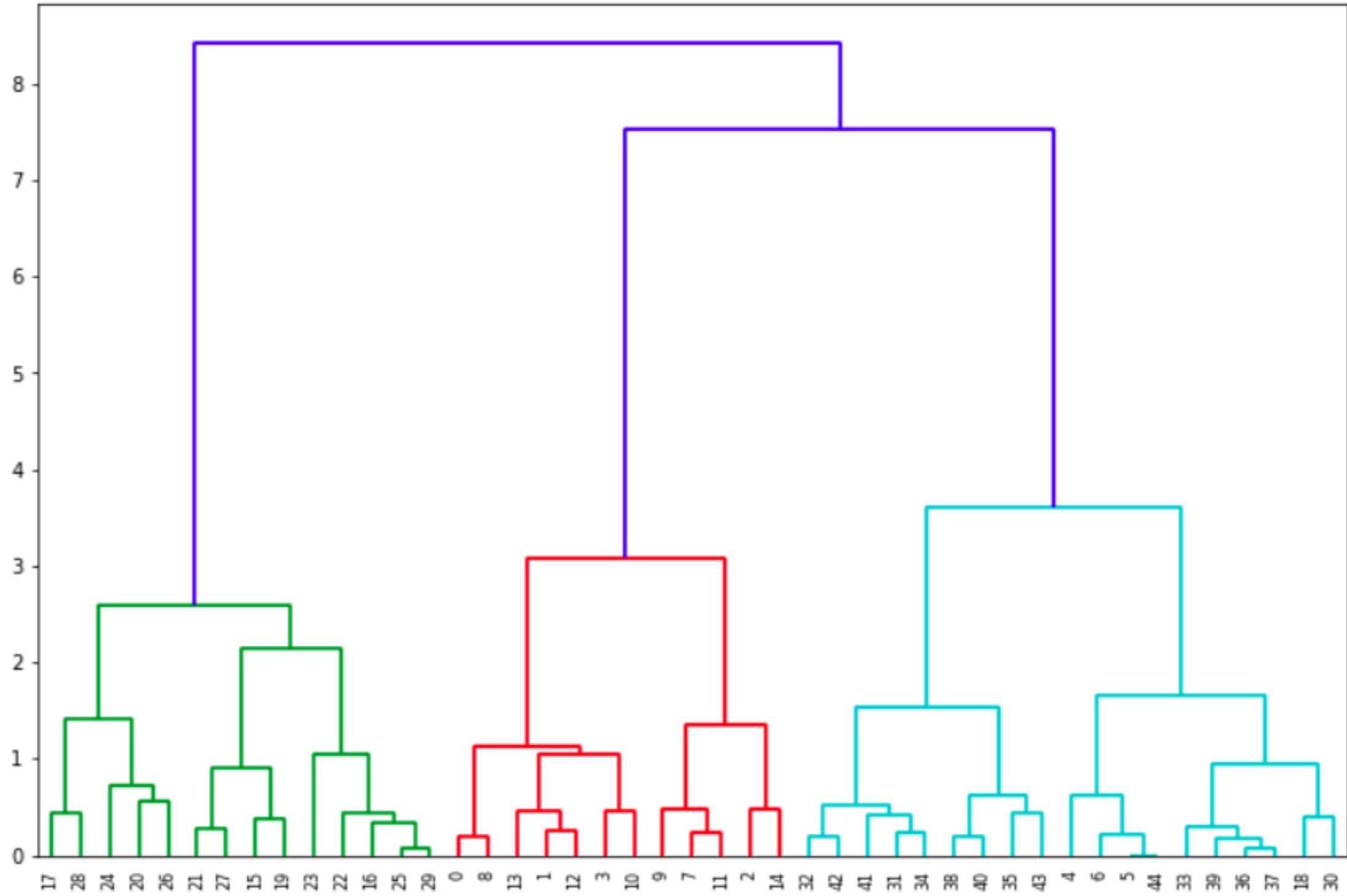
- Strategy till now - decide clusters on visual inspection
- Dendograms help in showing progressions as clusters are merged
- A dendrogram is a branching diagram that demonstrates how each cluster is composed by branching out into its child nodes

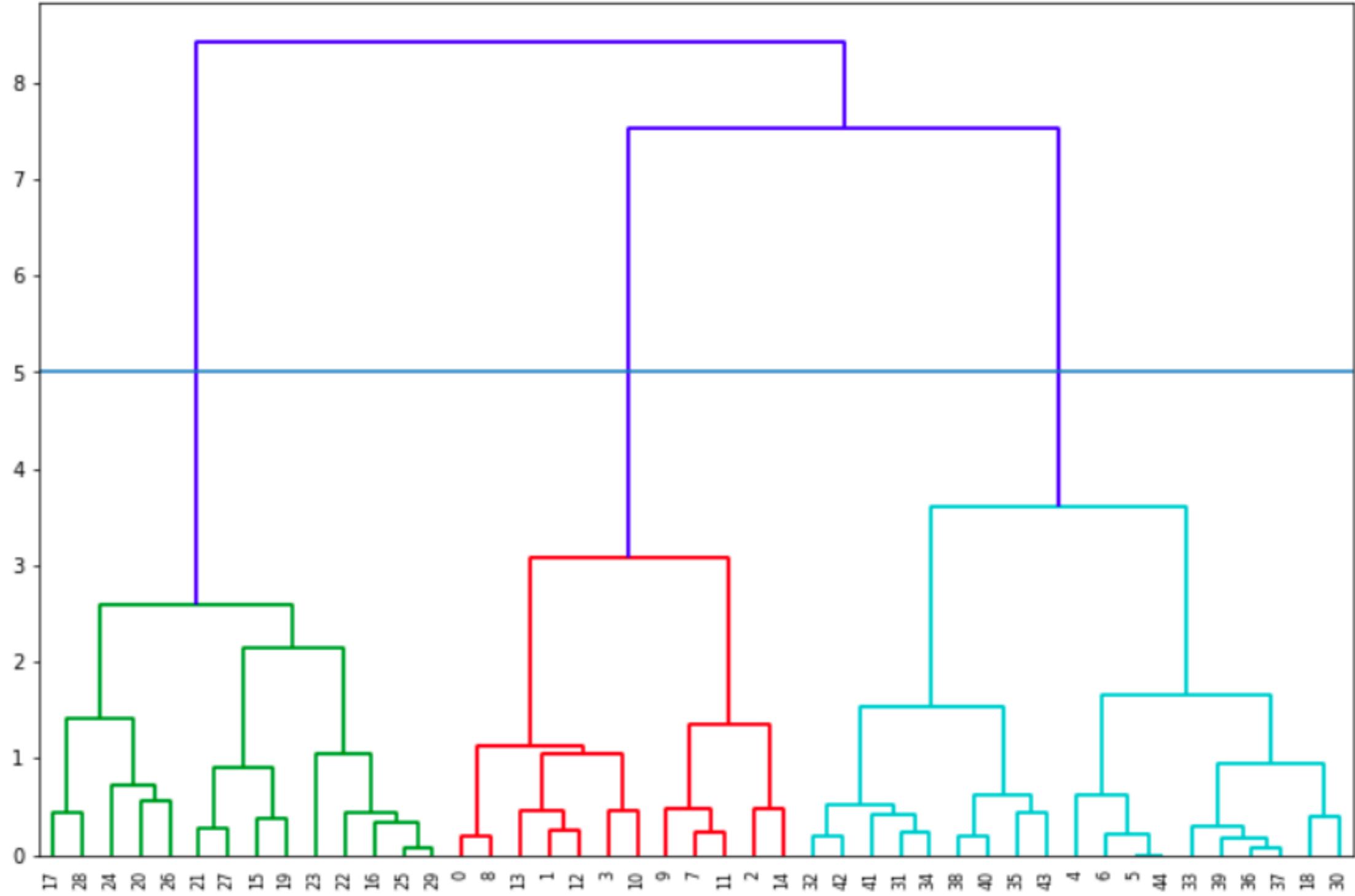


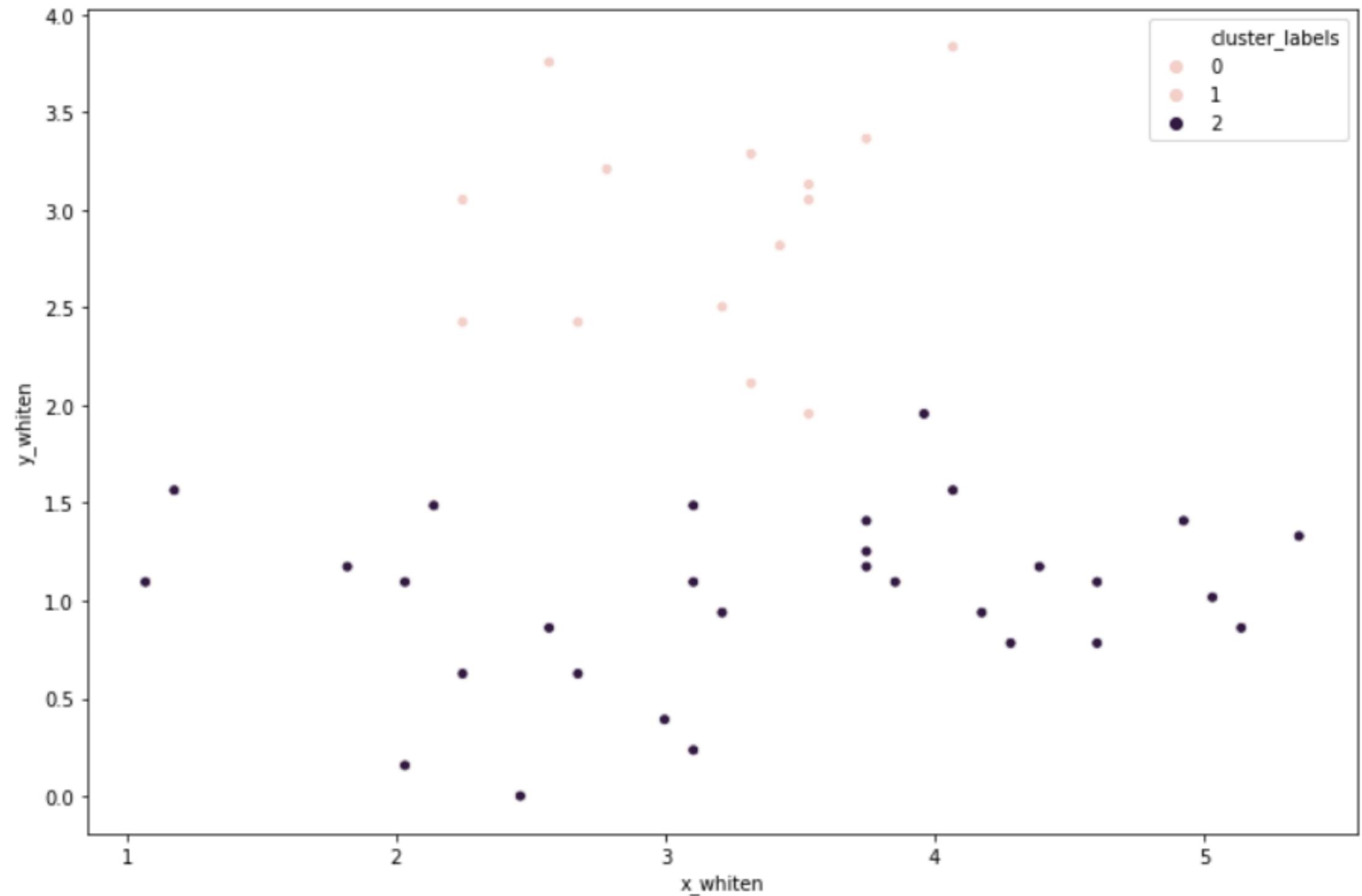
# Create a dendrogram in SciPy

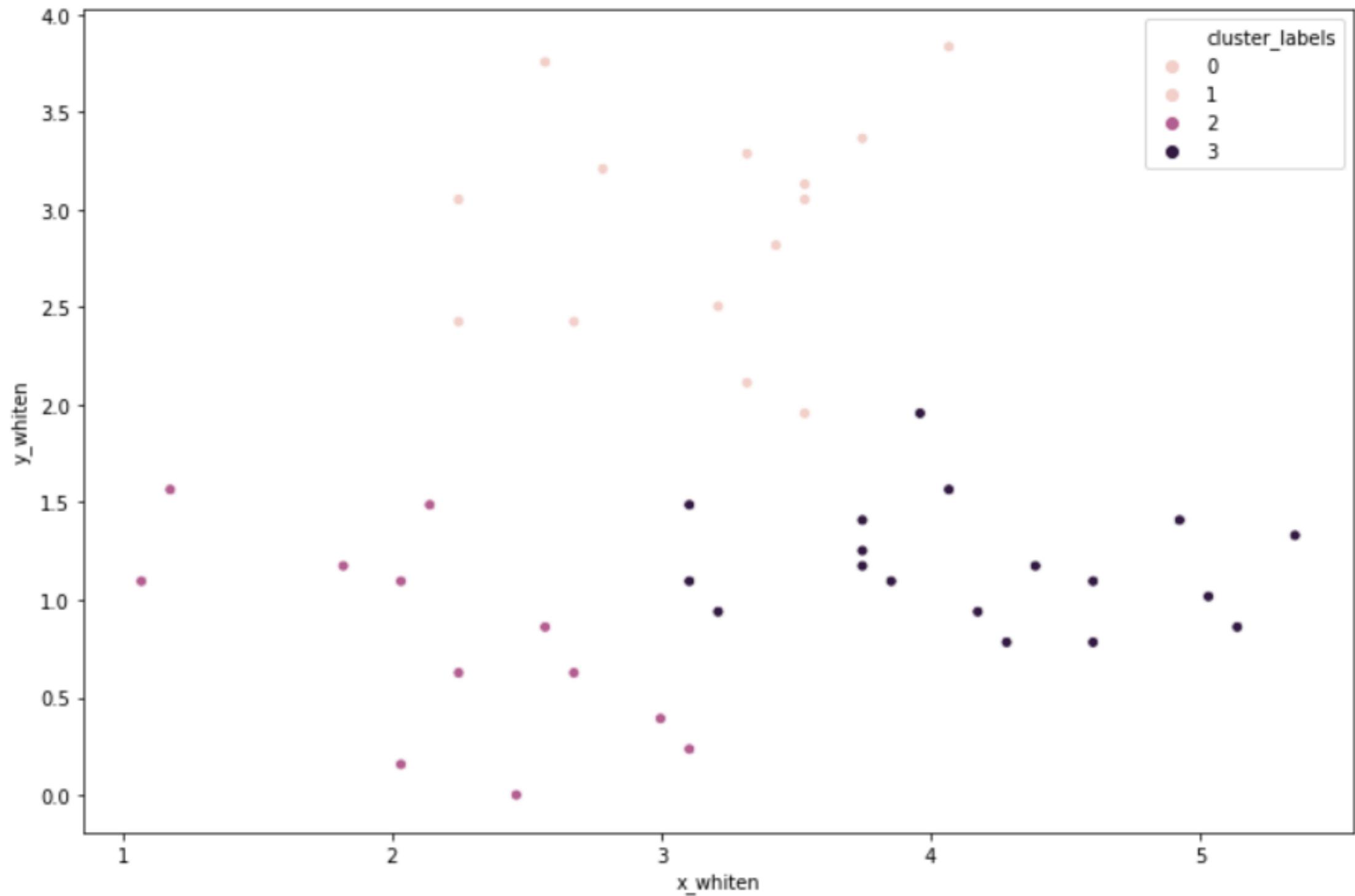
```
from scipy.cluster.hierarchy import dendrogram
```

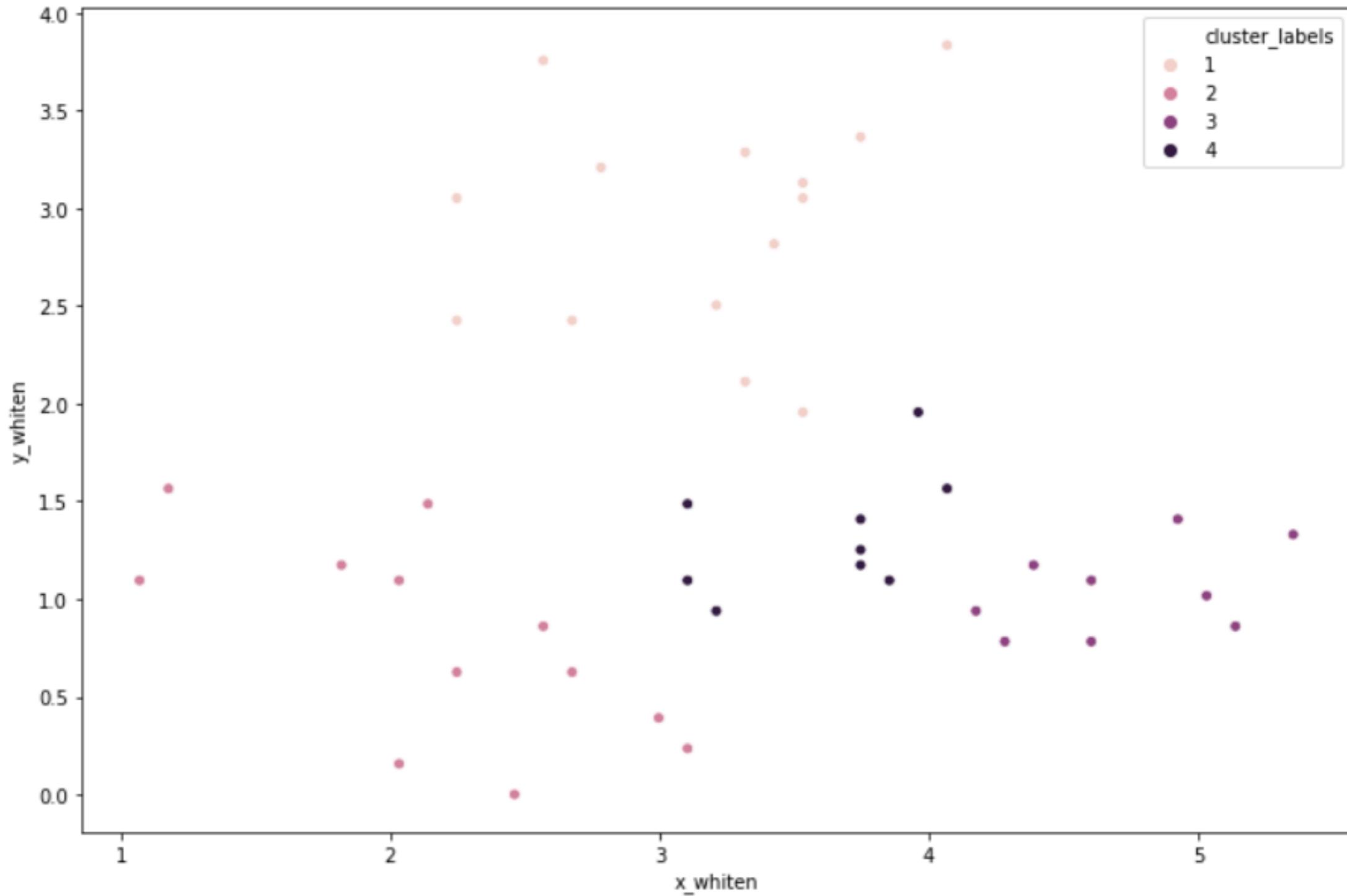
```
Z = linkage(df[['x_whiten', 'y_whiten']],
             method='ward',
             metric='euclidean')
dn = dendrogram(Z)
plt.show()
```









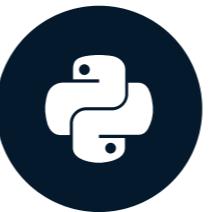


# **Next up - try some exercises**

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# Limitations of hierarchical clustering

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# Measuring speed in hierarchical clustering

- `timeit` module
- Measure the speed of `.linkage()` method
- Use randomly generated points
- Run various iterations to extrapolate

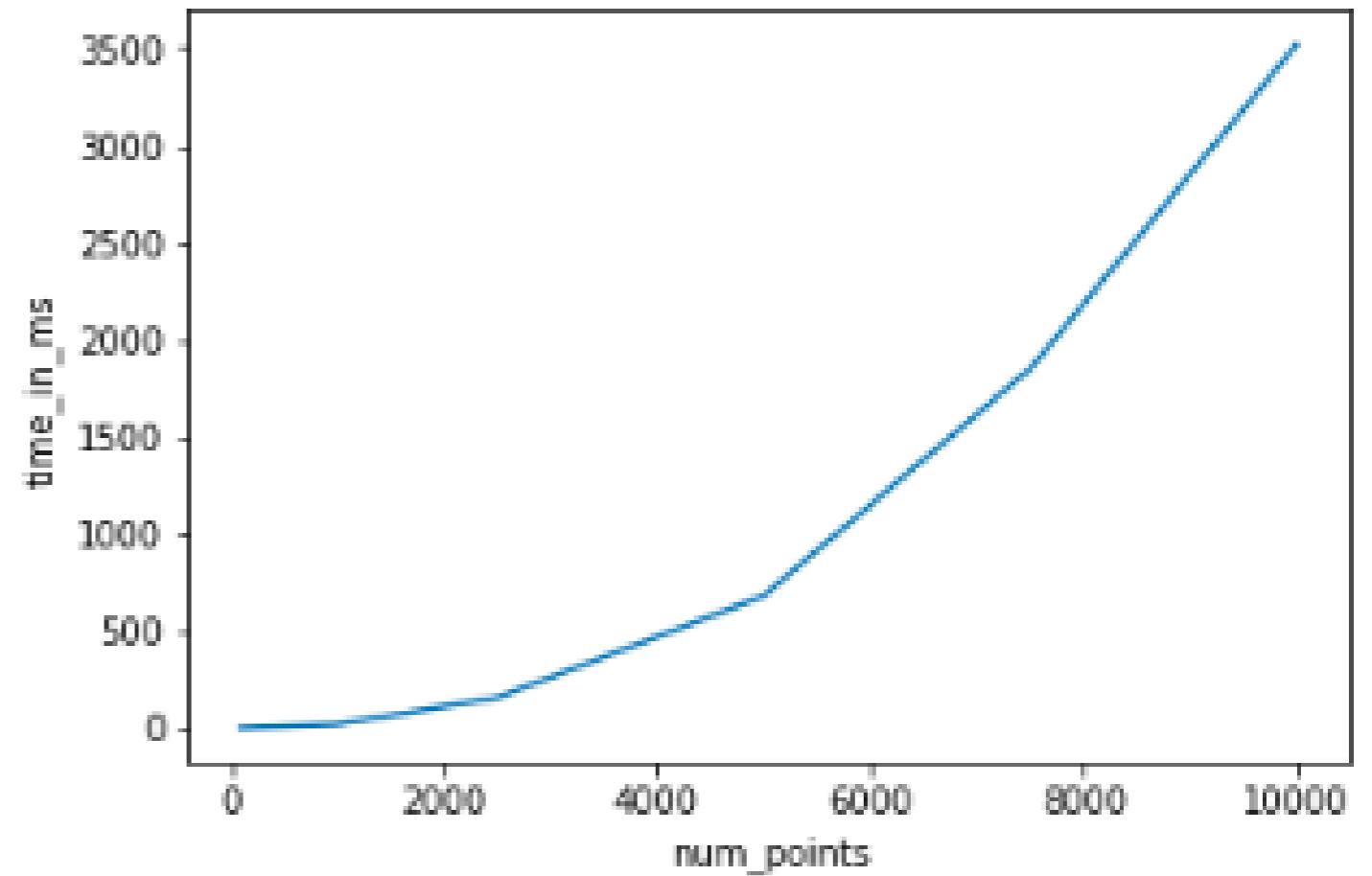
# Use of timeit module

```
from scipy.cluster.hierarchy import linkage
import pandas as pd
import random, timeit
points = 100
df = pd.DataFrame({'x': random.sample(range(0, points), points),
                    'y': random.sample(range(0, points), points)})
%timeit linkage(df[['x', 'y']], method = 'ward', metric = 'euclidean')
```

1.02 ms ± 133 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)

# Comparison of runtime of linkage method

- Increasing runtime with data points
- Quadratic increase of runtime
- Not feasible for large datasets



# **Next up - exercises**

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