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?

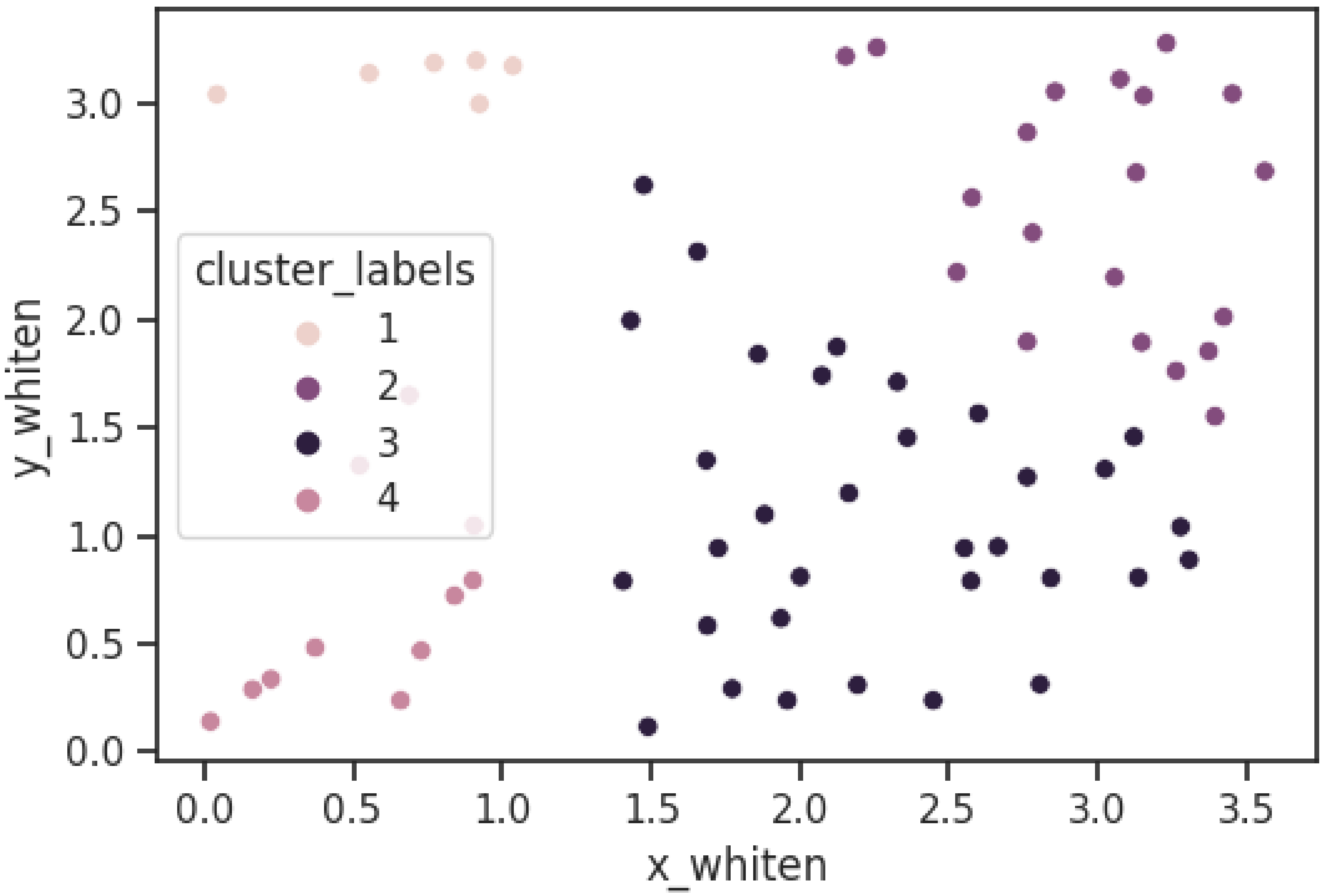
- `'single'` : based on two closest objects
- `'complete'` : based on two farthest objects
- `'average'` : based on the arithmetic mean of all objects
- `'centroid'` : based on the geometric mean of all objects
- `'median'` : based on the median of all objects
- `'ward'` : based on the sum of squares

Create cluster labels with fcluster

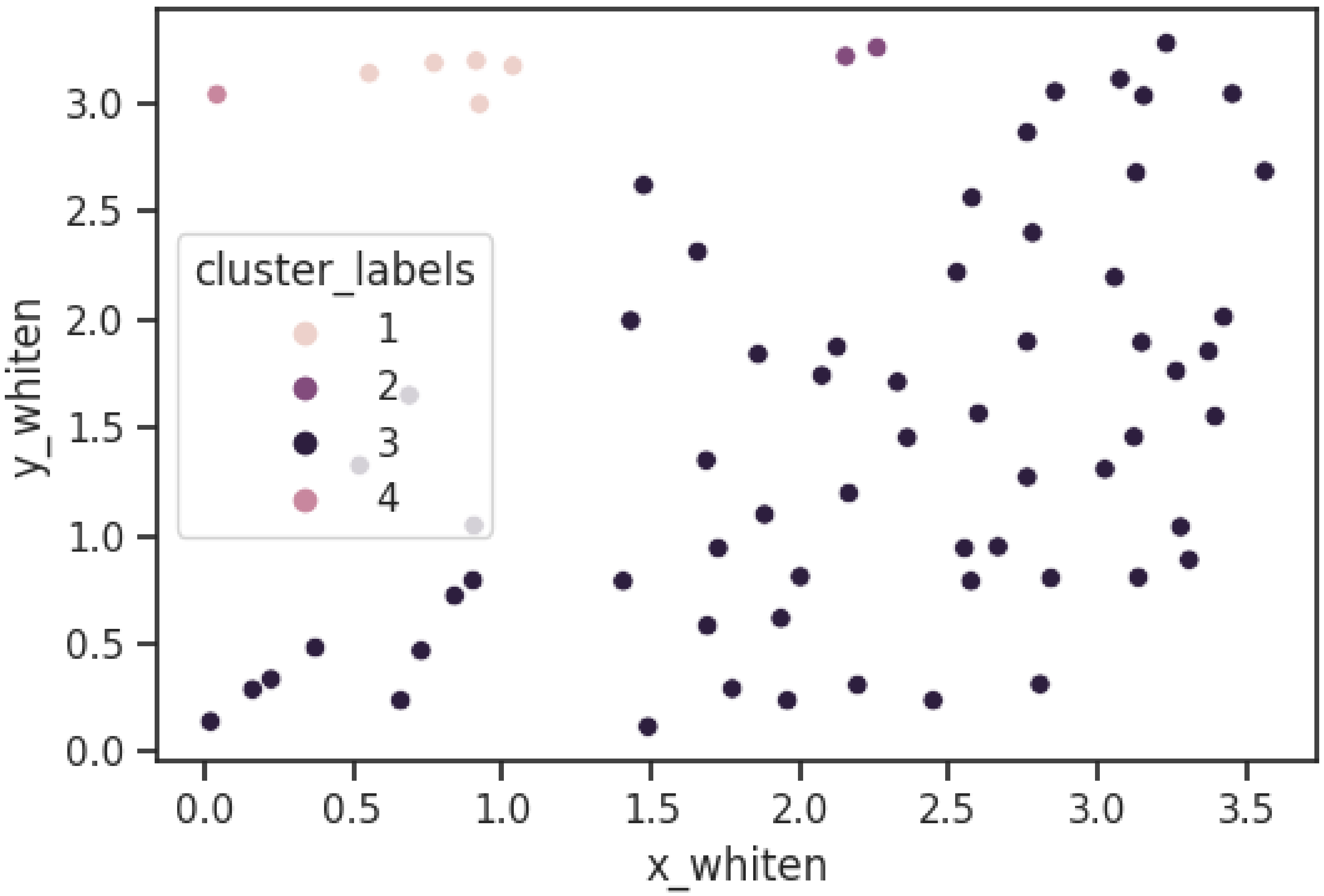
```
scipy.cluster.hierarchy.fcluster(distance_matrix,
                                 num_clusters,
                                 criterion
)
```

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

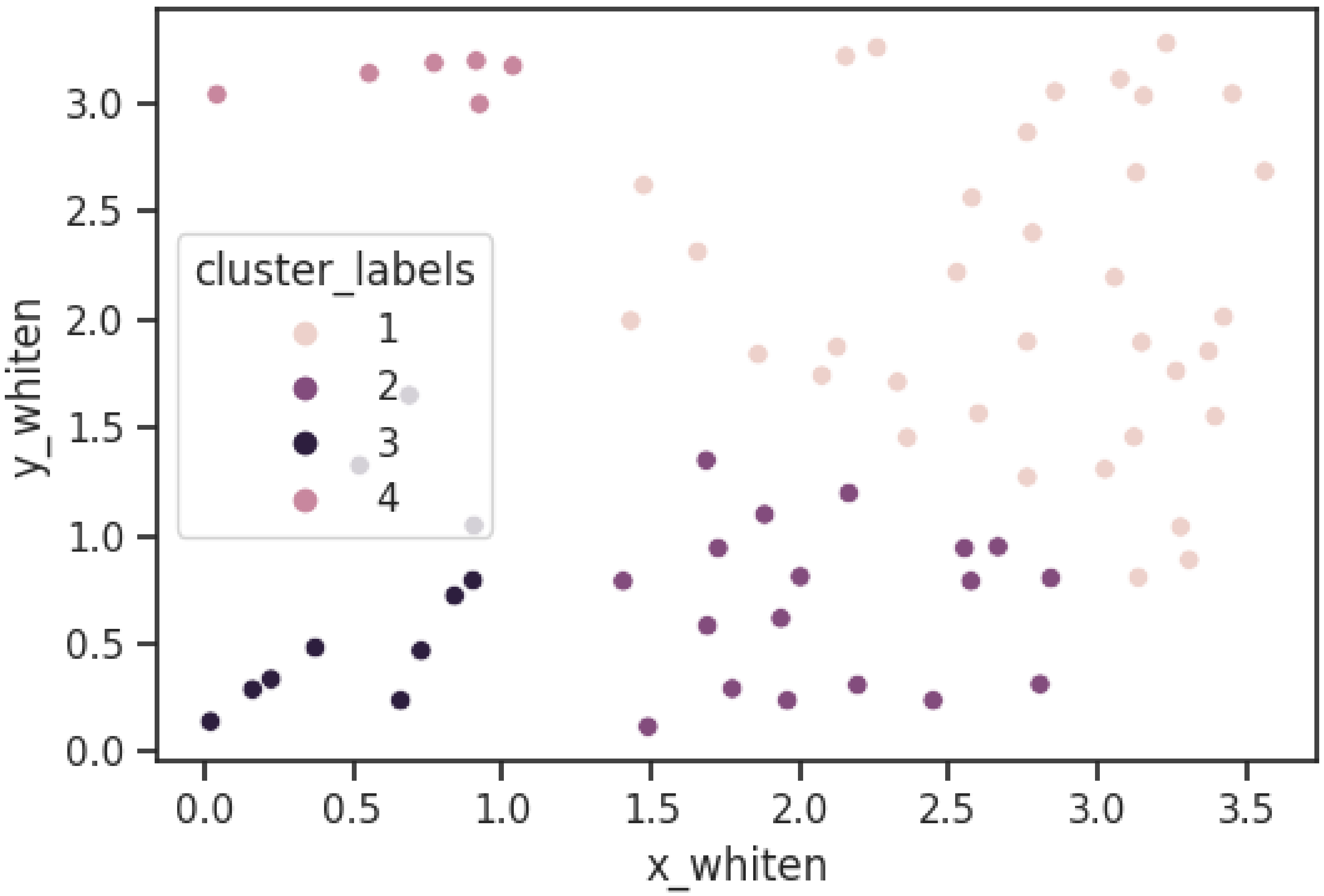
Hierarchical clustering with ward method



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()
```

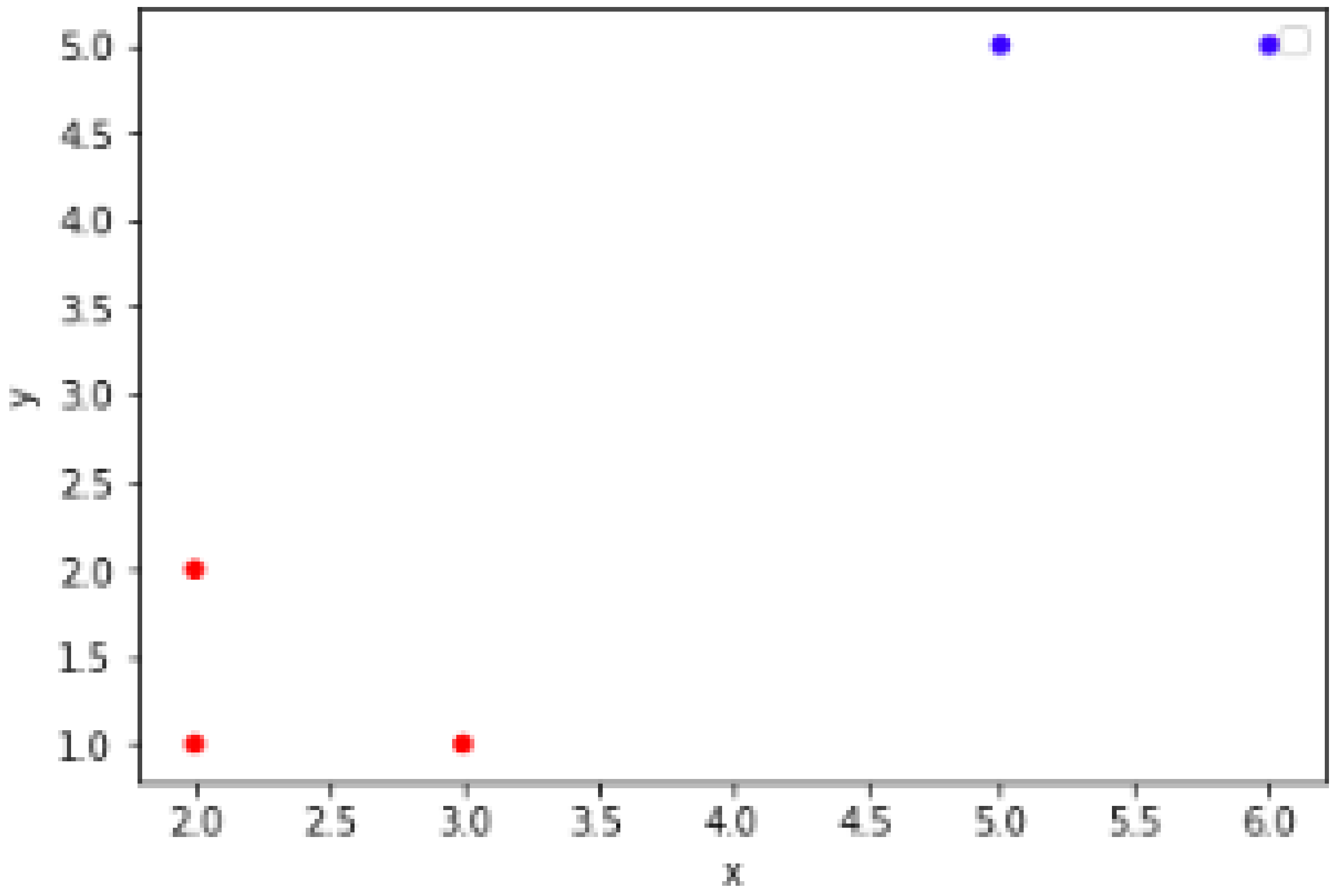
Visualize clusters with seaborn

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

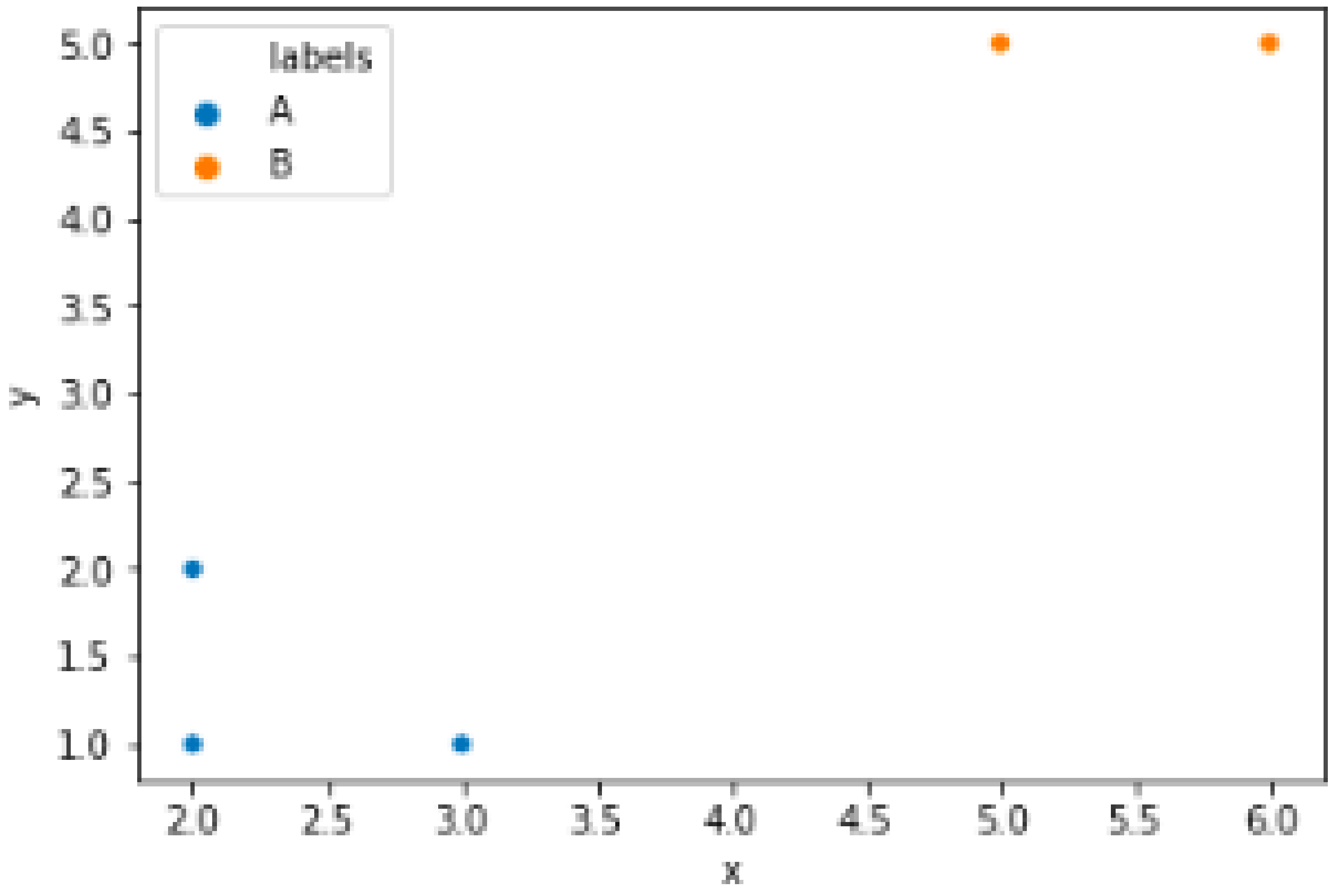
```
df = pd.DataFrame({'x': [2, 3, 5, 6, 2],
                   'y': [1, 1, 5, 5, 2],
                   'labels': ['A', 'A', 'B', 'B', 'A']})
sns.scatterplot(x='x',
                y='y',
                hue='labels',
                data=df)
plt.show()
```

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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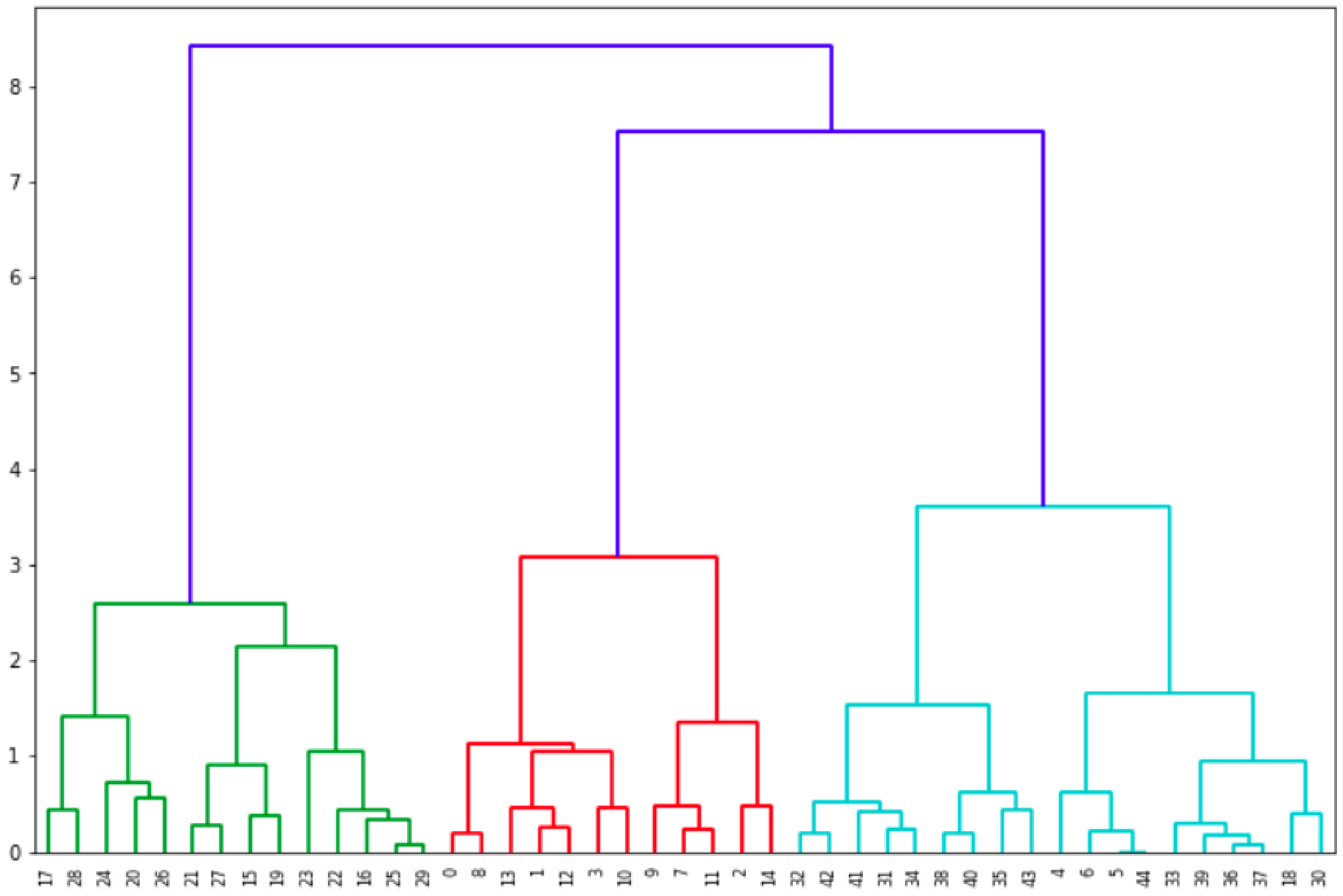
Introduction to dendrograms

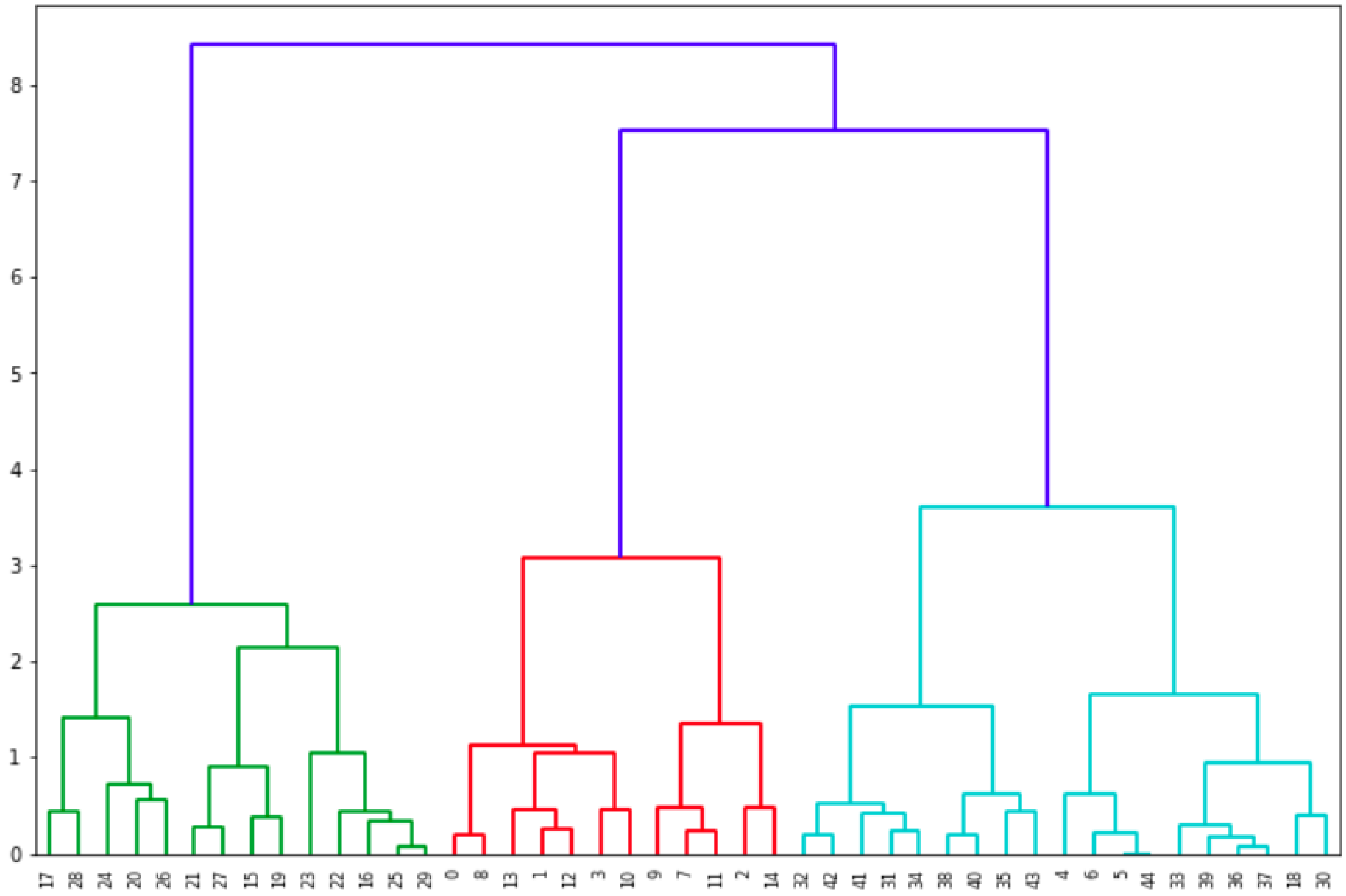
- Strategy till now - decide clusters on visual inspection
- Dendrograms help in showing progressions as clusters are merged
- A dendrogram is a branching diagram that demonstrates how each cluster is composed by branching out into its child nodes



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()
```


8
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5
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17
28
24
20
26
21
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29
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43
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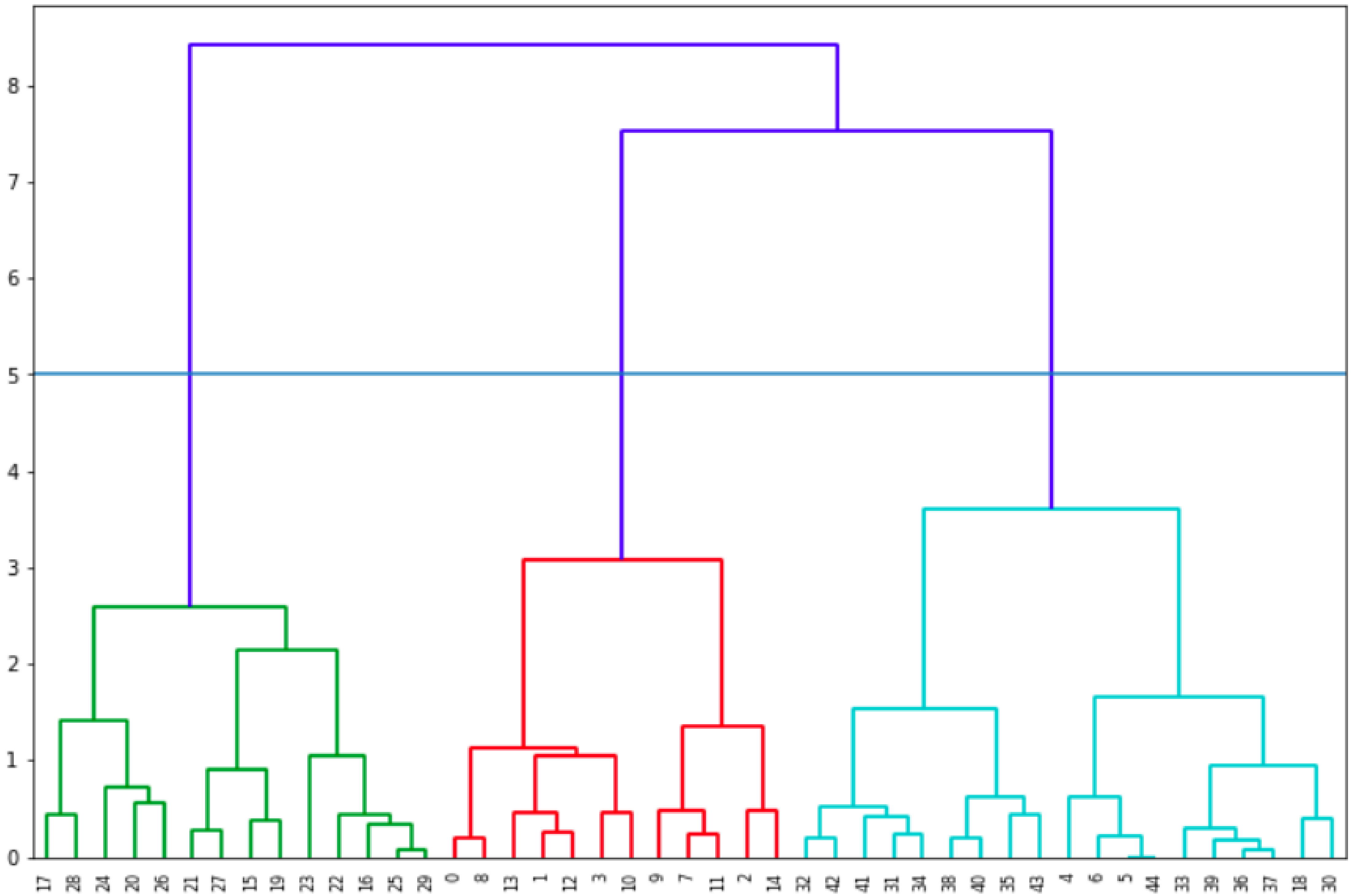
39
36
37
18
30



8
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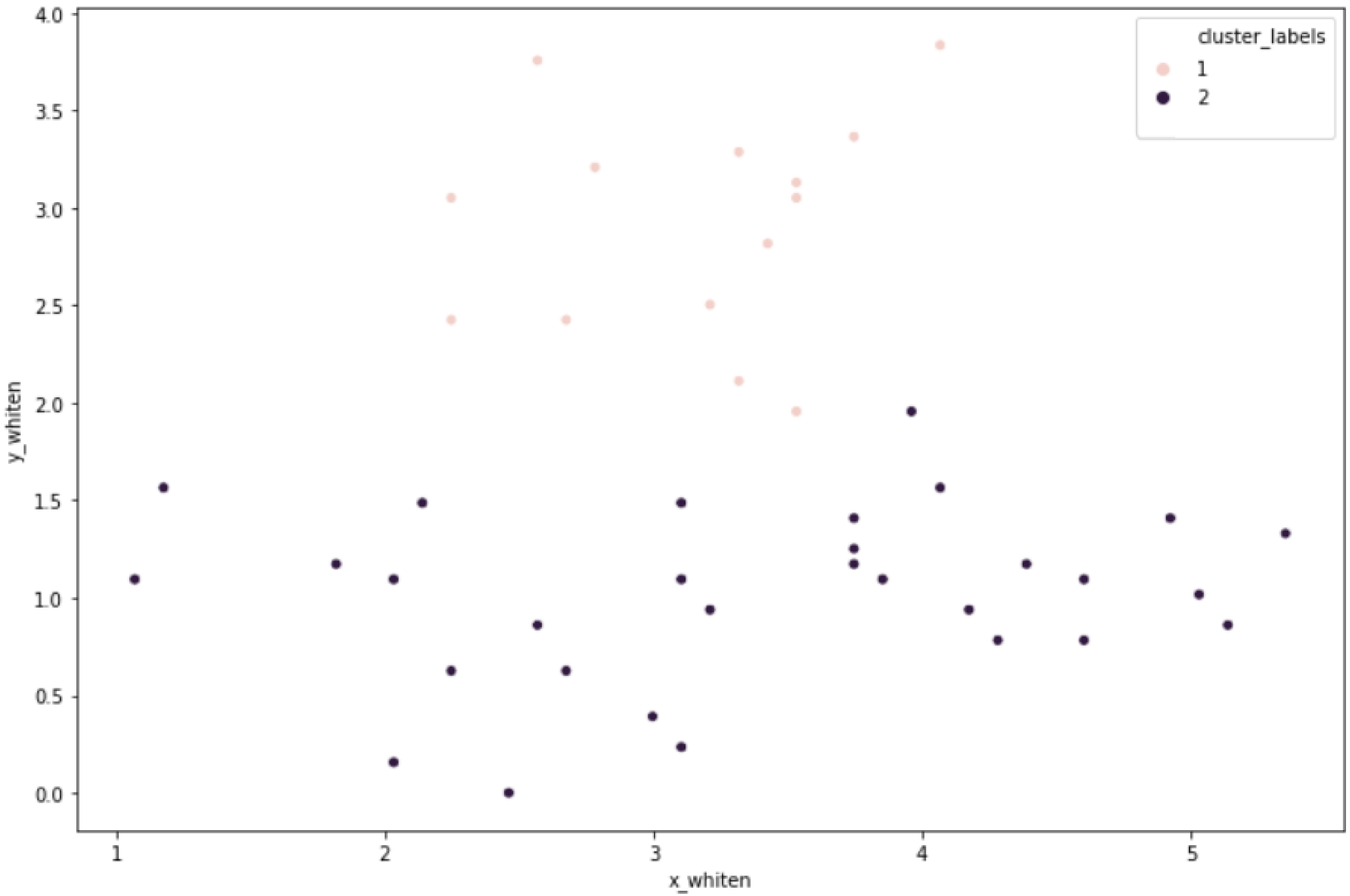
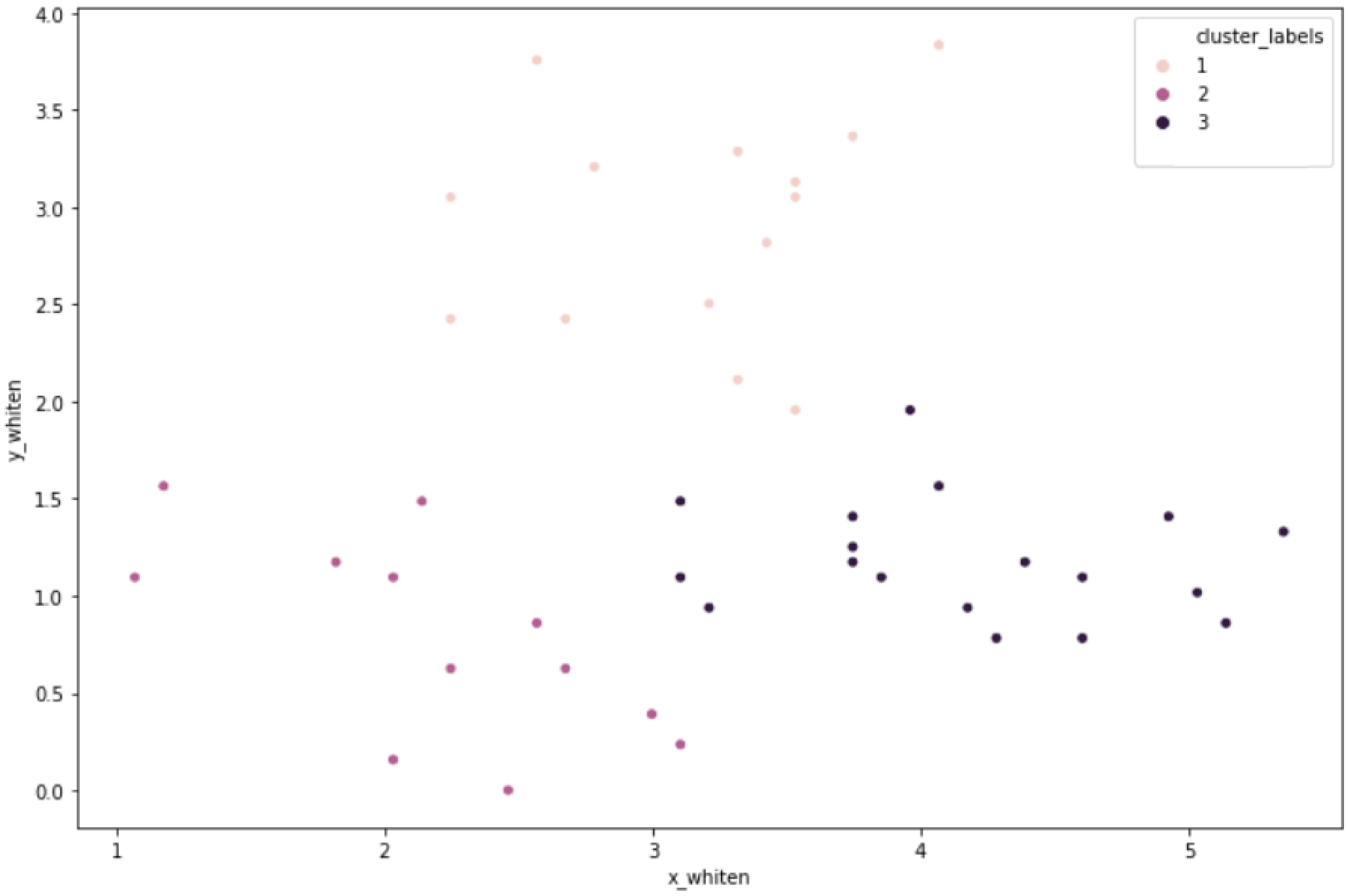
0
17 28 24 20 26 21 27 15 19 23 22 16 25 29 0 8 13 1 12 3 10 9 7 11 2 14 32 42 41 31 34 38 40 35 43 4 6 5 44 33 39 36 37 18 30


cluster_labels
1
2
y_whiten
x_whiten
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
2
3
4
5


cluster_labels
1
2
3
y_whiten
x_whiten
4.0
3.5
3.0
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1.5
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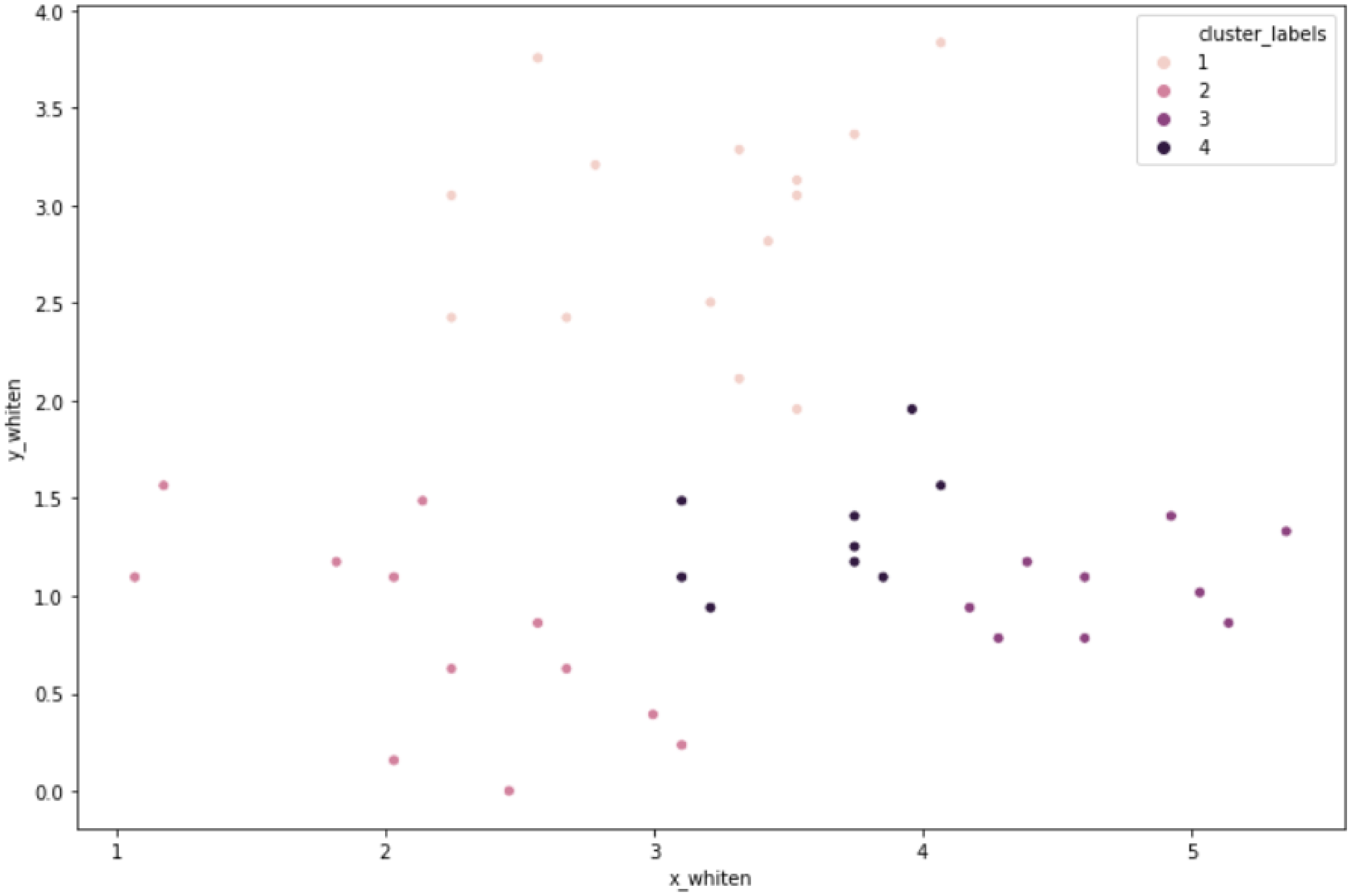

cluster_labels
1
2
3
4
y_whiten
x_whiten
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
2
3
4
5

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

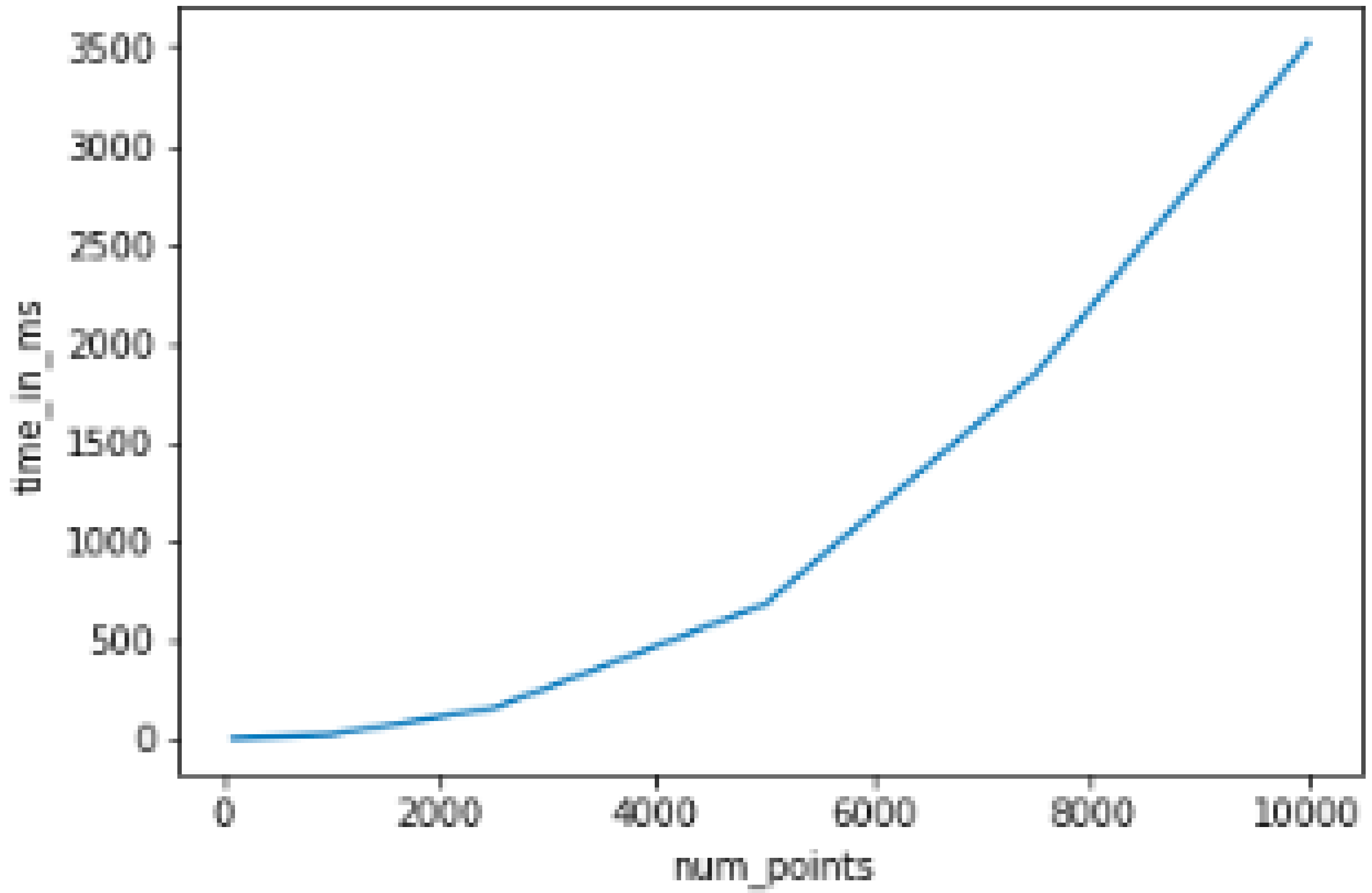
Use of timeit module

```
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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