Basics of k-means clustering

CLUSTER ANALYSIS IN PYTHON

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Why k-means clustering?

- A critical drawback of hierarchical clustering: runtime
- K means runs significantly faster on large datasets

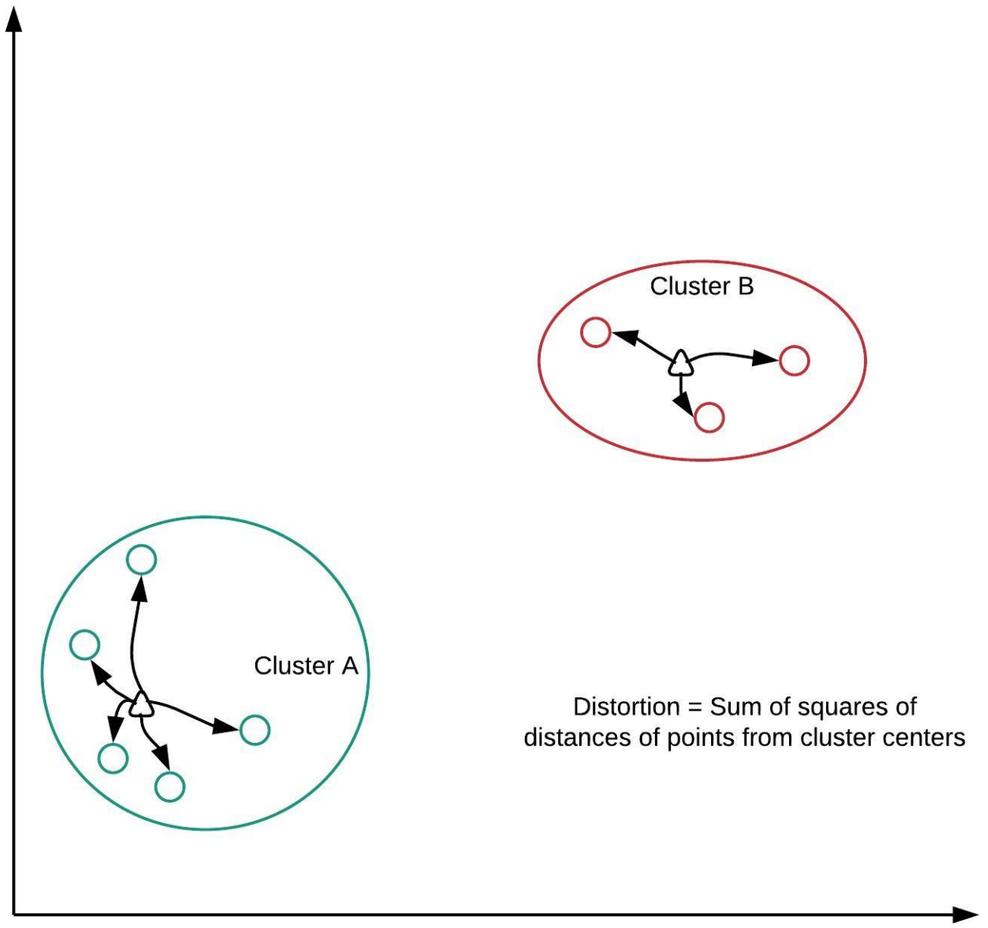
Step 1: Generate cluster centers

```
kmeans(obs, k_or_guess, iter, thresh, check_finite)
```

- `obs` : standardized observations
- `k_or_guess` : number of clusters
- `iter` : number of iterations (default: 20)
- `thres` : threshold (default: 1e-05)
- `check_finite` : whether to check if observations contain only finite numbers (default: True)

Returns two objects: cluster centers, distortion

How is distortion calculated?



Step 2: Generate cluster labels

```
vq(obs, code_book, check_finite=True)
```

- `obs` : standardized observations
- `code_book` : cluster centers
- `check_finite` : whether to check if observations contain only finite numbers (default: True)

Returns two objects: a list of cluster labels, a list of distortions

A note on distortions

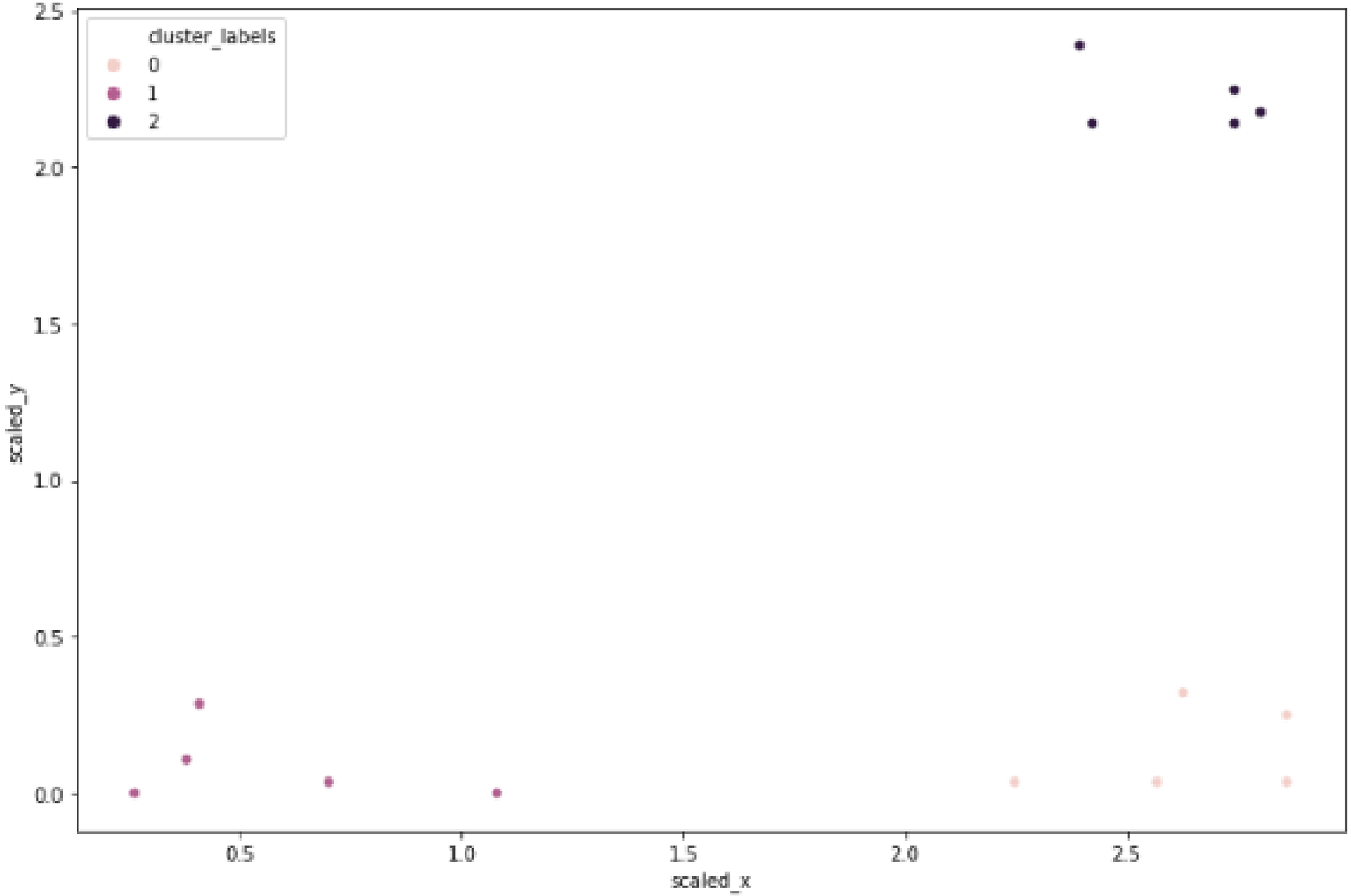
- `kmeans` returns a single value of distortions
- `vq` returns a list of distortions.

Running k-means

```
# Import kmeans and vq functions
from scipy.cluster.vq import kmeans, vq
```

```
# Generate cluster centers and labels
cluster_centers, _ = kmeans(df[['scaled_x', 'scaled_y']], 3)
df['cluster_labels'], _ = vq(df[['scaled_x', 'scaled_y']], cluster_centers)
```

```
# Plot clusters
sns.scatterplot(x='scaled_x', y='scaled_y', hue='cluster_labels', data=df)
plt.show()
```


cluster_labels
0
1
2
2.5
2.0
1.5
1.0
0.5
0.0
scaled_y
0.5
1.0
1.5
2.0
2.5
scaled_x

Next up: exercises!

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How many clusters?

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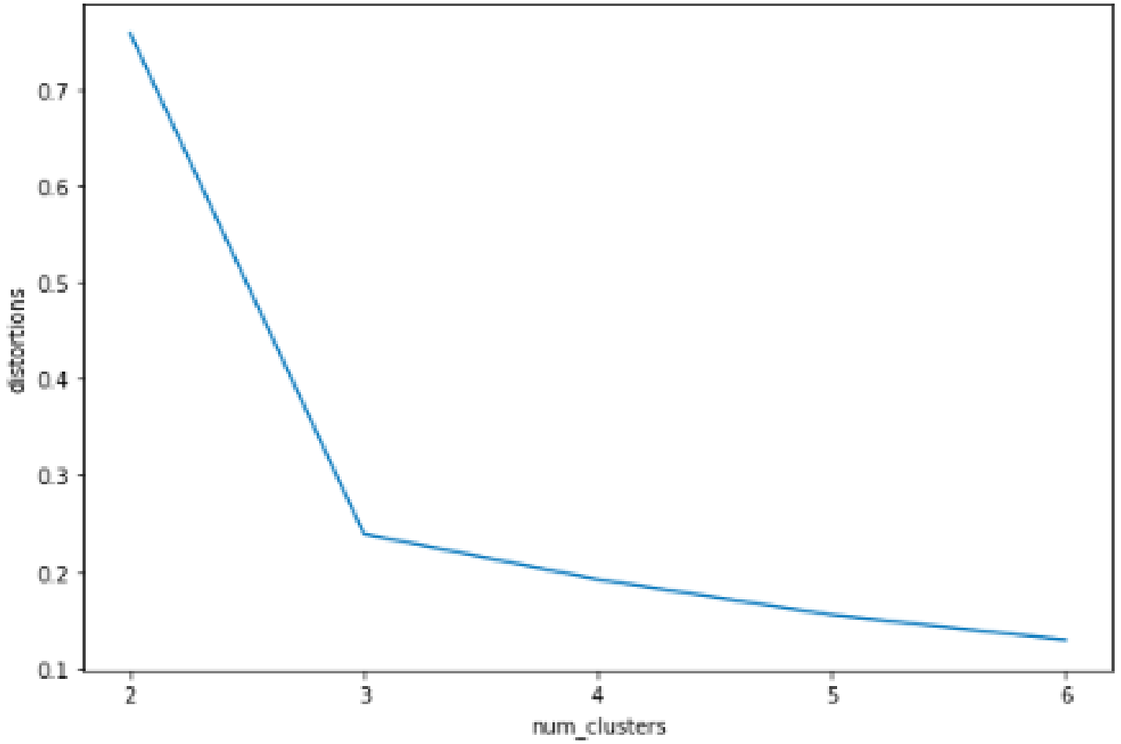
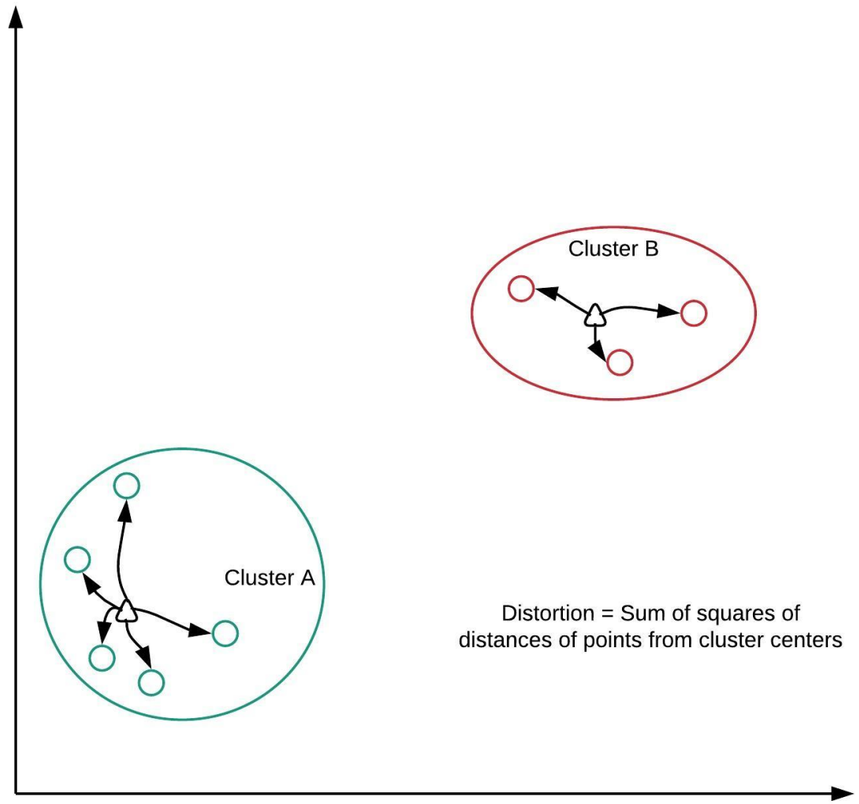
How to find the right k?

- No *absolute* method to find right number of clusters (k) in k-means clustering
- Elbow method



Distortions revisited

- Distortion: sum of squared distances of points from cluster centers
- Decreases with an increasing number of clusters
- Becomes zero when the number of clusters equals the number of points
- Elbow plot: line plot between cluster centers and distortion



Elbow method

- Elbow plot: plot of the number of clusters and distortion
- Elbow plot helps indicate number of clusters present in data

Elbow method in Python

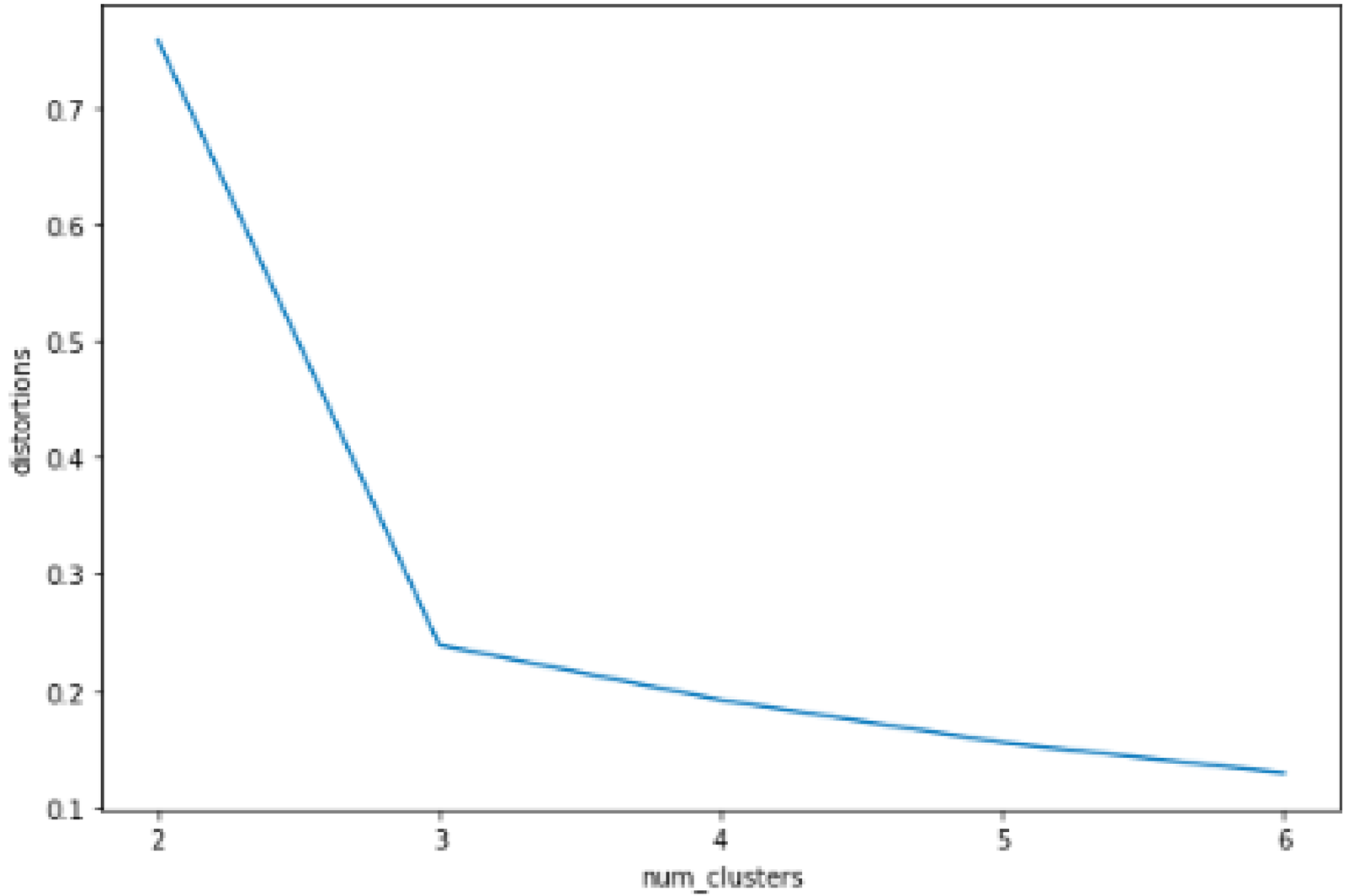
```
# Declaring variables for use
distortions = []

num_clusters = range(2, 7)
```

```
# Populating distortions for various clusters
for i in num_clusters:
    centroids, distortion = kmeans(df[['scaled_x', 'scaled_y']], i)
    distortions.append(distortion)
```

```
# Plotting elbow plot data
elbow_plot_data = pd.DataFrame({'num_clusters': num_clusters,
                                'distortions': distortions})

sns.lineplot(x='num_clusters', y='distortions',
             data = elbow_plot_data)
plt.show()
```


0.7
0.6
0.5
0.4
0.3
0.2
0.1
distortions
2
3
4
5
6
num_clusters

Final thoughts on using the elbow method

- Only gives an indication of optimal _k_ (numbers of clusters)
- Does not always pinpoint how many _k_ (numbers of clusters)
- Other methods: average silhouette and gap statistic

Next up: exercises

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Limitations of k-means clustering

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Limitations of k-means clustering

- How to find the right _K_ (number of clusters)?
- Impact of seeds
- Biased towards equal sized clusters

Impact of seeds

Initialize a random seed

```
from numpy import random
random.seed(12)
```

Seed: `np.array(1000, 2000)`

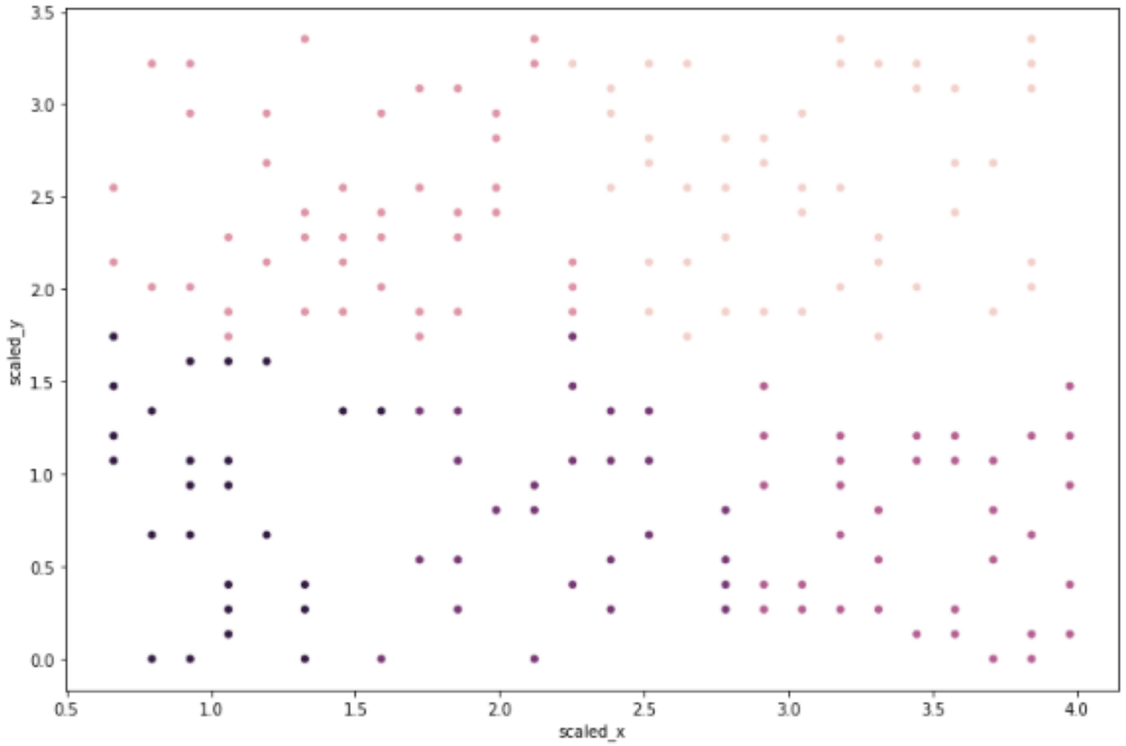
Cluster sizes: 29, 29, 43, 47, 52

Seed: `np.array(1,2,3)`

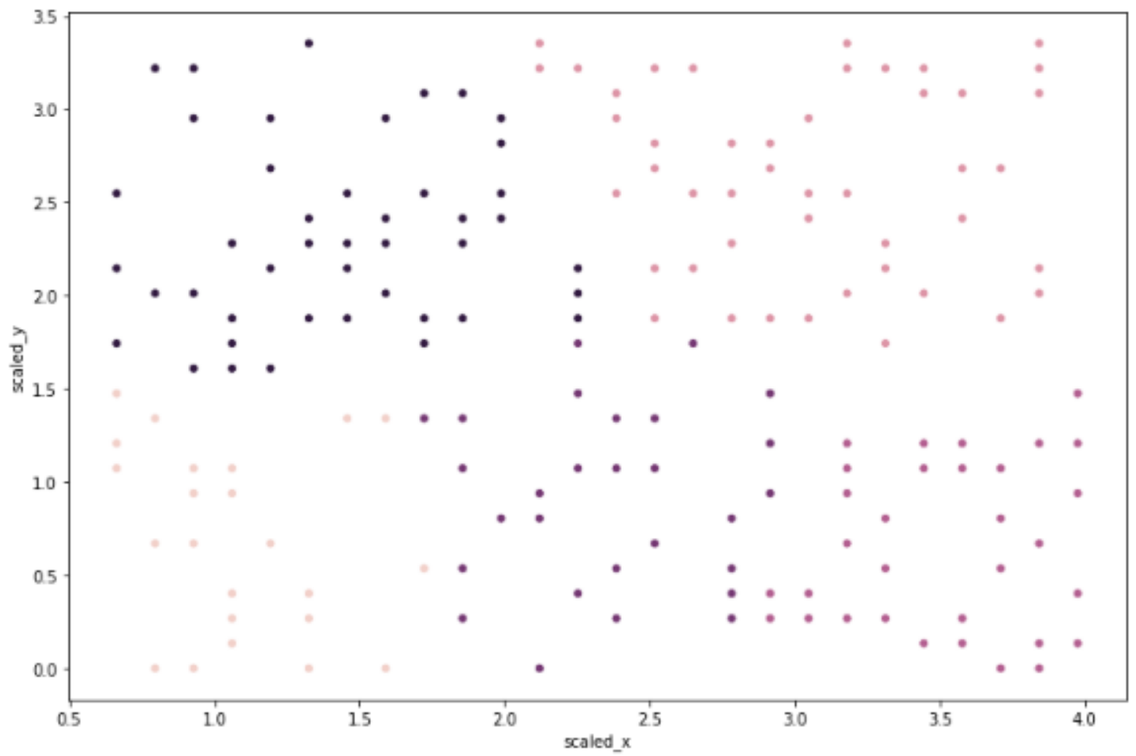
Cluster sizes: 26, 31, 40, 50, 53

Impact of seeds: plots

Seed: `np.array(1000, 2000)`

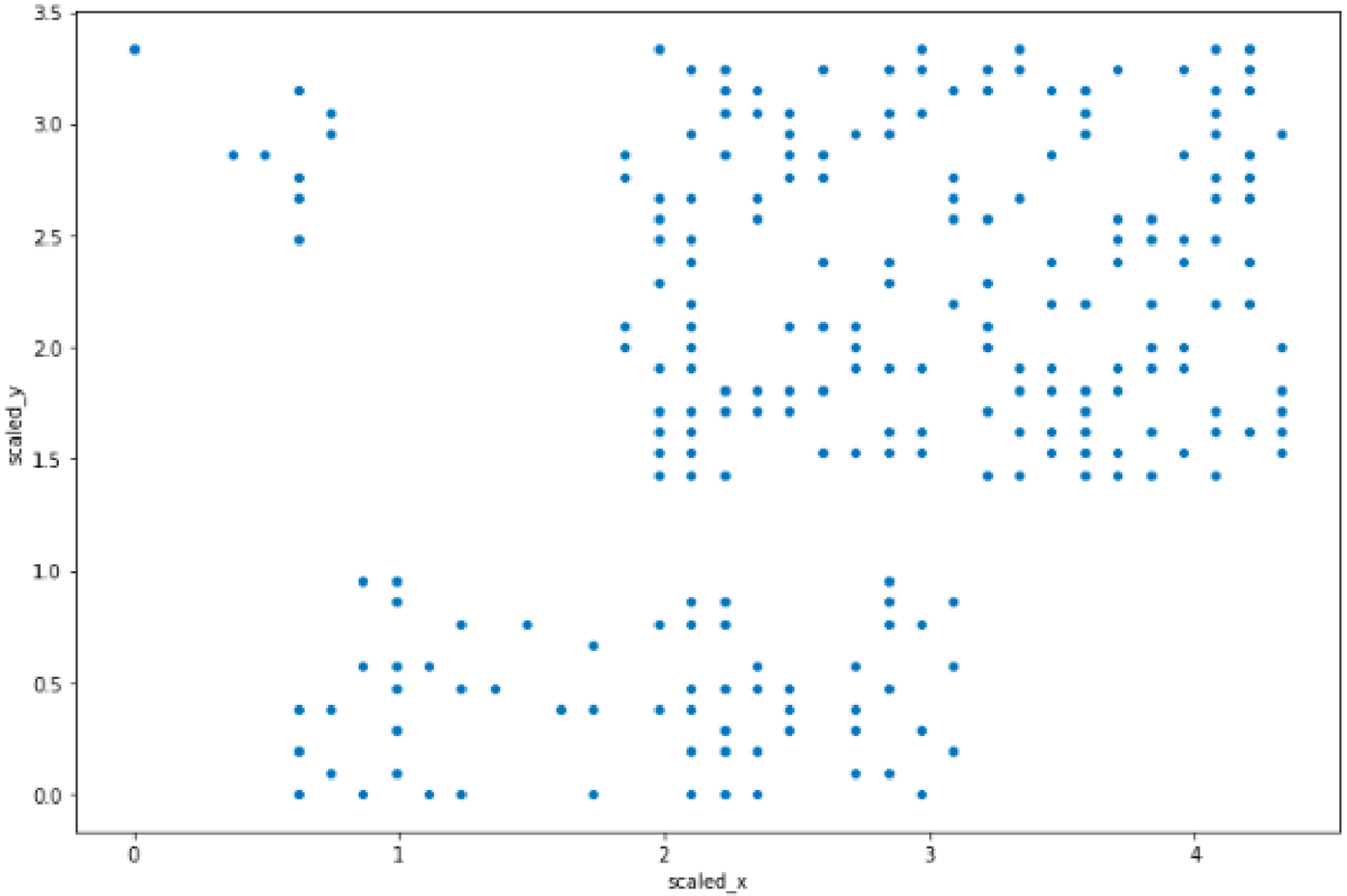


Seed: `np.array(1,2,3)`



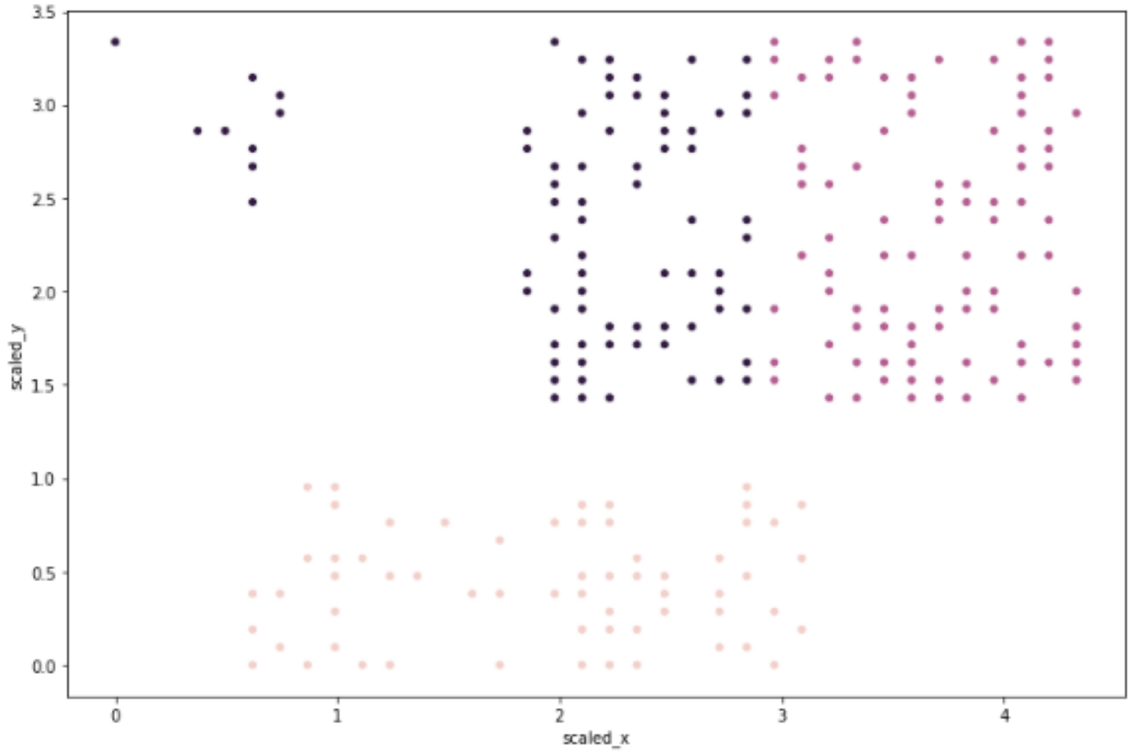
You will notice that many points along the cluster boundaries have interchanged clusters. Interestingly, the effect of seeds is only seen when the data to be clustered is fairly uniform. If the data has distinct clusters before clustering is performed, the effect of seeds will not result in any changes in the formation of

Uniform clusters in k means

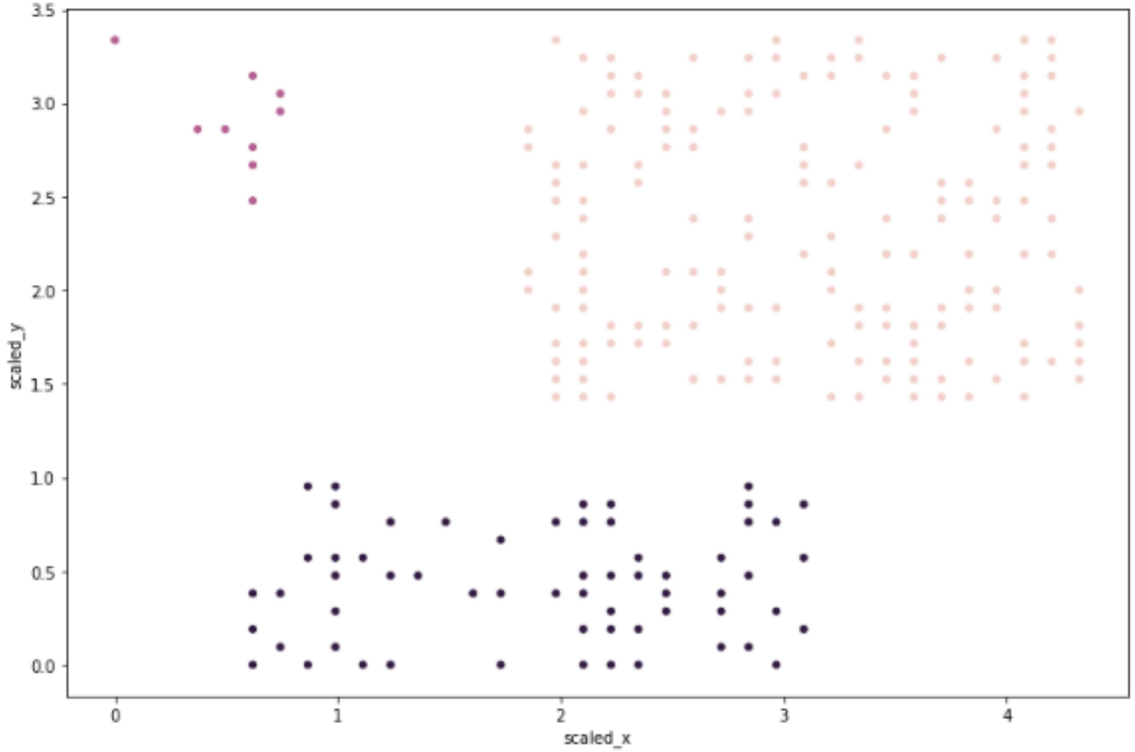


Uniform clusters in k-means: a comparison

K-means clustering with 3 clusters



Hierarchical clustering with 3 clusters



Final thoughts

- Each technique has its pros and cons
- Consider your data size and patterns before deciding on algorithm
- Clustering is exploratory phase of analysis

Next up: exercises

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