LECTURE 21

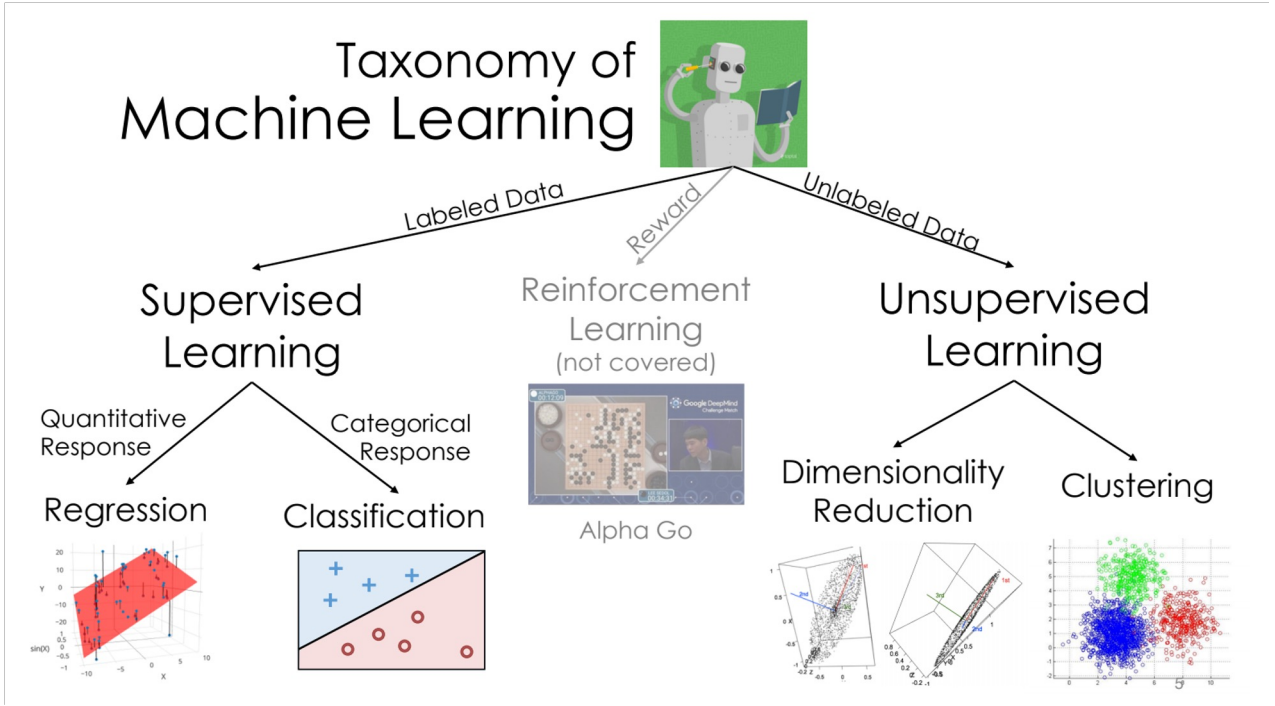
Clustering

Using clustering algorithms to identify patterns in our data.

Machine learning taxonomy

Regression and Classification are both forms of **supervised learning**.

Logistic regression, the topic of this lecture, is mostly used for **classification**, even though it has “regression” in the name.



Today's Roadmap

Introduction to Clustering

Taxonomy of Clustering Approaches

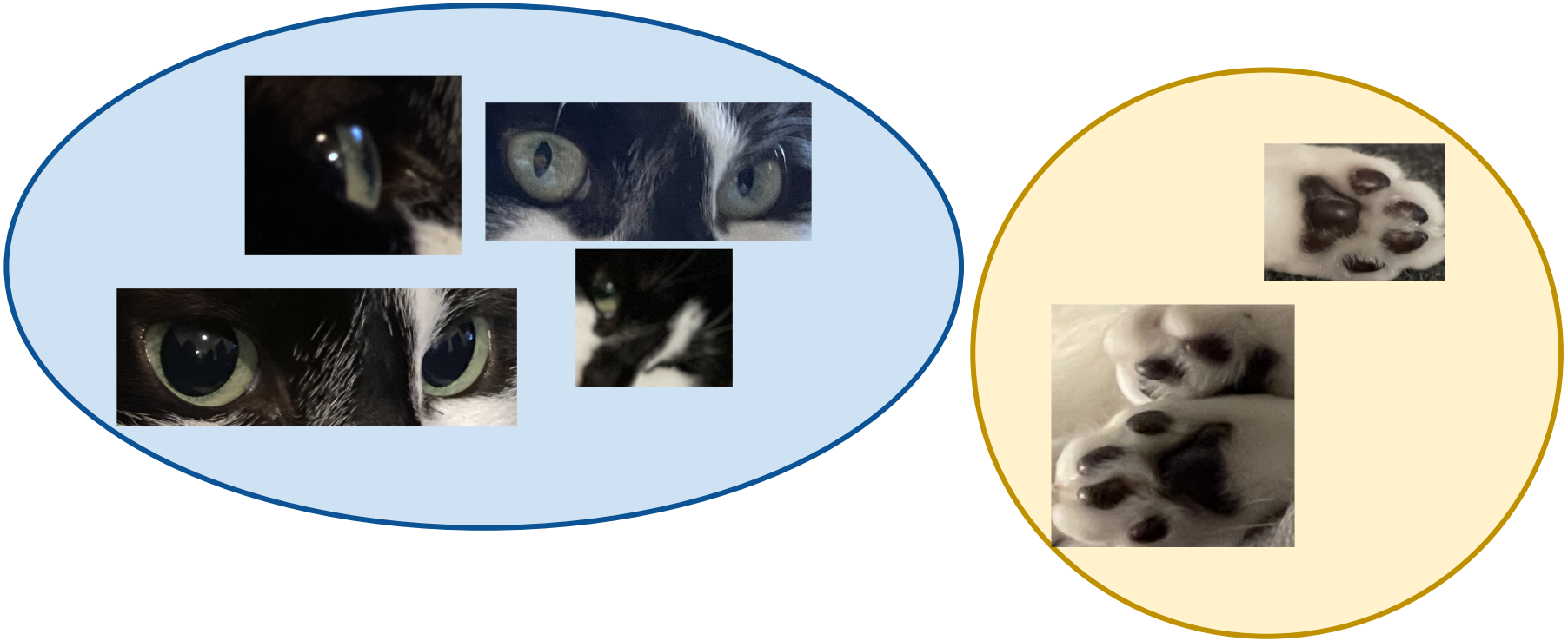
K-Means Clustering

Minimizing Inertia

Hierarchical Agglomerative Clustering

Picking K

Clustering Example - 0

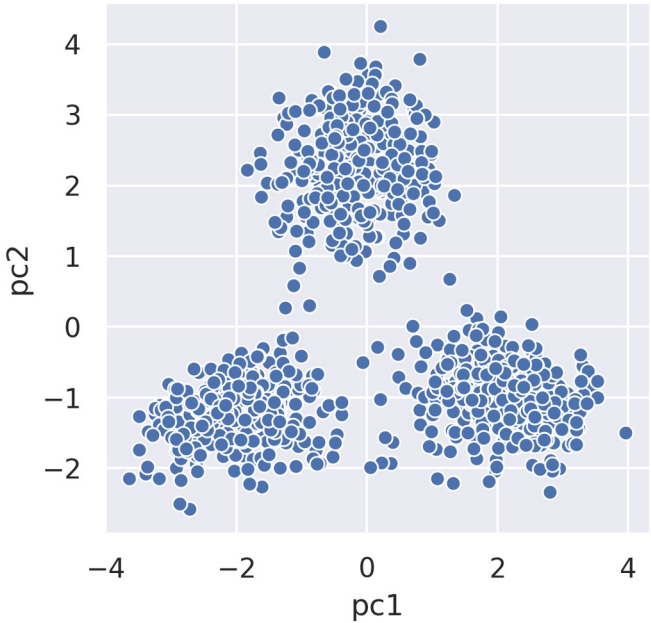


Clustering Example - 1

Goal of clustering: Assign each point to a cluster.

This is an unsupervised task.

- We don’t have labels for each visitor.
- Want to infer pattern even without labels.



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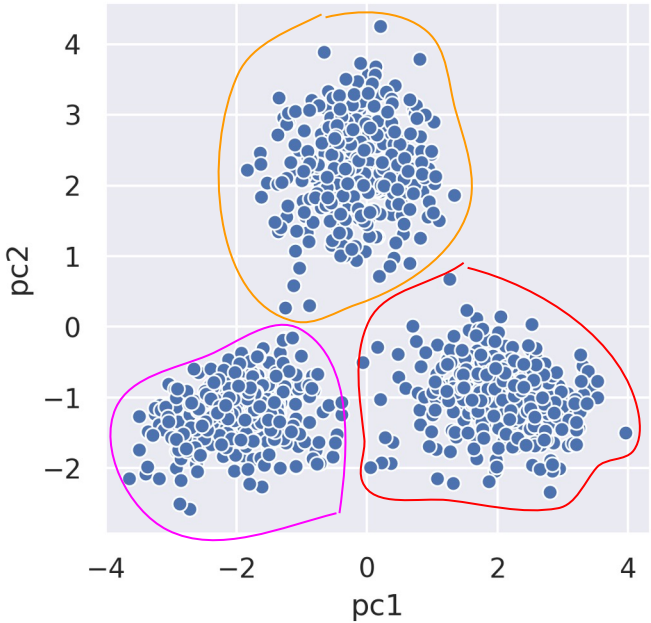


Clustering Example 2: Netflix

Suppose you're Netflix and have information on customer viewing habits.

- Can use clustering to assign each person or show to a "cluster".
- Don't have to define clusters in advance.

Clustering is different from classification.

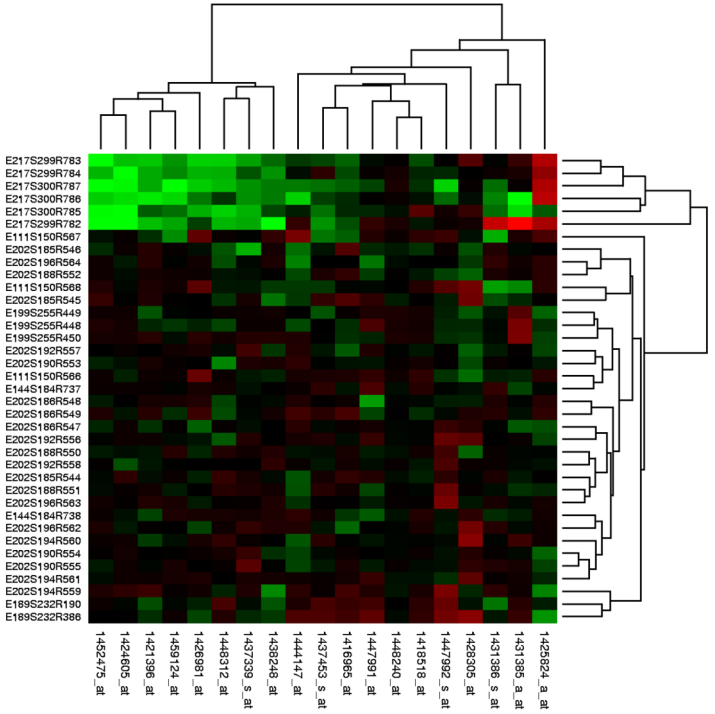
- With classification, you have to decide on labels in advance.
- Clustering discovers groups automatically.

Note: We're not certain that Netflix actually uses ML clustering to identify these categories, but they could in principle.

Clustering Example 3: Reverse Engineering Biology

In plot to the right:

- Rows are conditions (e.g. a row might be: “poured acid on the cells”).
- Columns are genes.



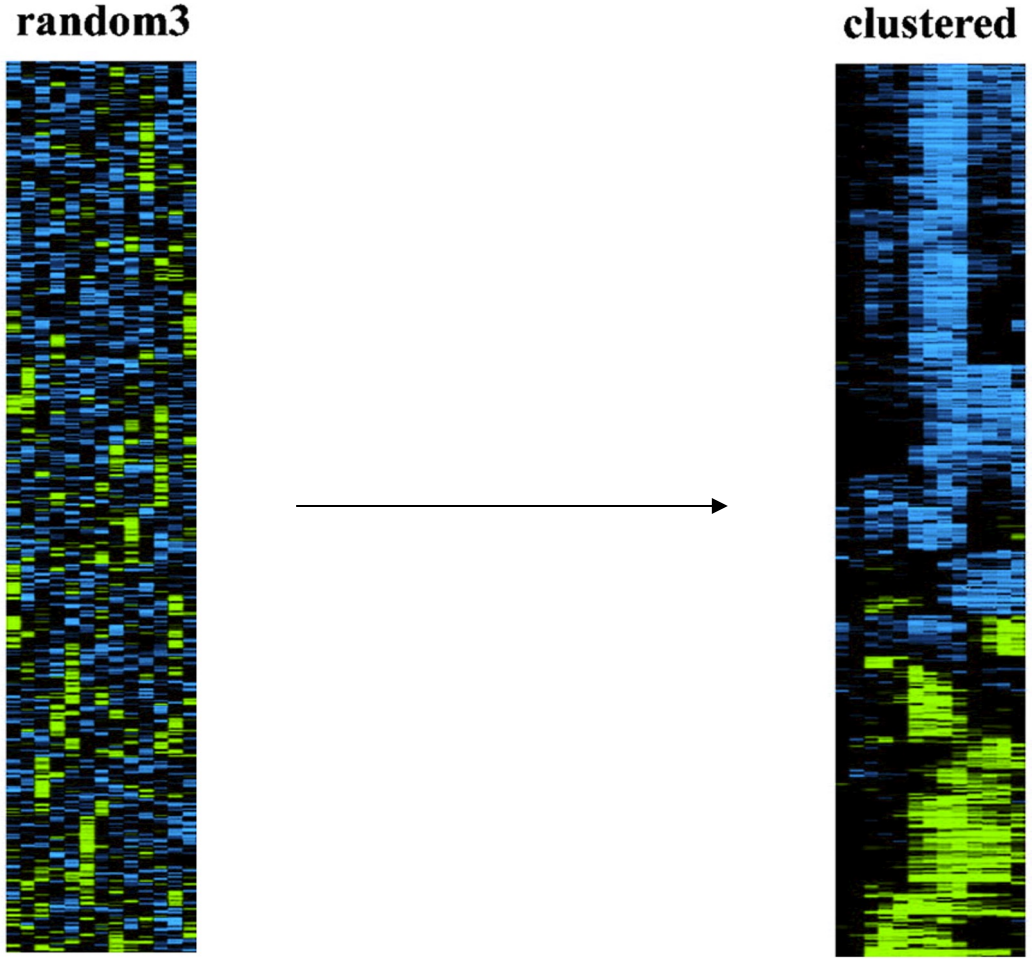
Green indicates that the gene was ~off.

- The ~9 genes on the left all got turned off by the 6 experiments at the top.

Clustering brings similar observations together.

Note: There is also red in this image indicating genes which were especially “on”.

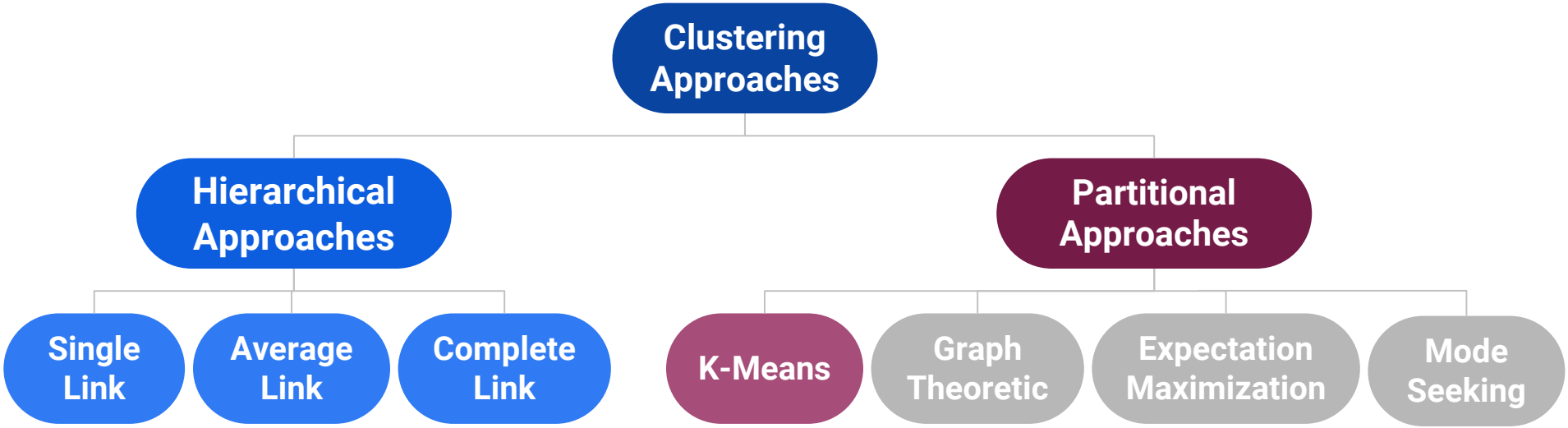
Clustering Example 3: Before and After Clustering



From: Cluster analysis and display of genome-wide expression patterns by Michael Eisen, et. al

Taxonomy of Clustering Approaches

Taxonomy of Clustering Approaches



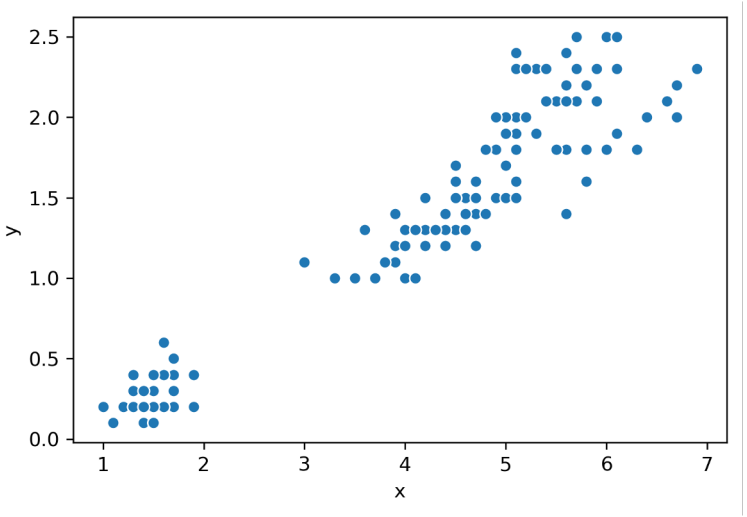
K-Means Clustering

K-Means Clustering

Most popular clustering approach. The algorithm:

- Pick an arbitrary **k**, and randomly place **k "centers"**, each a different color.
- Repeat until convergence:
  - Color points according to the closest center.
  - Move center for each color to center of points with that color.

Raw data →



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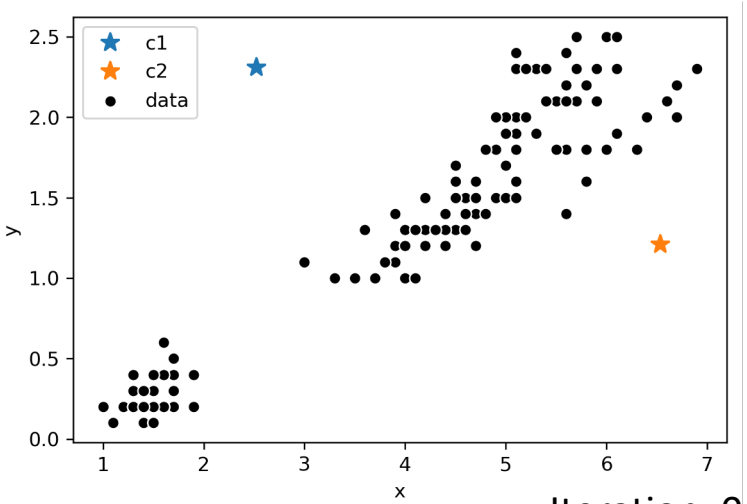
Initial random placement of two centers



Iteration: 0

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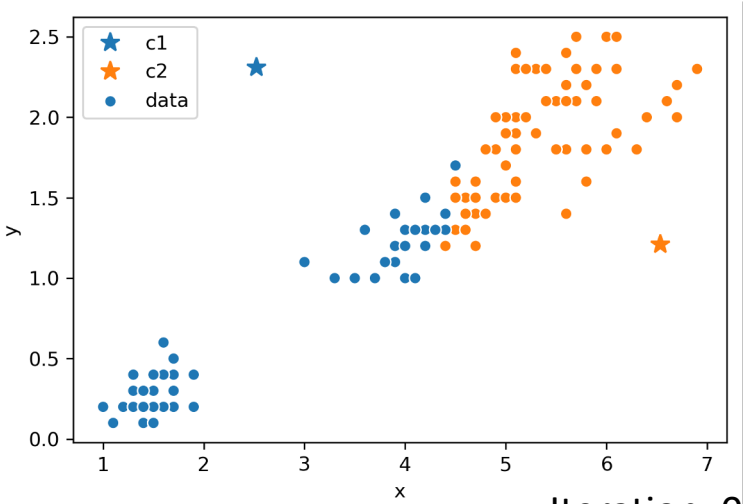
Data colored by closest center



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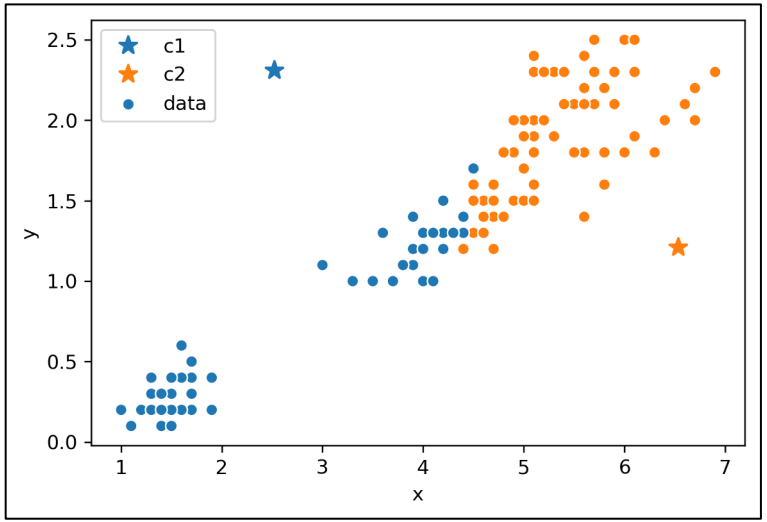
Where should the centers go next?



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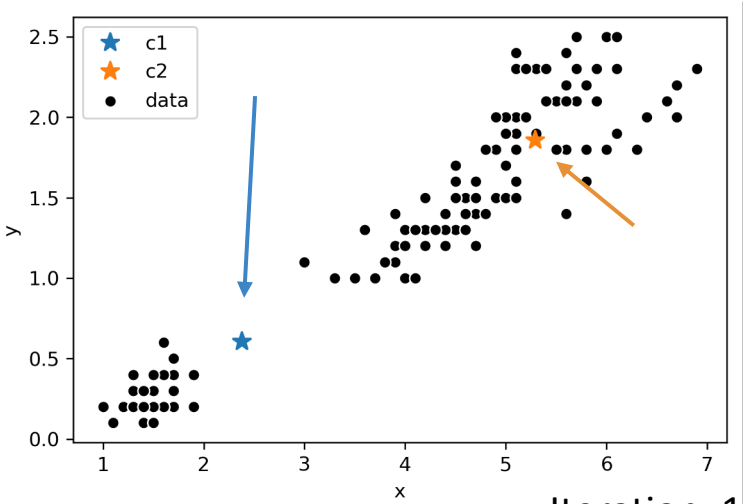
Centers moved to their new homes



Iteration: 1

K-Means Clustering

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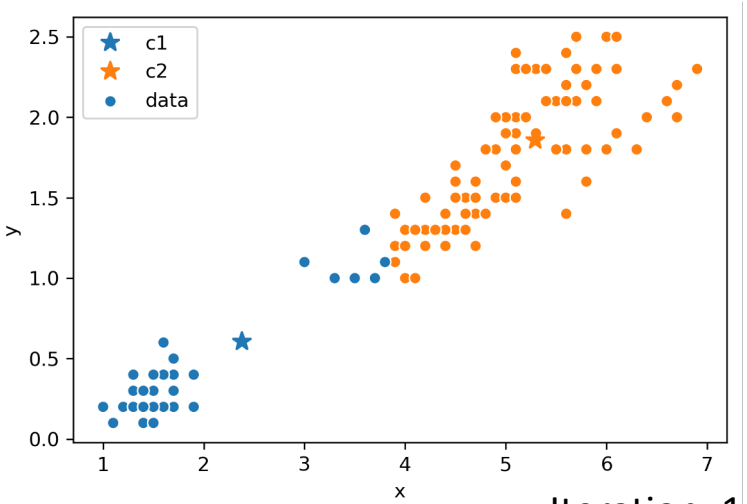
Data colored by closest center (in new position)



Iteration: 1

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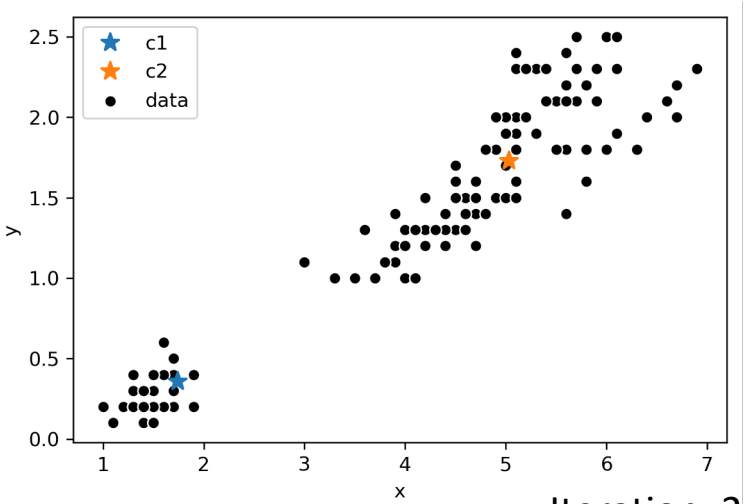

Iteration: 2

K-Means Clustering

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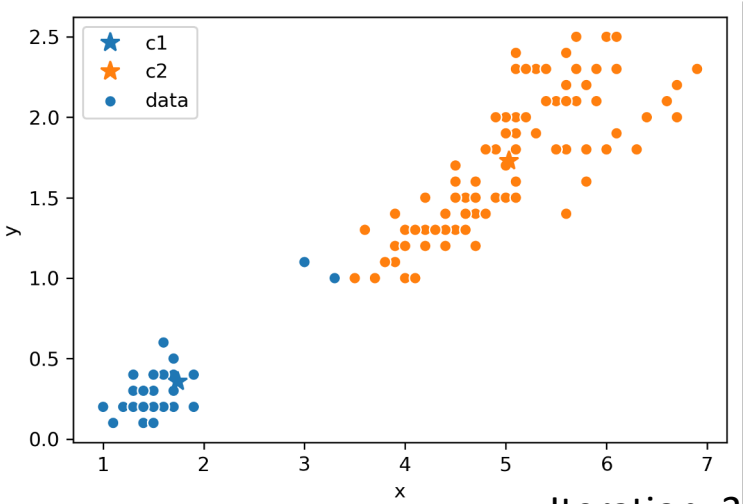

Iteration: 3

K-Means Clustering

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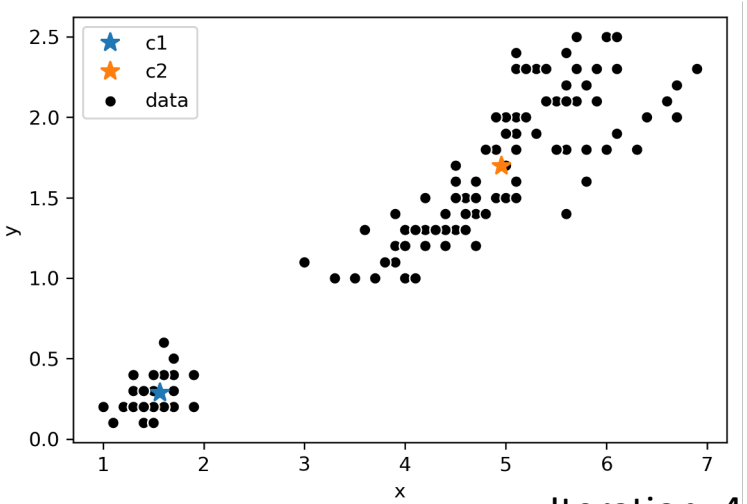
Centers moved to new position



Iteration: 4

K-Means Clustering

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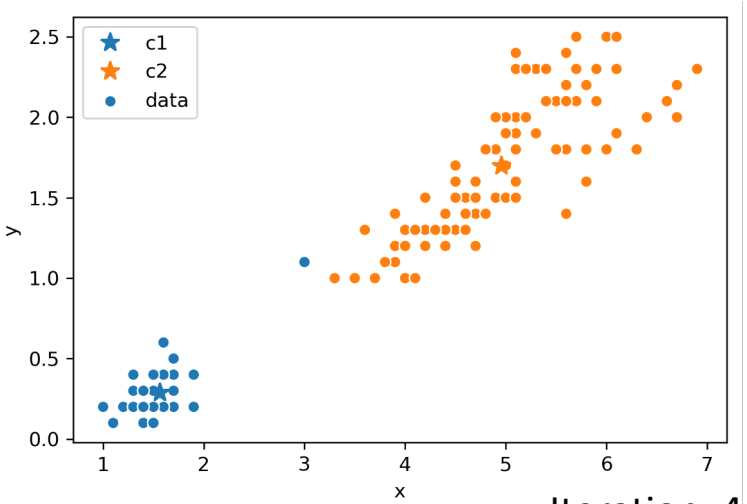
Data colored by closest center (in new position)



Iteration: 4

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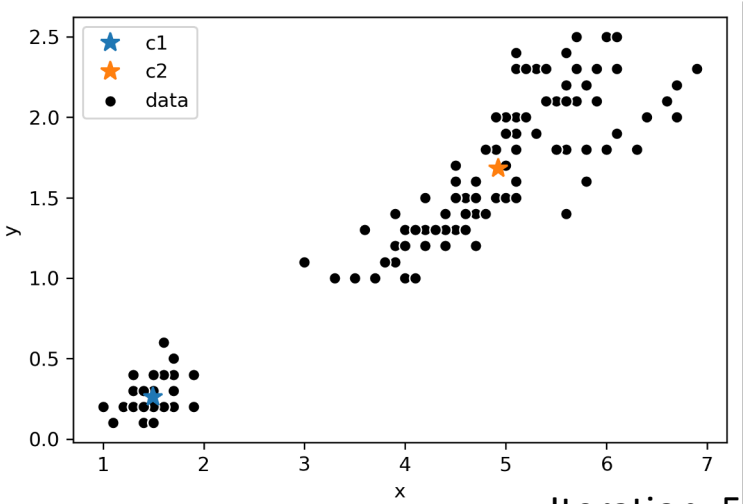

Iteration: 5

K-Means Clustering

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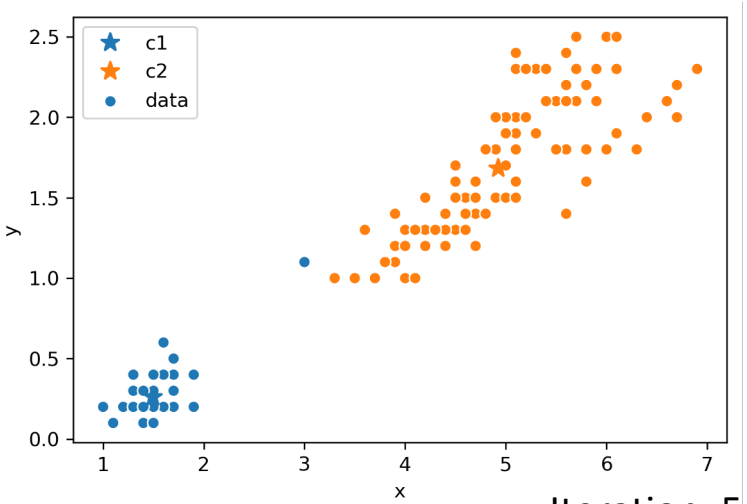
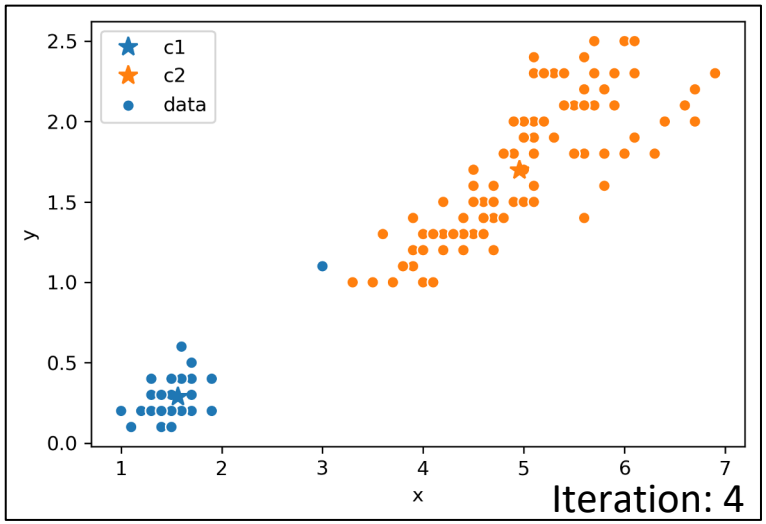
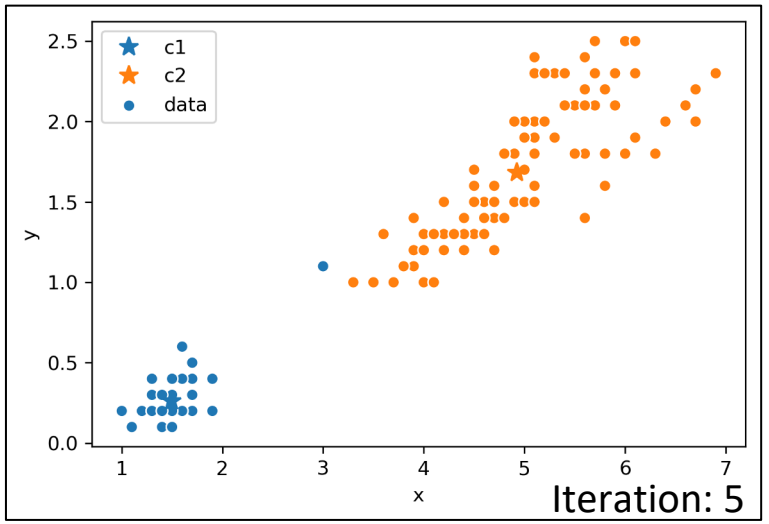
Data colored by closest center (in new position)



Iteration: 5

K-Means Clustering

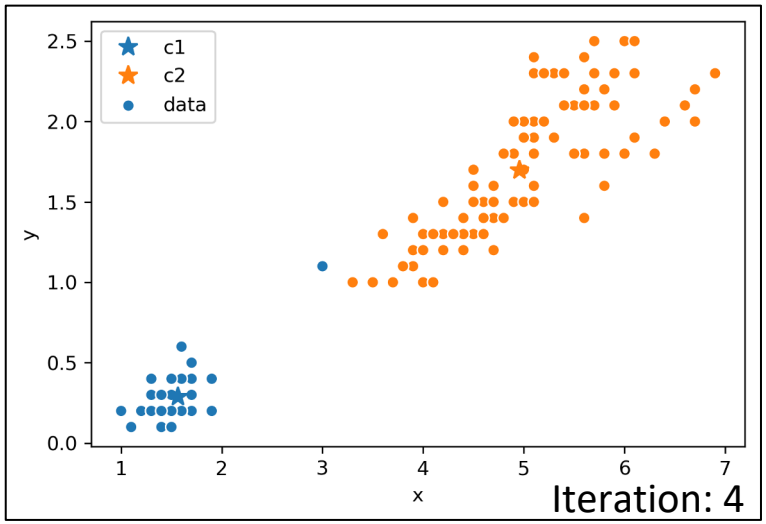


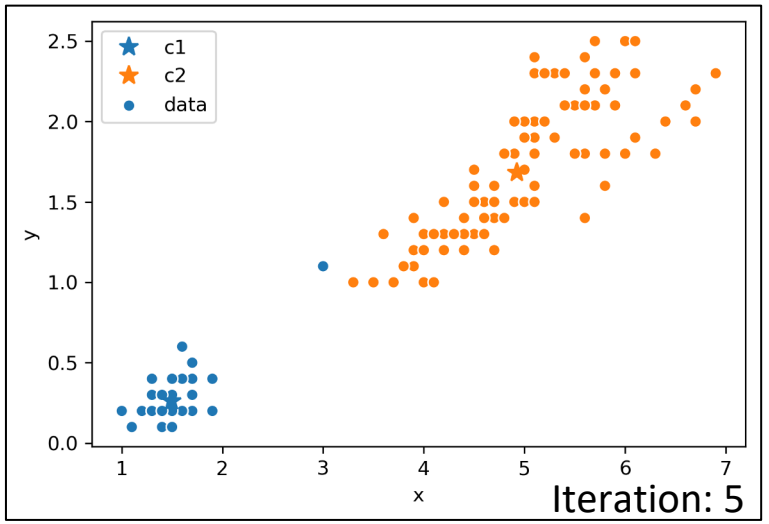


Above, we see the results after iteration 4 and 5:

- Centers moved slightly between iteration 4 and 5.
- But no points changed color.
- Are we done?

K-Means Clustering





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- Are we done?
  - Yes! If we tried iteration 6, we'd see that centers don't move at all.

K-Means vs. K-Nearest Neighbors

Quick note: **K-Means** is a totally different algorithm than "**K-Nearest Neighbors**".

- **K-Means**: For clustering:
  - Assigns each point to one of K clusters.
- **K-Nearest Neighbors**: For Classification (or less often, Regression):
  - Prediction is the most common class among the k-nearest data points in the training set.

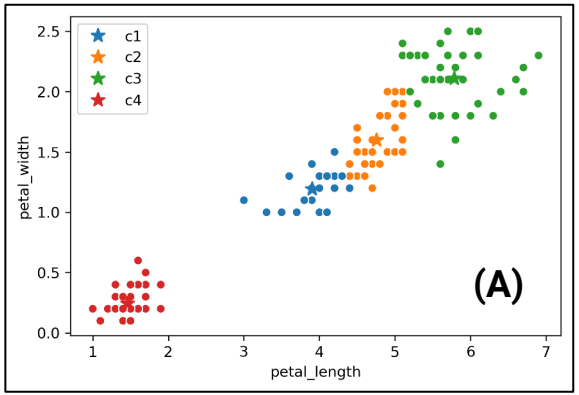
The names may be similar, but there isn't really anything in common.

Minimizing Inertia

K-Means Clustering for K = 4

Each time you run K-Means, you get a different output, depending on where centers started.

`random.seed(25)`



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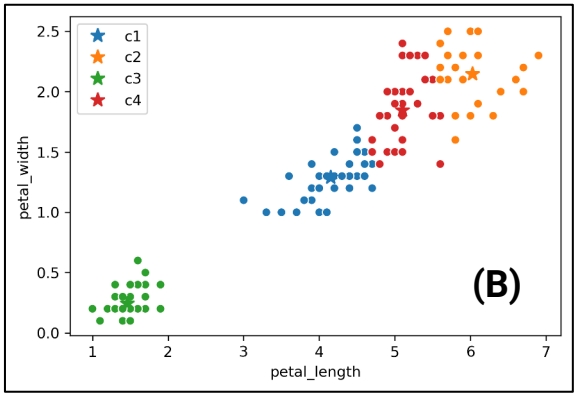
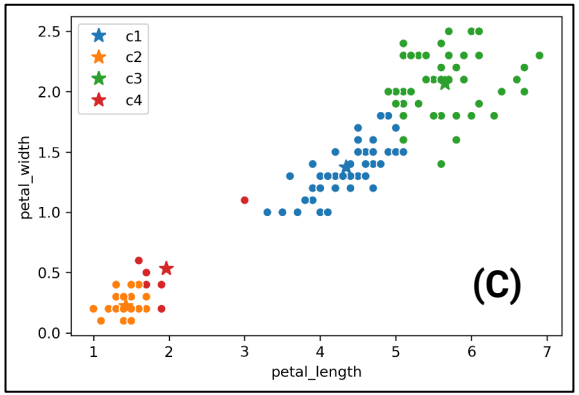


`random.seed(40)`



Which is best?

- One approach: Define some sort of loss function.

Goal: Come up with a loss function for clustering.

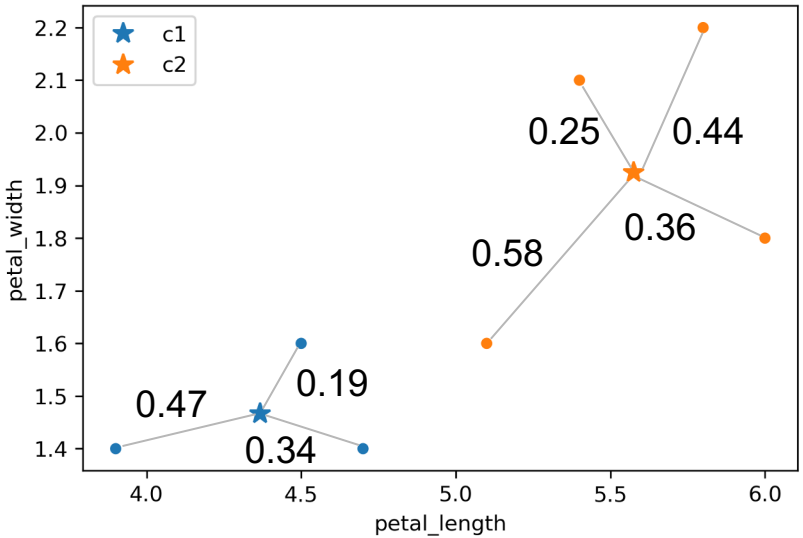
- What is “good” about the leftmost clustering, but “bad” about the right clustering?

K-Means Clustering for K = 4

To evaluate different clustering results, we need a loss function.

Two common loss functions:

- **Inertia**: Sum of squared distances from each data point to its center.
- **Distortion**: Weighted sum of squared distances from each data point to its center.



Example:

- **Inertia**: $0.47^2 + 0.19^2 + 0.34^2 + 0.25^2 + 0.58^2 + 0.36^2 + 0.44^2$
- **Distortion**: $(0.47^2 + 0.19^2 + 0.34^2)/3 + (0.25^2 + 0.58^2 + 0.36^2 + 0.44^2)/4$

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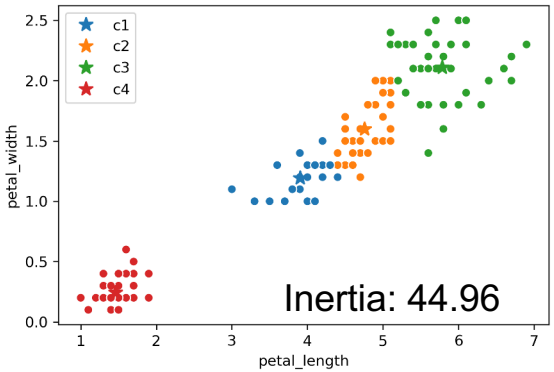

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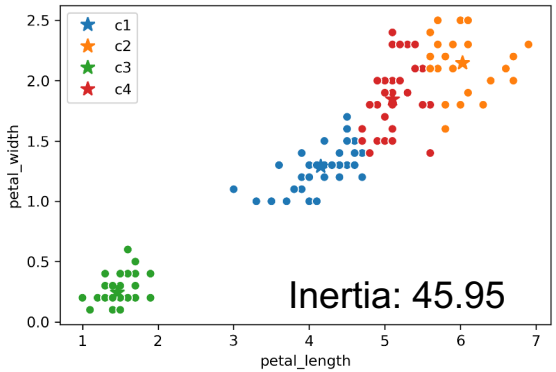

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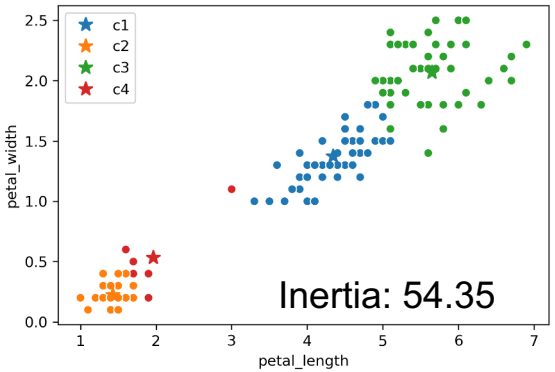


Among these three choices, our **inertia** loss function says that the leftmost clustering is best (inertia: 44.96) and rightmost clustering (inertia: 54.35) is worst.

K-Means and Inertia

It turns out that the function K-Means is trying to minimize is **inertia**…

… but often fails to find global optimum. Why?

Can think of K-means as a pair of optimizers that take turns:

- First optimizer:
  - Holds center positions constant.
  - Optimizes data colors.
- Second optimizer:
  - Holds data colors constant.
  - Optimizes center positions.
- Neither gets total control!

Optimizing Inertia

Hard problem: Give an algorithm that optimizes inertia FOR A GIVEN K. K is picked in advance.

- Your algorithm should return the EXACT best centers and colors.
- Don't worry about runtime.

A "coloring" is just a choice of color for every point, e.g. point 1 = red, point 2 = green, point 3 = orange, point 4 = blue

Algorithm:

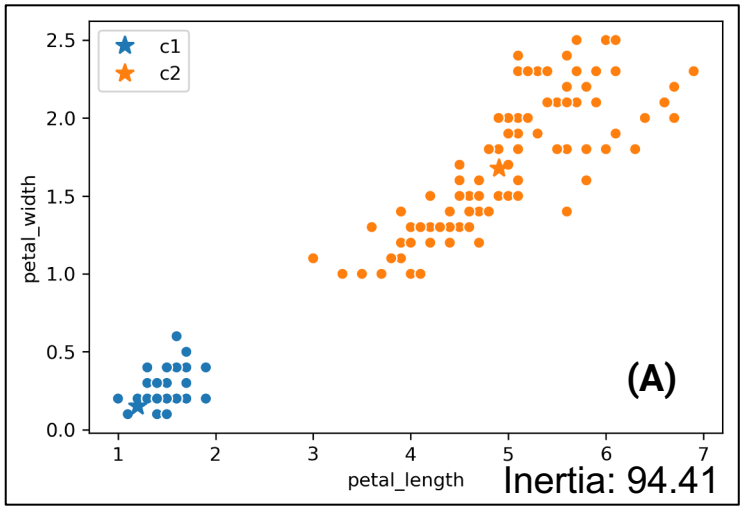
- For all possible k^n **colorings**:
  - Compute the k centers for that coloring.
  - Compute the inertia for the k centers.
    - If current inertia is better than best known, write down the current centers and coloring and call that the new best known.

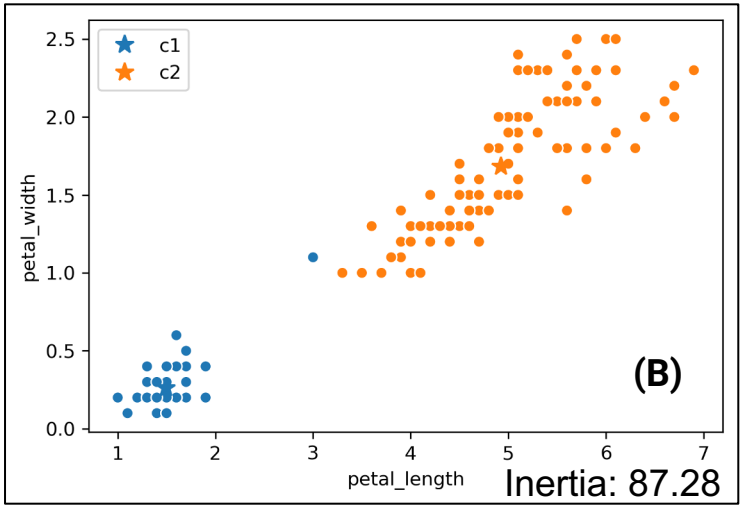
No better algorithm has been found for solving the problem of minimizing exactly.

For those who know what this means:
K-Means is known to be an NP-hard problem

K-Means

Which clustering result do you like better?



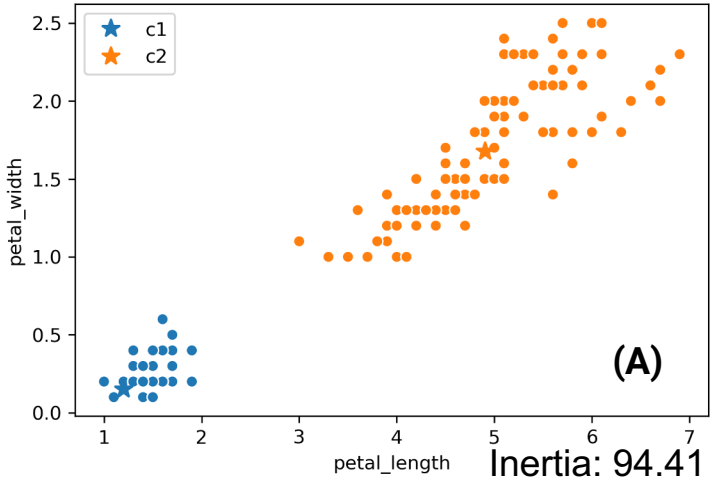


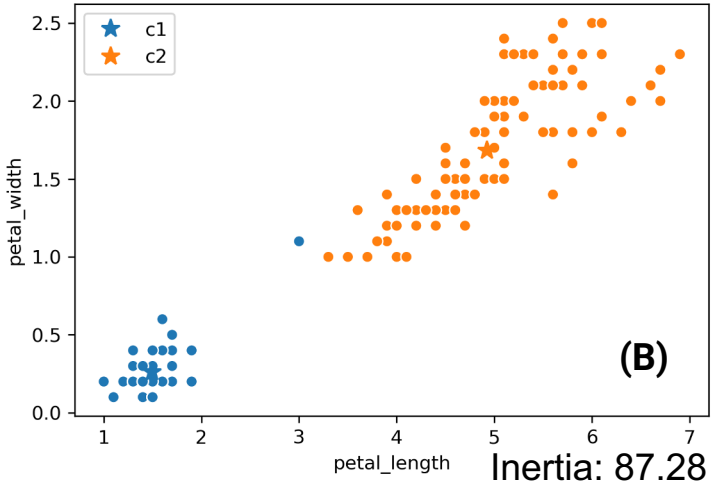
K-Means likes the one on the right better because it has lower inertia: sum of squared distances from each data point to its center.

- Why is the inertia on the right lower?
- Is clustering on the right “wrong”?

K-Means

Which clustering result do you like better?



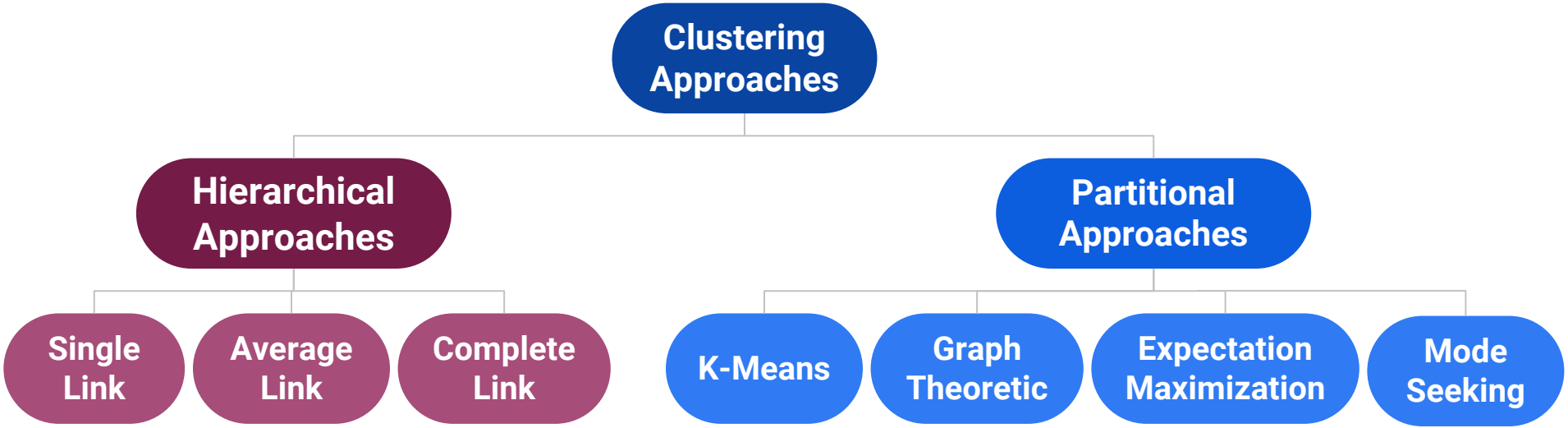


K-Means likes the one on the right better because it has lower inertia: sum of squared distances from each data point to its center.

- Why is the inertia on the right lower? K-Means optimizes for distance, not “blobbiness”.
- Is clustering on the right “wrong”? Good question!

Hierarchical Agglomerative Clustering

Taxonomy of Clustering Approaches

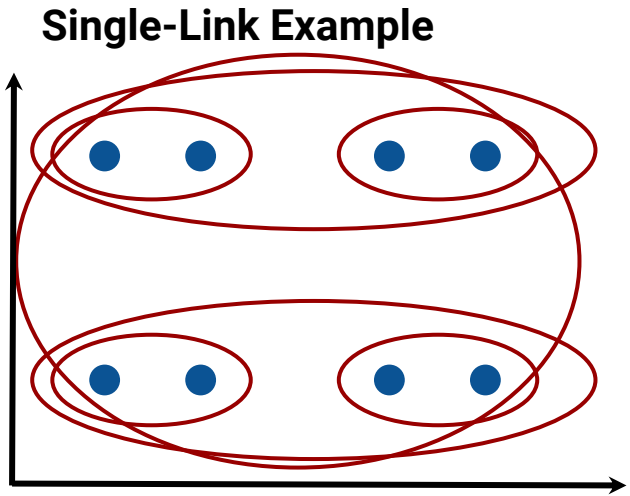


Hierarchical Agglomerative Clustering

- We start with every data point in a separate cluster.
- We keep merging the most similar pairs of data points/clusters until we have one big cluster left.
- This is called a **bottom-up** or **agglomerative** method.
- There are various ways to decide the order of combining clusters called **Linkage Criterion**.

Approaches for Merging Clusters: Linkage Criteria

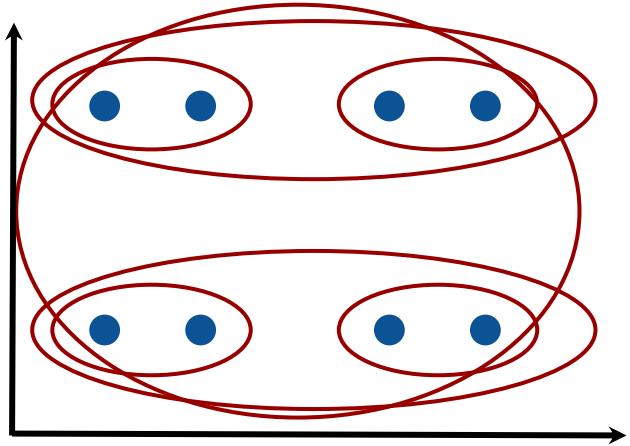
- **Single linkage:** Similarity of the most similar: the distance between two clusters as the **minimum** distance between a point in the first cluster and a point in the second.



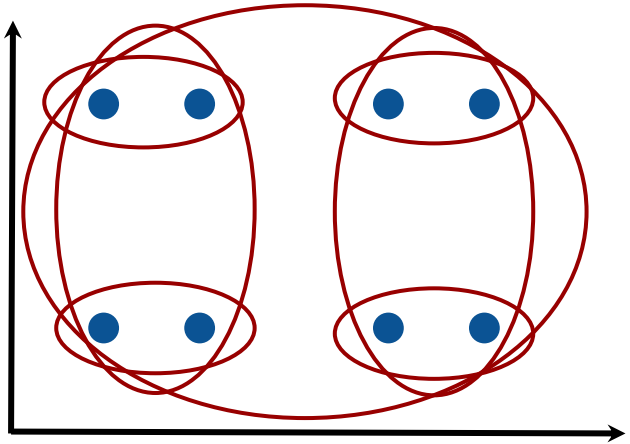
Approaches for Merging Clusters: Linkage Criteria

- **Single linkage:** Similarity of the most similar: the distance between two clusters as the **minimum** distance between a point in the first cluster and a point in the second.
- **Average linkage:** **Average** similarity of pairs of points in clusters.
- **Complete linkage:** Similarity of the least similar: the distance between two clusters as the **maximum** distance between a point in the first cluster and a point in the second.

Single-Link Example



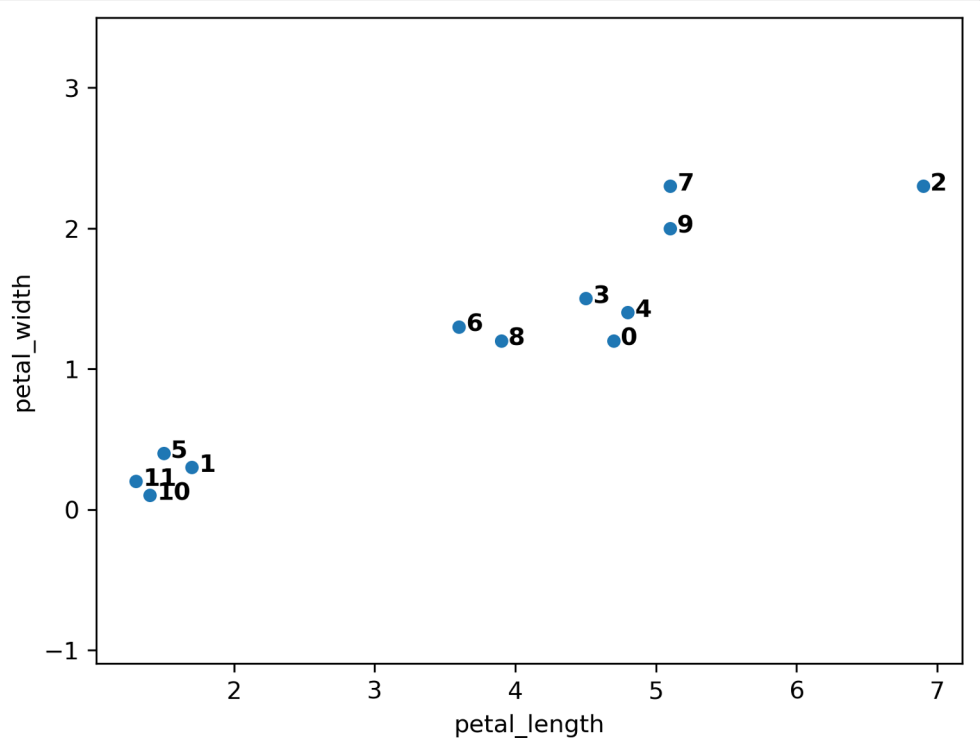
Complete-Link Example



Agglomerative Clustering Example

When the algorithm starts, every data point is in its own cluster.

- Below, 12 data points, so 12 clusters.
- Closest clusters are 10 and 11, so merge them.



Agglomerative Clustering Example

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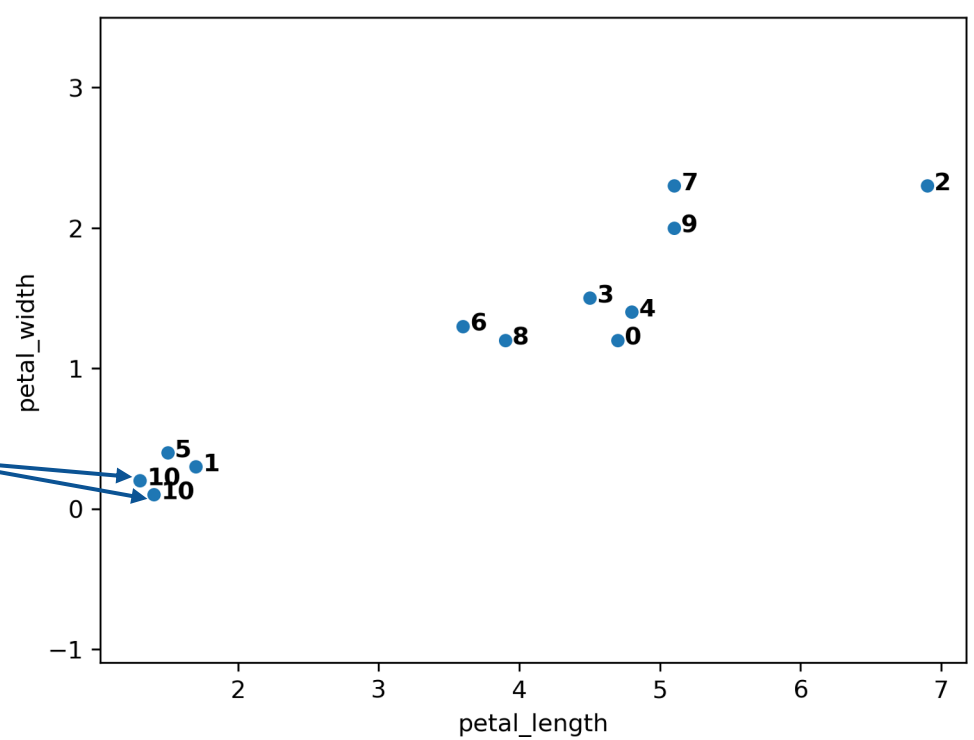
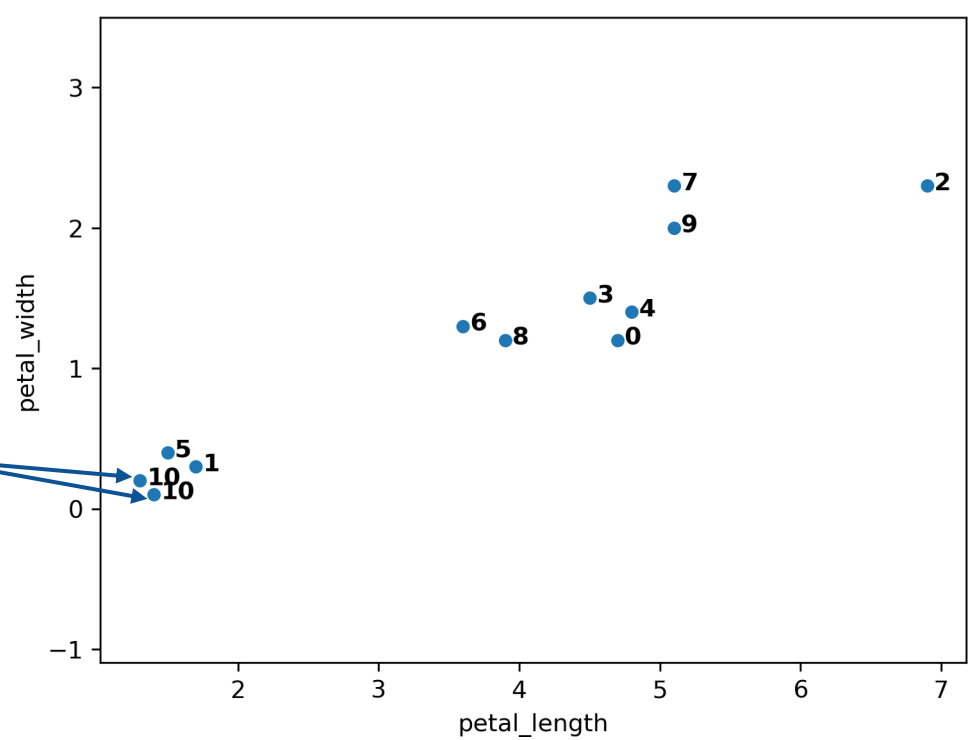


Two points in the same cluster

Agglomerative Clustering Example

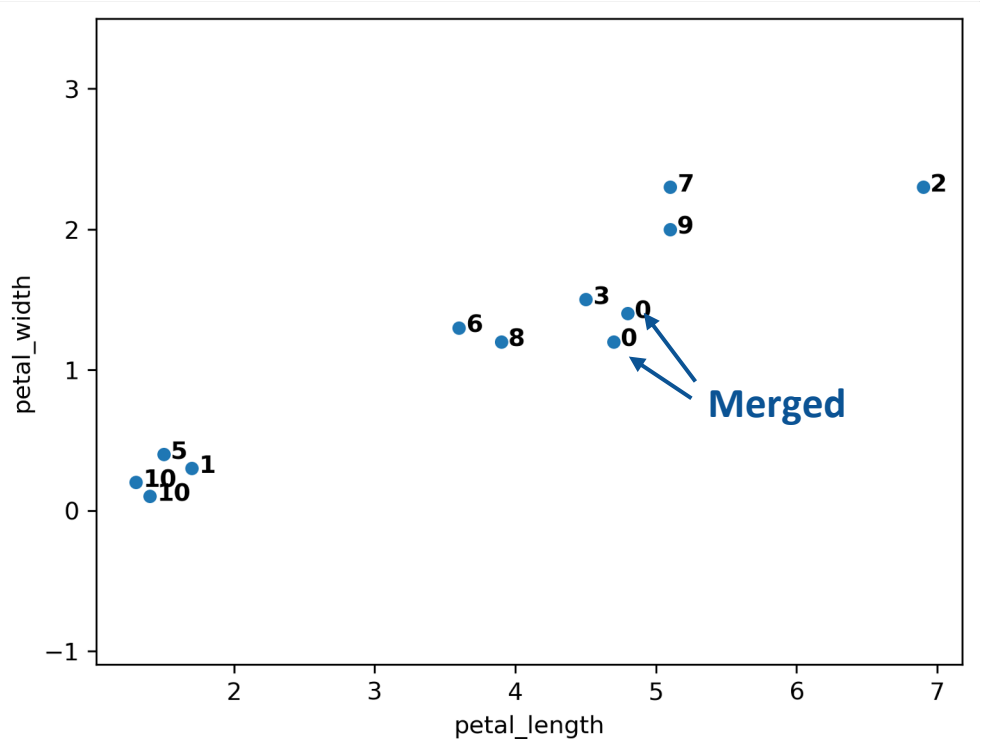
Next two closest are 0 and 4, so merge them.

Two points in the same cluster



Agglomerative Clustering Example

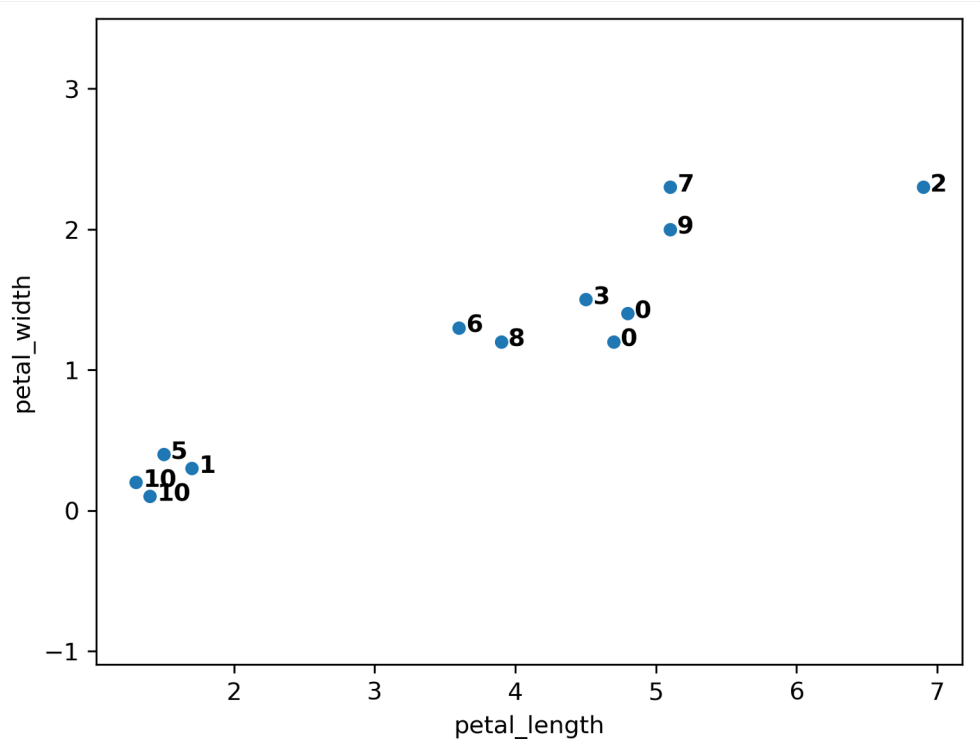
Next two closest are 0 and 4, so merge them.



Agglomerative Clustering Example

At this point we have 10 clusters:

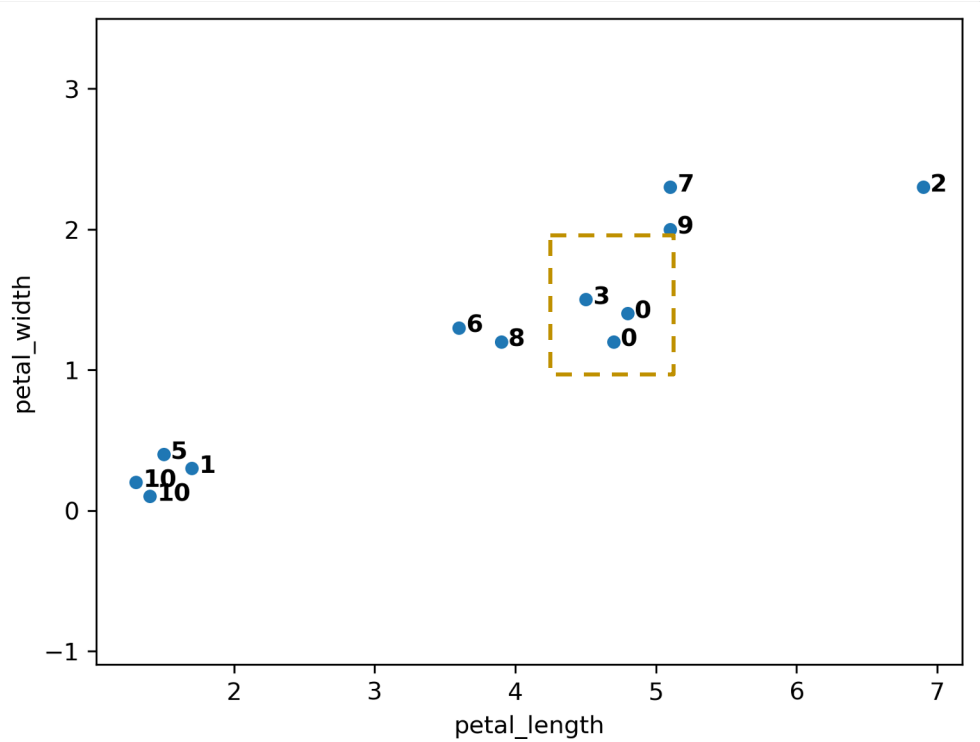
- 8 with a single point {1, 2, 3, 5, 6, 7, 8, 9}
- 2 with two points {0/0, 10/10}



Agglomerative Clustering Example

Tricky question:

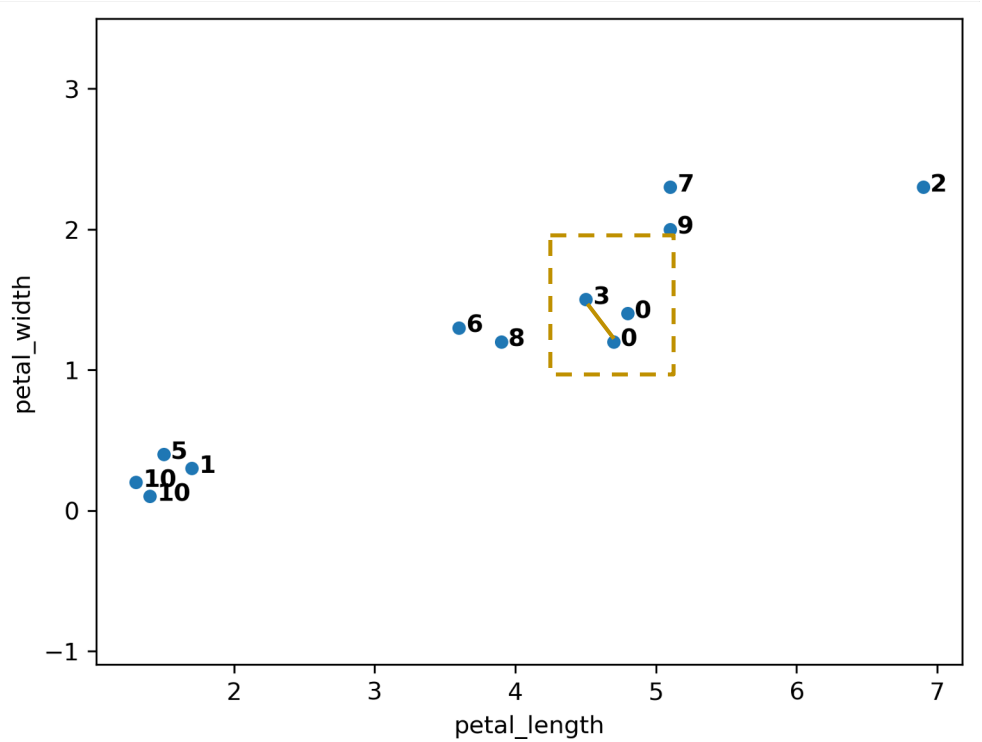
- What is the distance between clusters 0 and 3?



Agglomerative Clustering Example

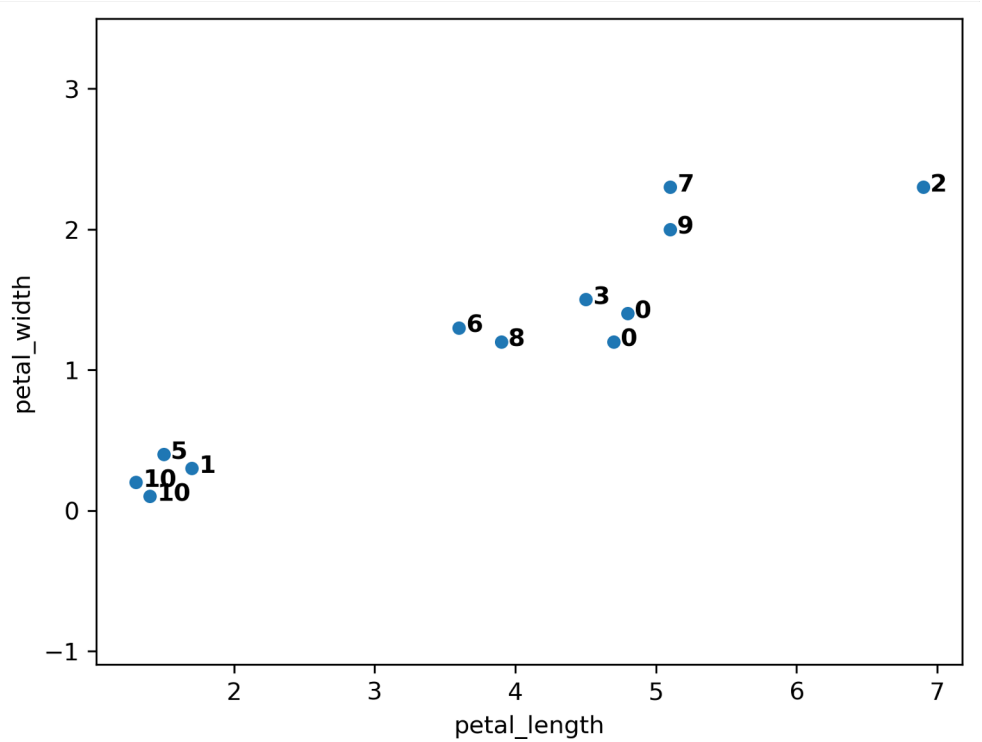
Tricky question:

- What is the distance between clusters 0 and 3?
- We can use the **Complete-Link** approach that uses the **max** distance amongst all pairs.



Agglomerative Clustering Example

Next two closest clusters are 1 and 5.



Agglomerative Clustering Example

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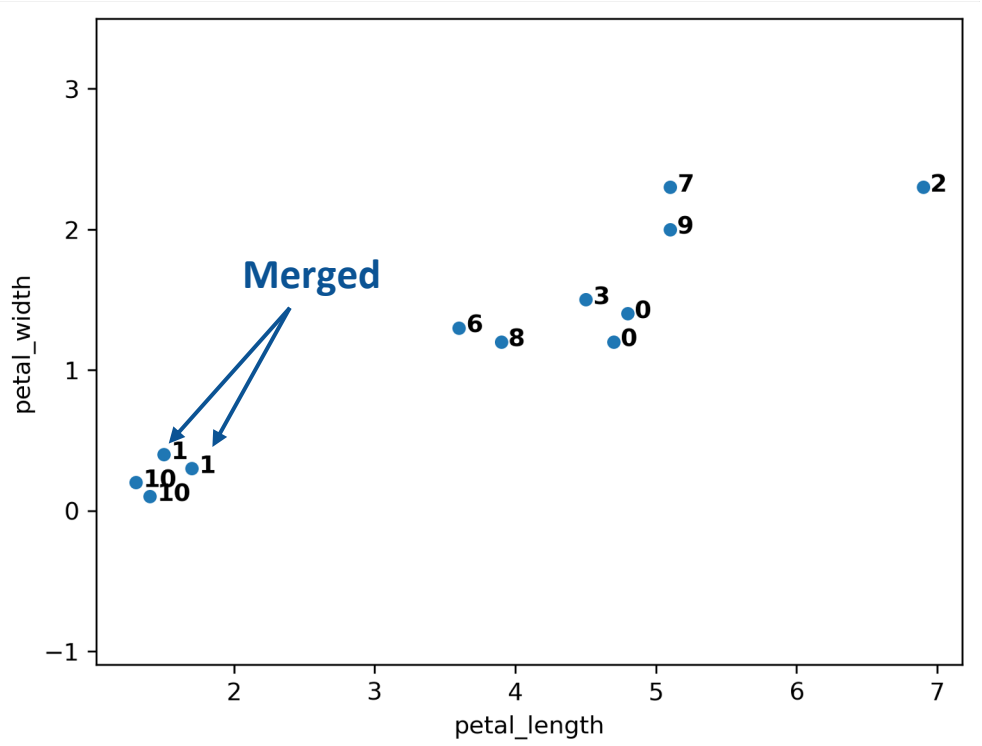
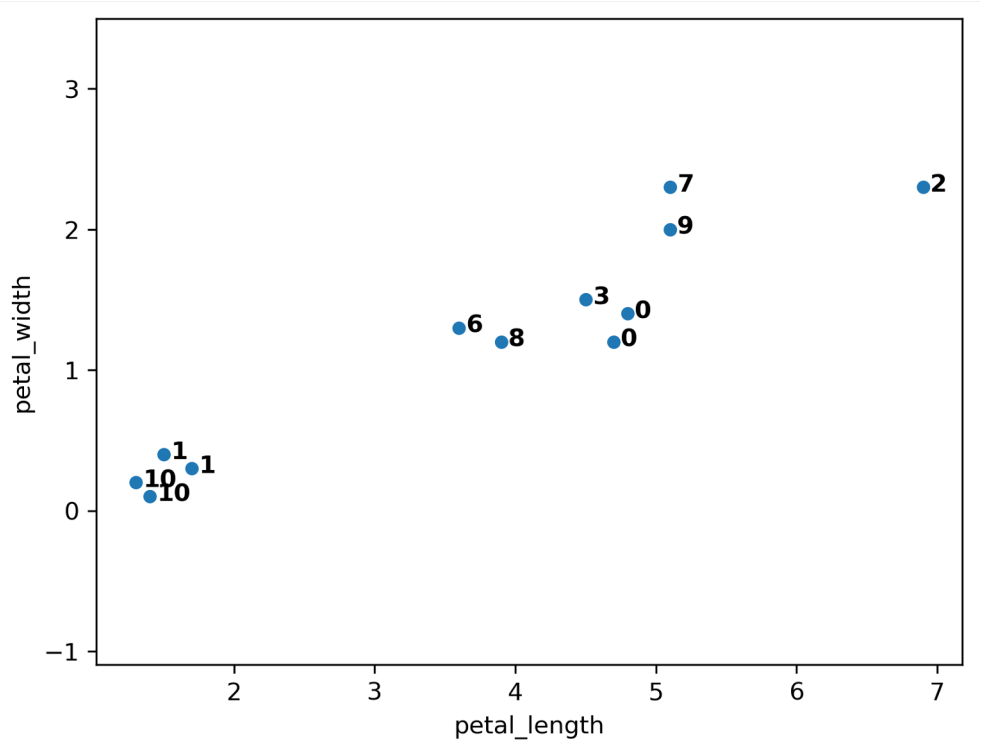


Agglomerative Clustering Example

Next two closest clusters are 7 and 9.



Agglomerative Clustering Example

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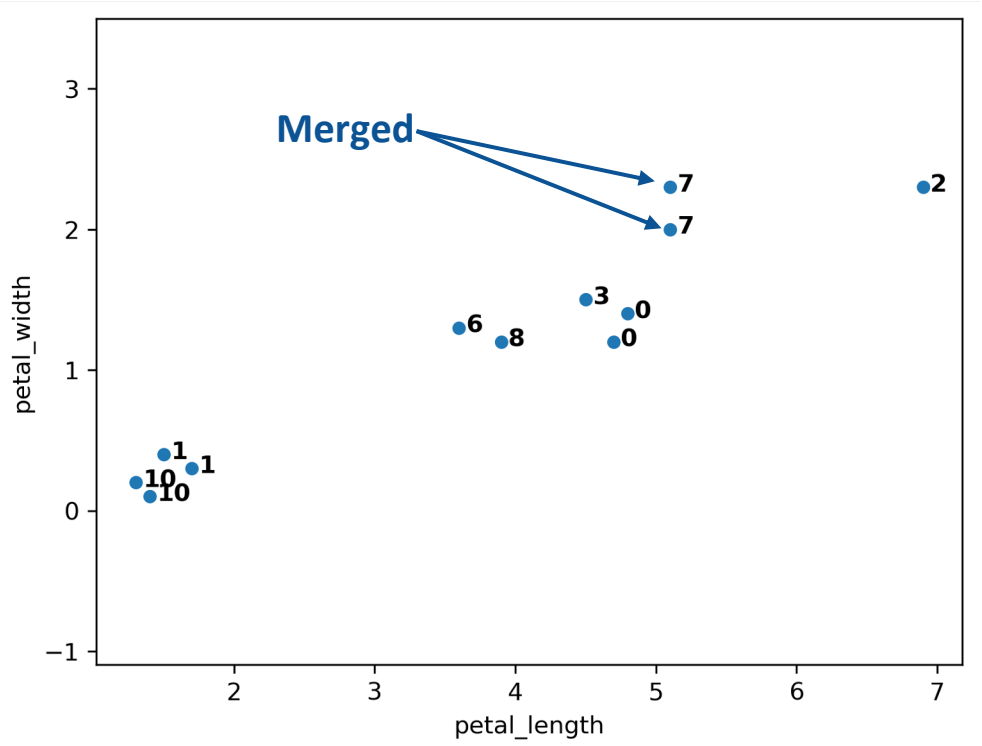
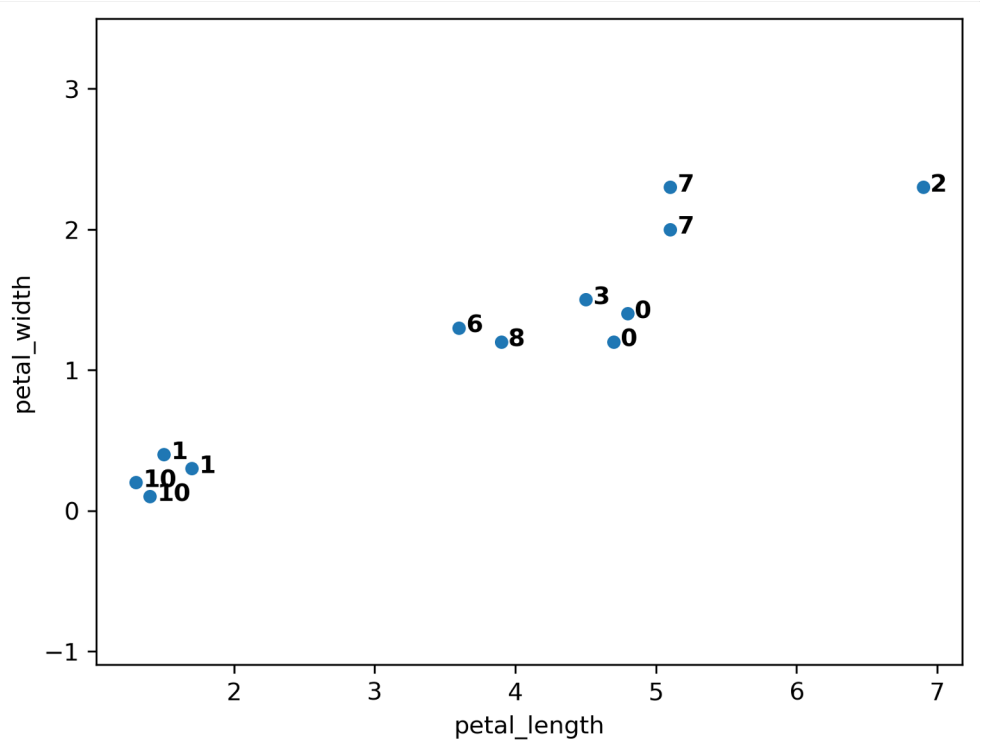


Agglomerative Clustering Example

Next closest are 6 and 8.



Agglomerative Clustering Example

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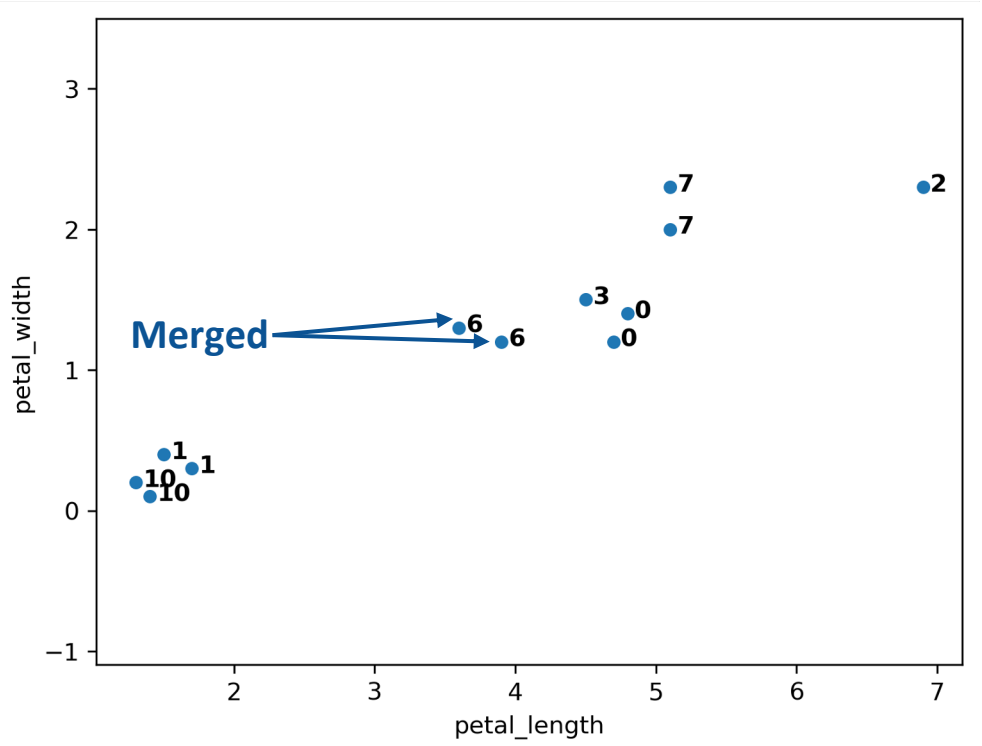
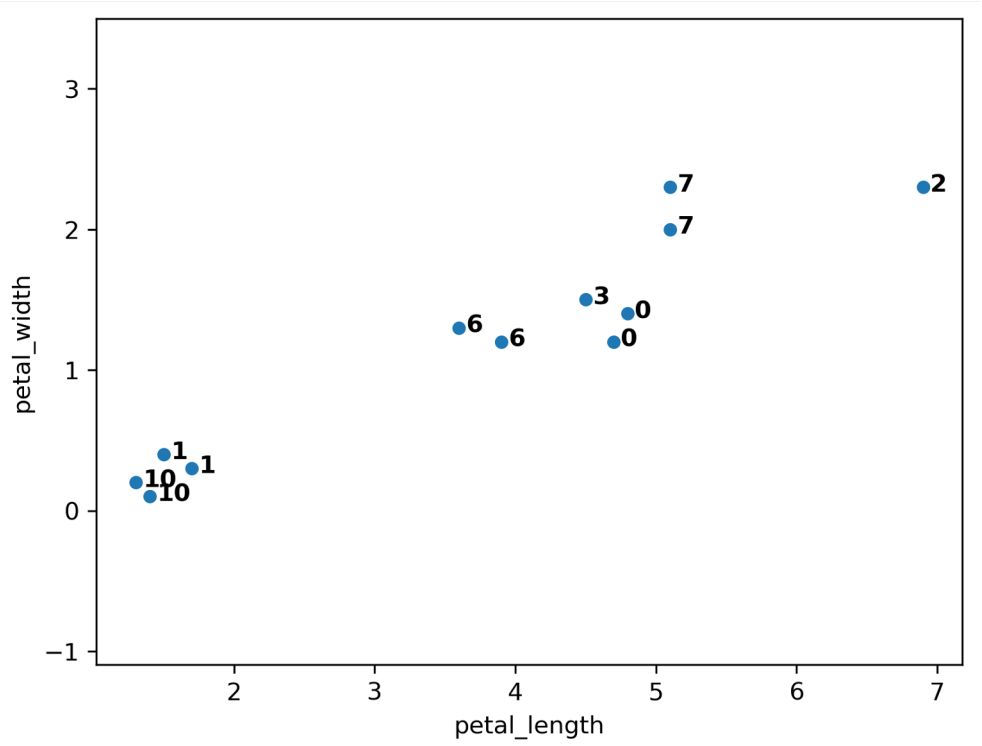


Agglomerative Clustering Example

Now 0 and 3 are closest. Merge them next.



Agglomerative Clustering Example

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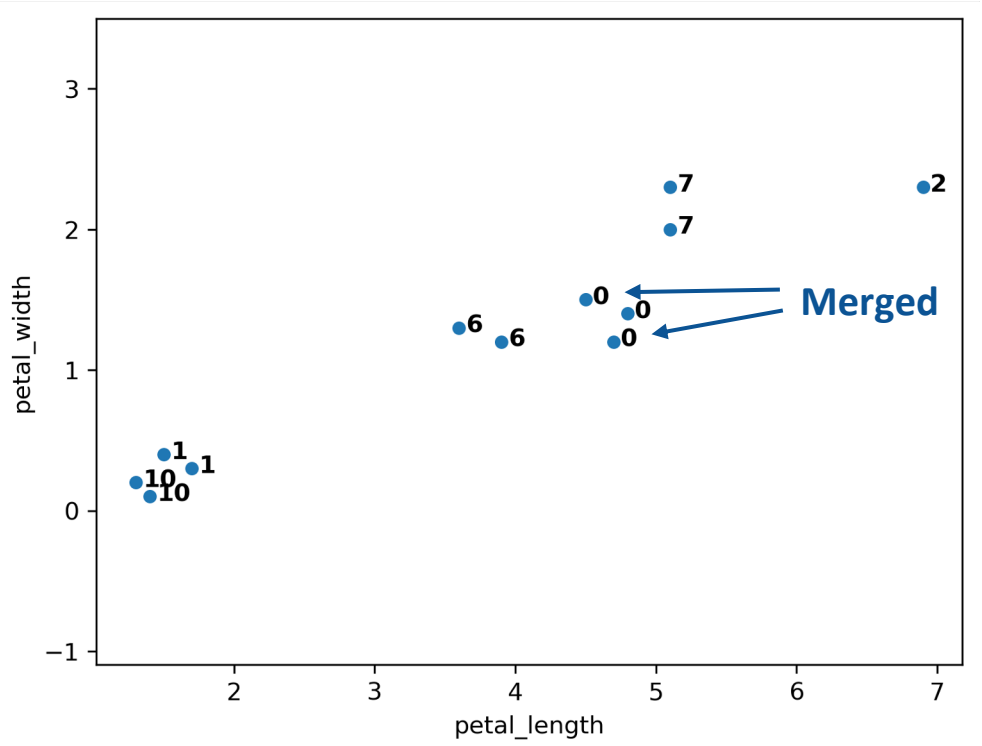
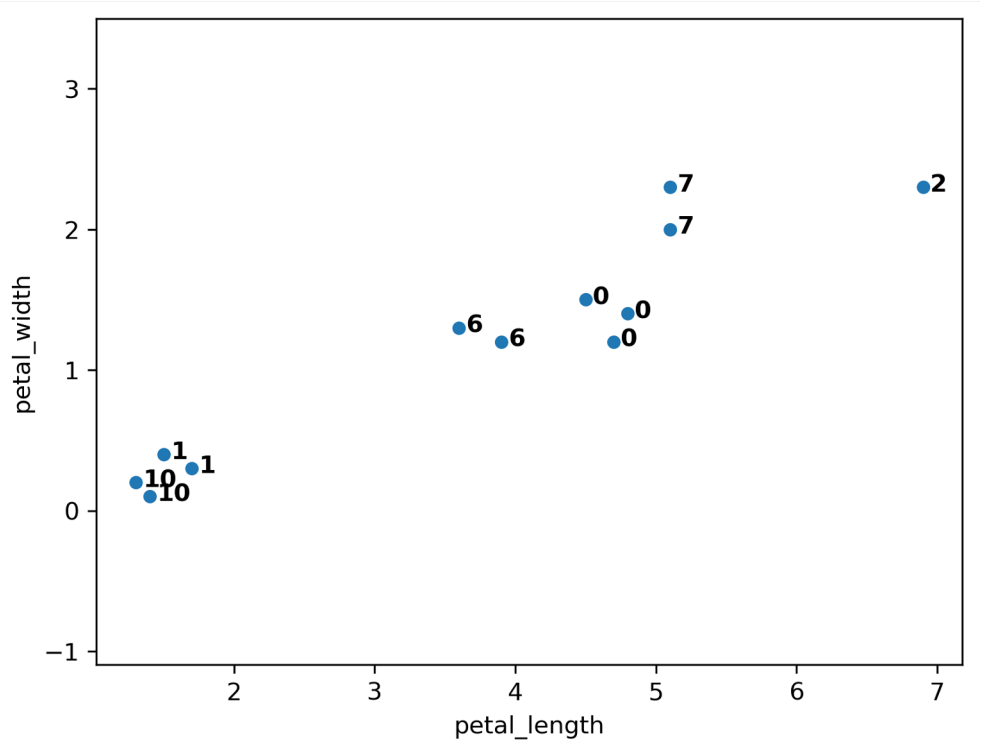


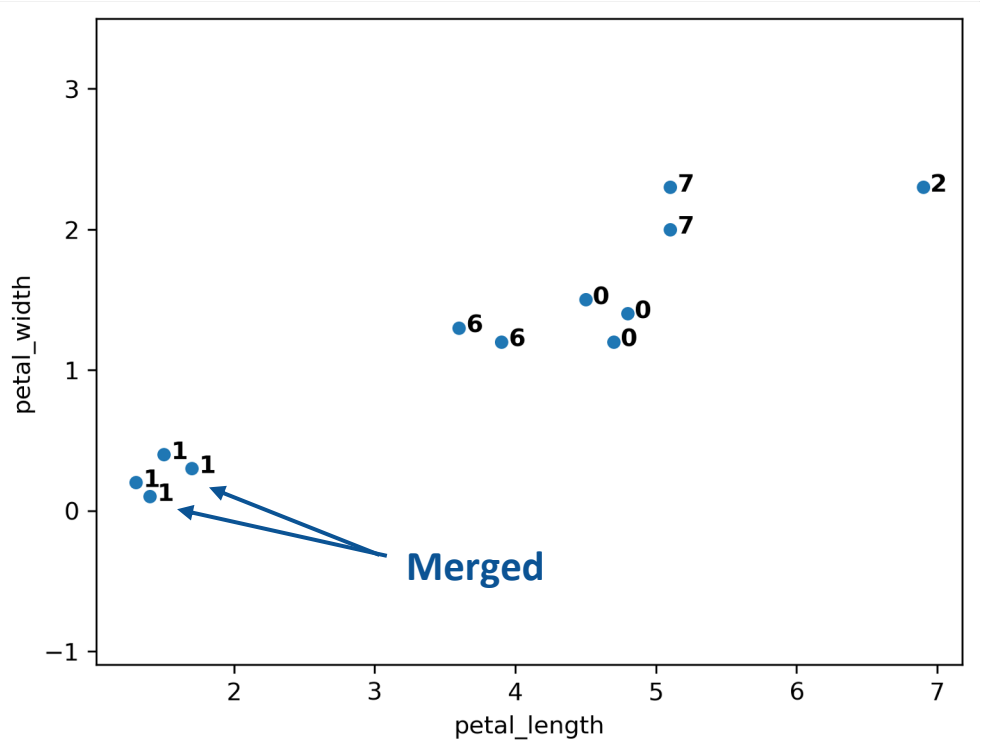
Agglomerative Clustering Example

Next up are 1 and 10.



Agglomerative Clustering Example

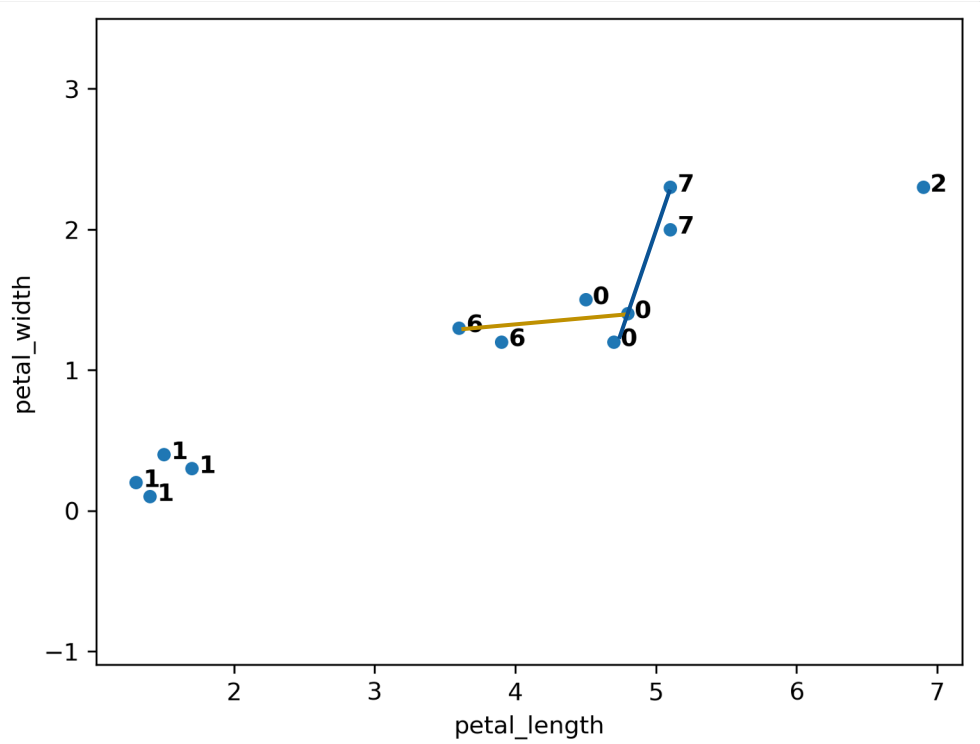
Next up are 1 and 10.



Agglomerative Clustering Example

Next up are 0 and 7. Why?

- **Max line between any member of 0 and 6** is longer than **max line between any member of 0 and 7.**



Blue line is shorter than **gold line**.

Note: Is not ***visually*** trivial to compare the difference in length of the two lines.

Agglomerative Clustering Example

Next up are 0 and 7. Why?

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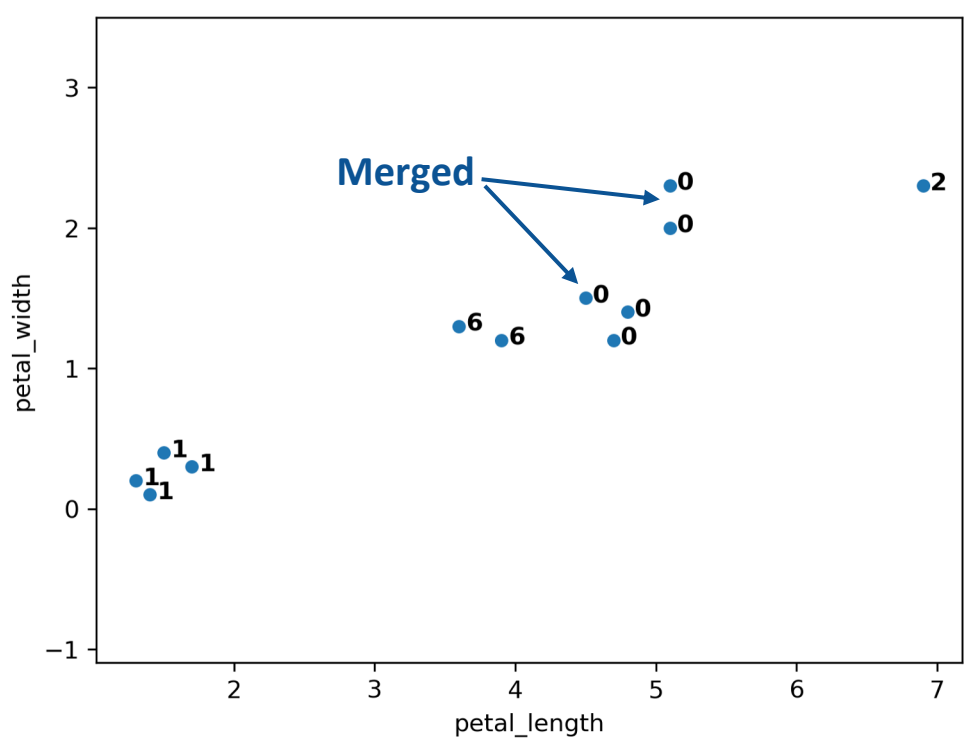

Agglomerative Clustering Example

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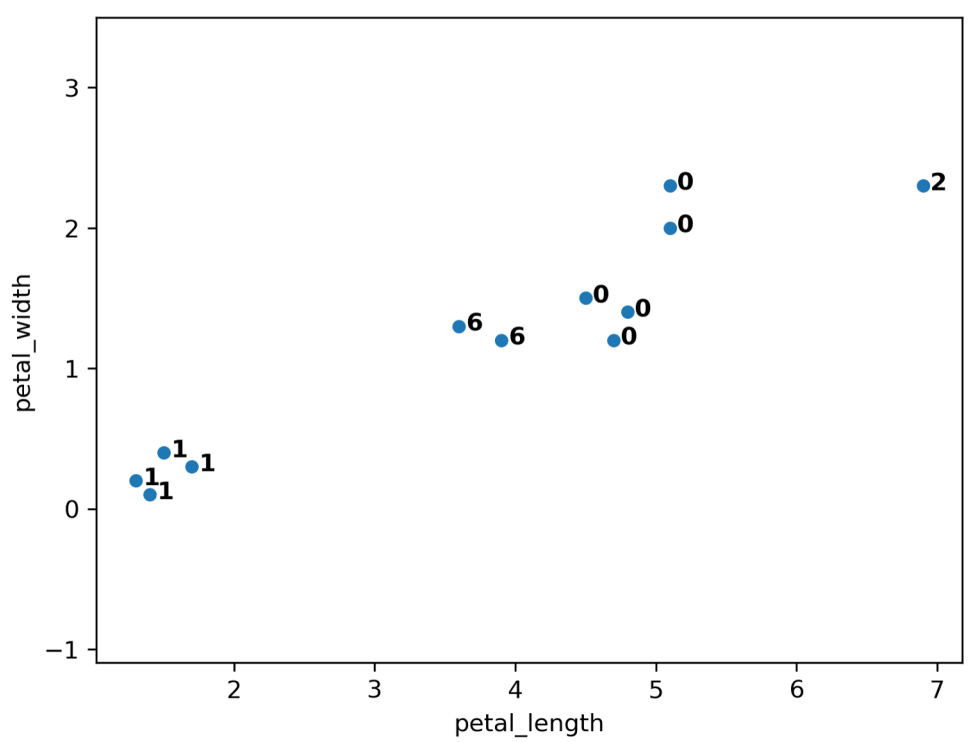
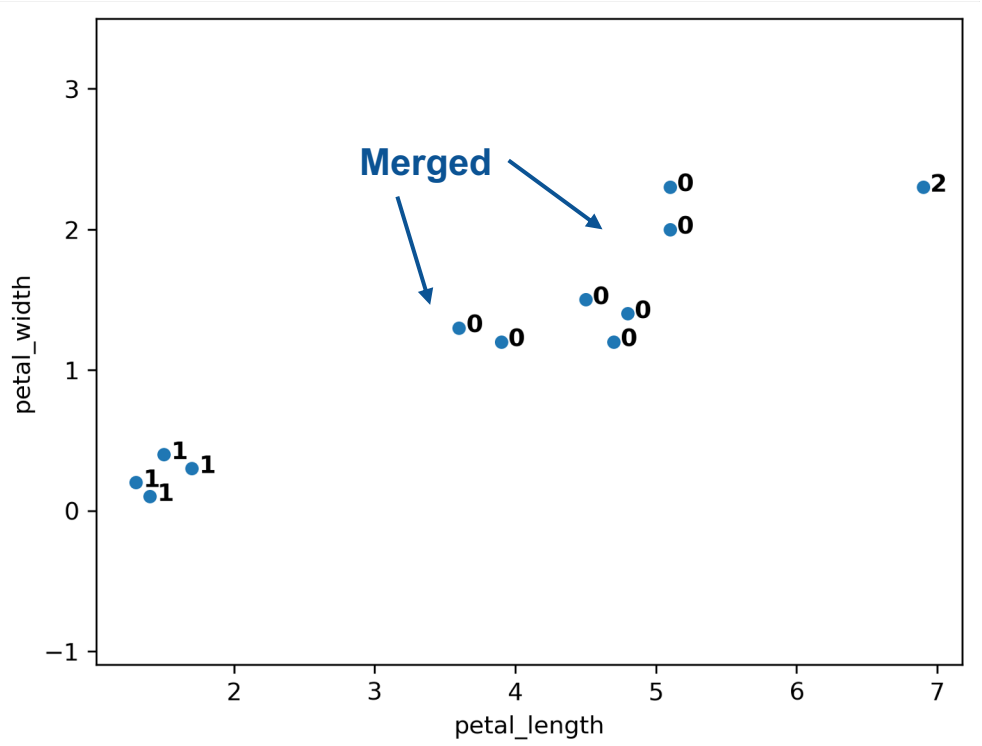


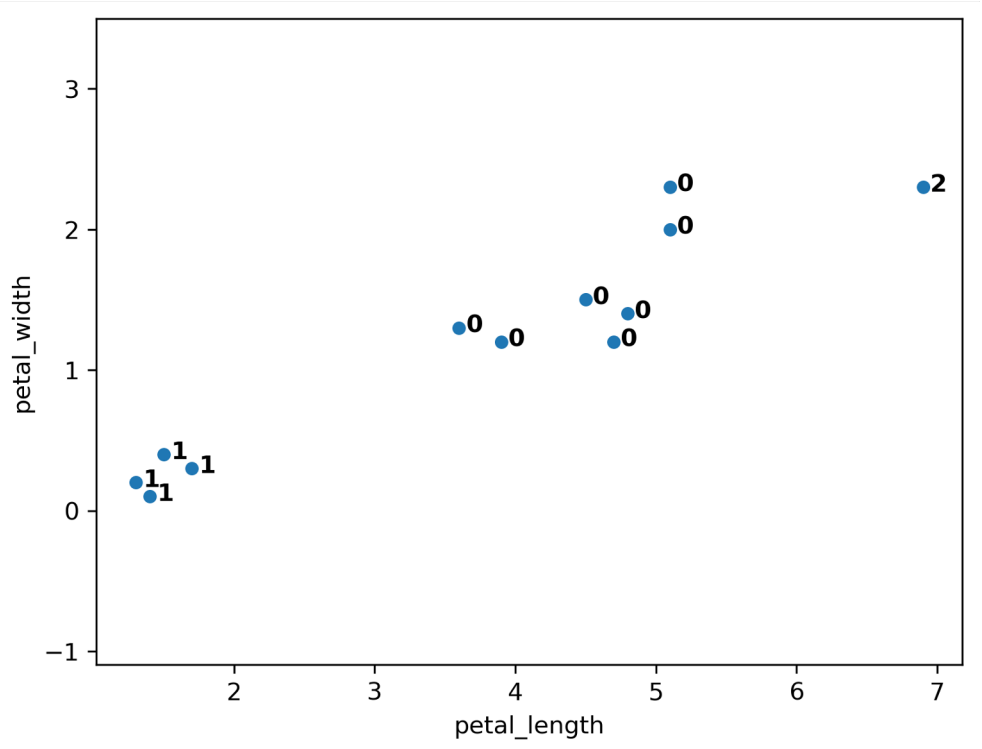
Agglomerative Clustering Example

Next up are 0 and 6.



Agglomerative Clustering Example

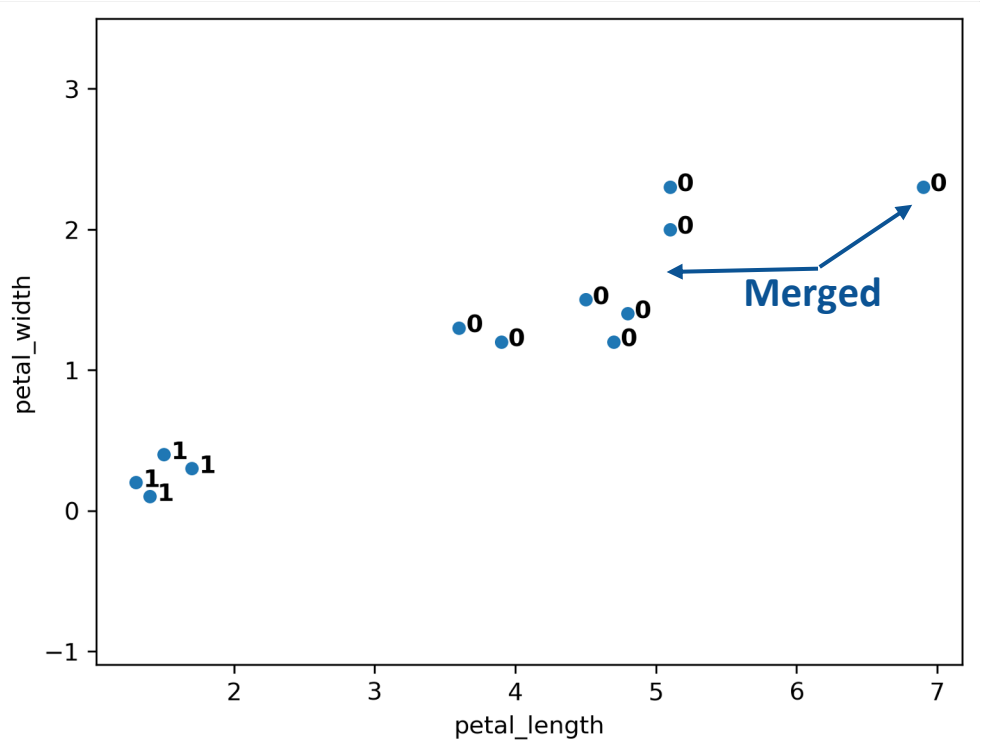
Next up are 0 and 2.



Agglomerative Clustering Example

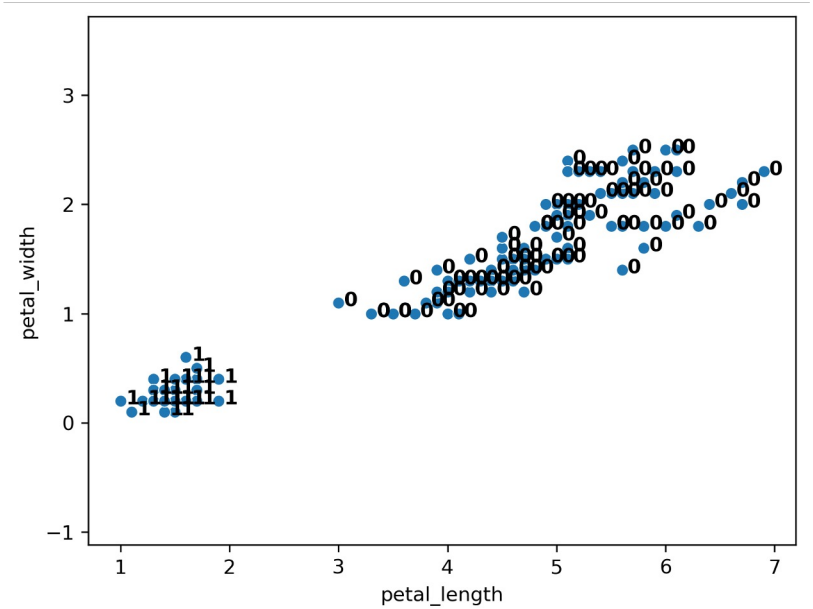
Next up are 0 and 2.

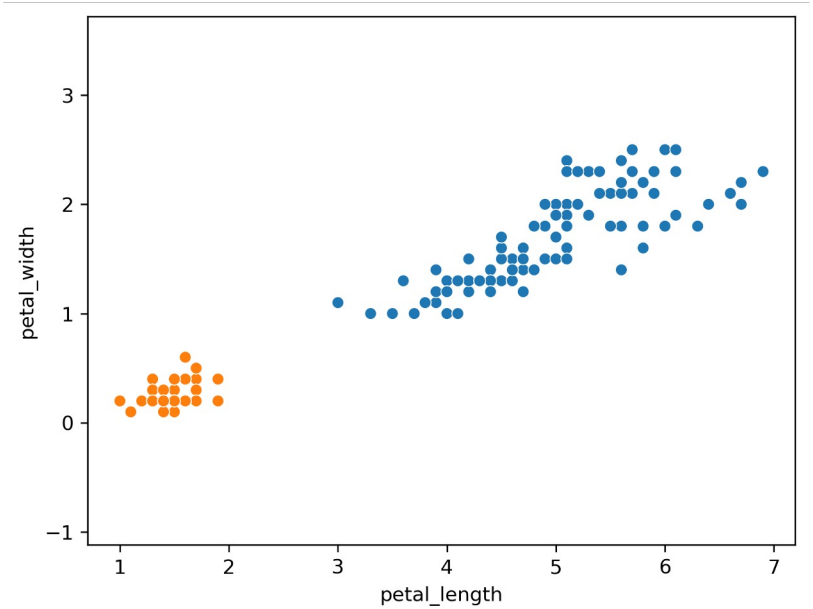
- At this point, we are done, because we only have two clusters left!
- Reminder: We arbitrarily chosen two clusters at the start.



Agglomerative Clustering Example

On the full dataset, our agglomerative clustering algorithm gets the “correct” output.

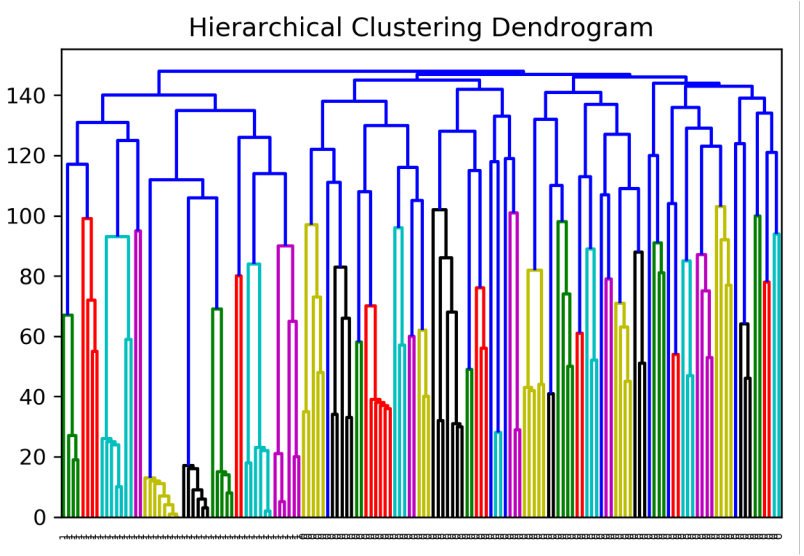


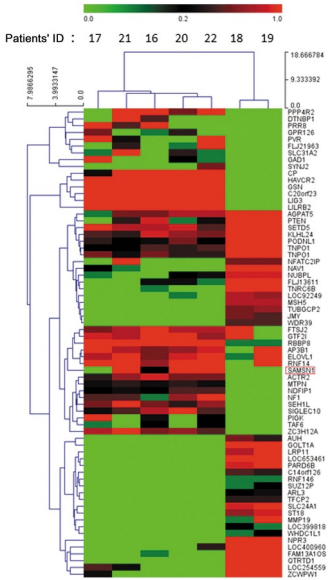


Clustering and Dendrograms

Agglomerative clustering is one form of “hierarchical clustering.”

- Can keep track of when two clusters got merged.
  - Each cluster is a tree.
- Can visualize merging hierarchy, resulting in a “dendrogram.”
  - Won’t discuss any further, but you might see these in the wild.





Picking K

Picking K

The algorithms we've discussed today require us to pick a K before we start.

- But how do we pick K?

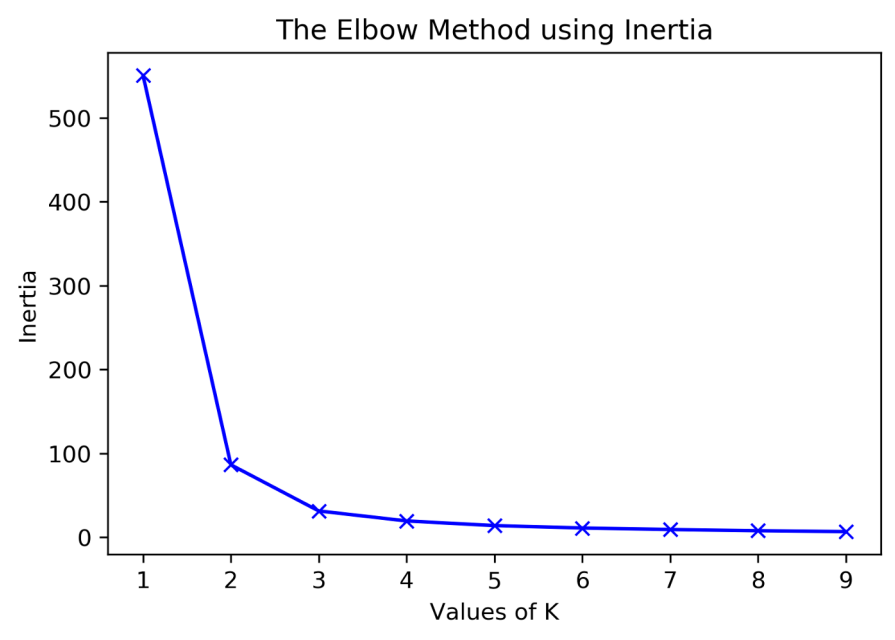
Often, best K is subjective:

- Example: State plot.
- How many clusters are there here?

Picking K: Elbow Method

For K-Means, one approach is to plot inertia versus many different K values.

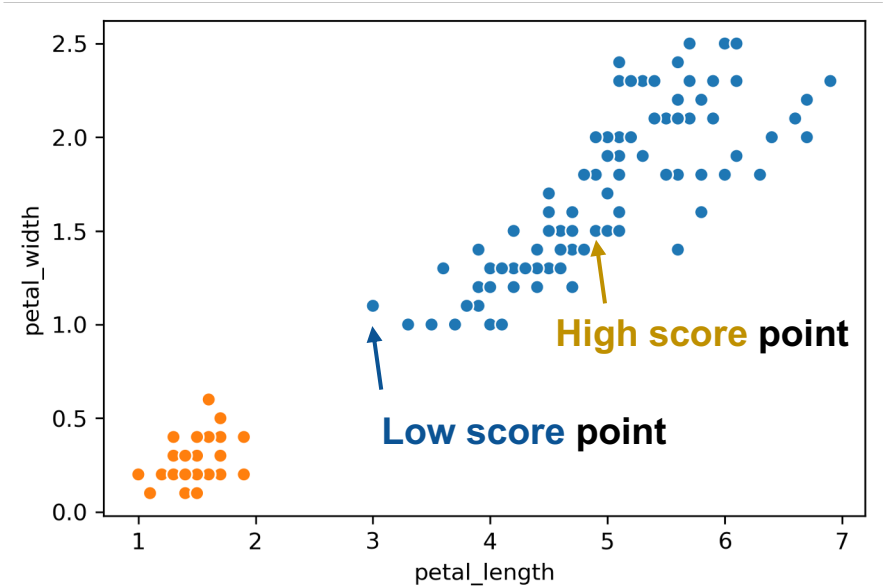
- Pick the K in the “elbow”, where we get diminishing returns afterwards.
- Note: Big complicated data often lacks an elbow.



Silhouette Scores

To evaluate how “well-clustered” a specific data point is, we can use the “silhouette score”, a.k.a. the “silhouette width”.

- **High score**: Near the other points in its cluster.
- **Low score**: Far from the other points in its cluster.



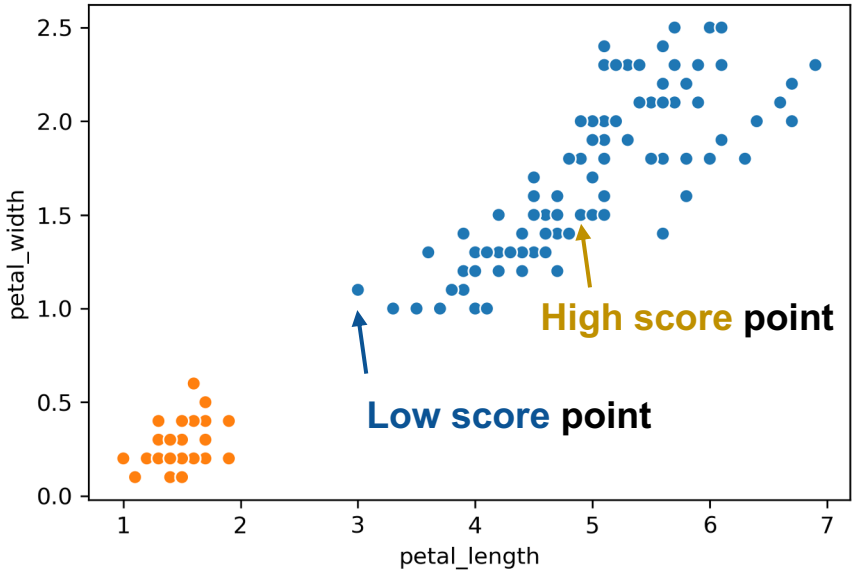
For a data point X, score S is:

- A = avg distance to other points in cluster.
- B = avg distance to points in closest cluster.
- S = (B - A) / max(A, B)

Silhouette Scores

For a data point X:

- A = average distance to other points in X's cluster.
- B = average distance to points in closest cluster.
- S = (B - A) / max(A, B).



What is the highest possible S?

- How can this happen?

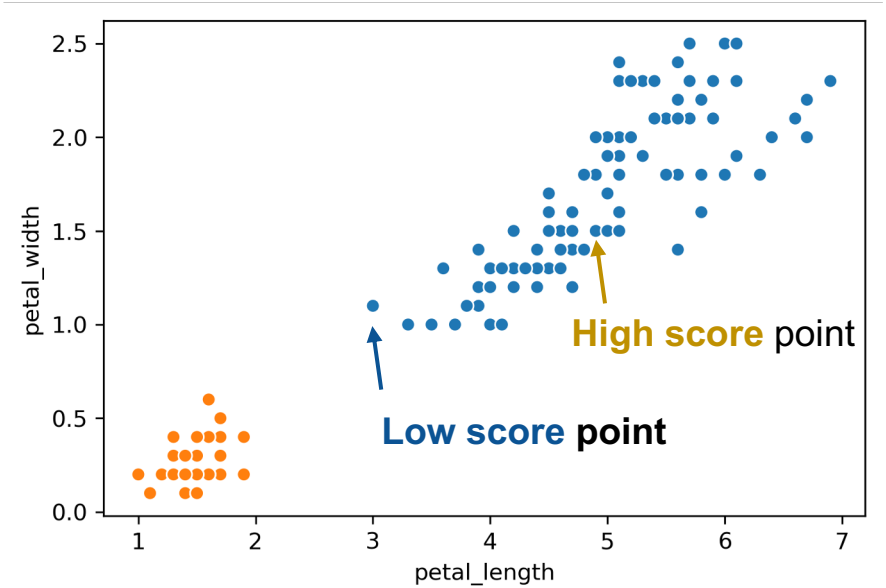
Highest possible S is 1.

- This happens if every point in X's cluster is right on top of X.
  - Average distance to other points in X's cluster is 0 (all equal to zero!), so A = 0.
  - B / max(0, B) = B / B = 1
  - Or B >> A

Silhouette Scores

For a data point X:

- A = average distance to other points in X's cluster.
- B = average distance to points in closest cluster.
- S = (B - A) / max(A, B).



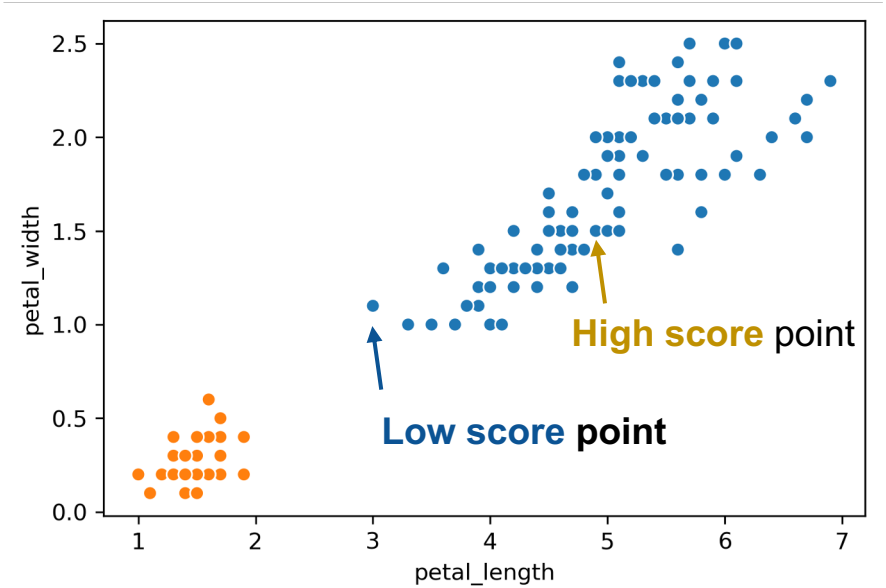
Can S be negative?

- Yes. If the average distance to X's clustermates is larger than distance to the closest cluster.

Silhouette Scores

For a data point X:

- A = average distance to other points in X's cluster.
- B = average distance to points in closest cluster.
- S = (B - A) / max(A, B).



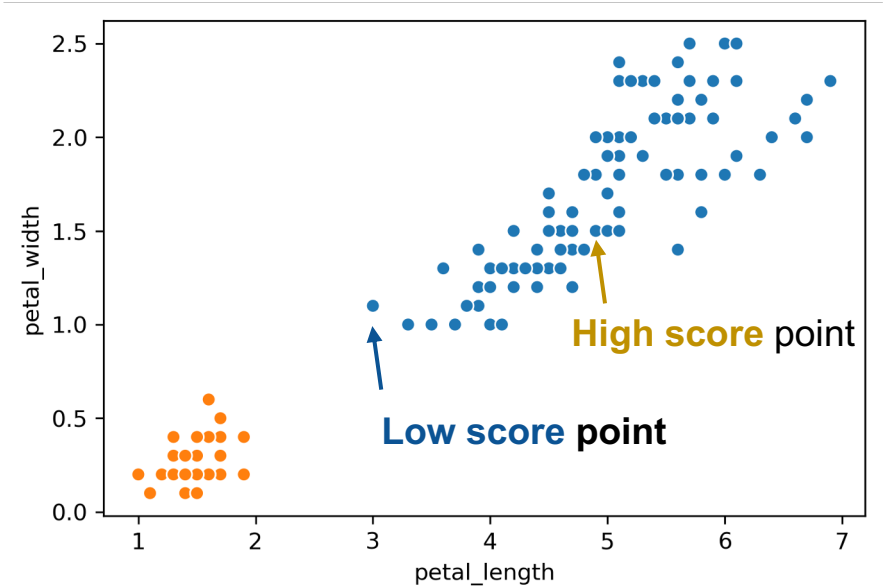
Can S be negative?

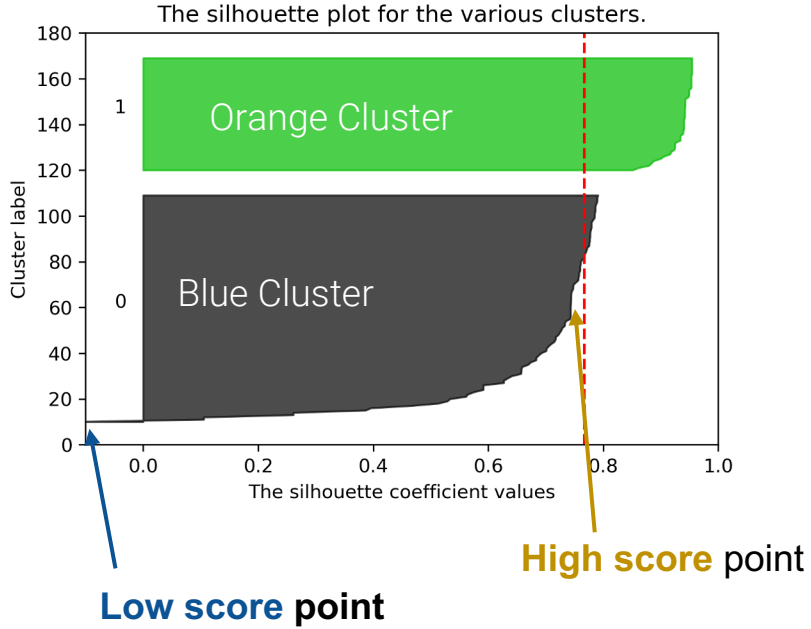
- Yes. If the average distance to X's clustermates is larger than distance to the closest cluster.
- Example: The "low score" point on the right has S = -0.13

Silhouette Plot

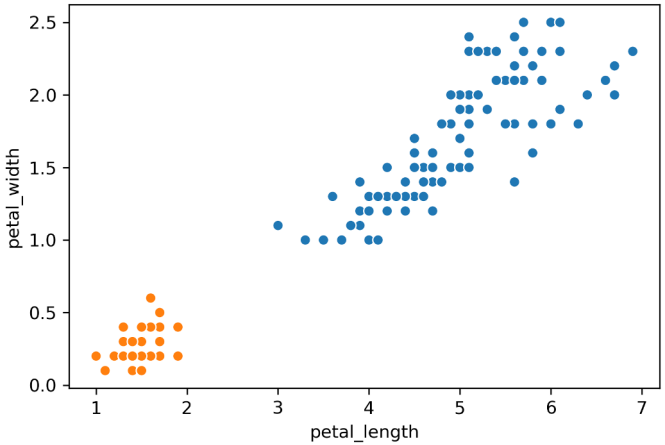
We can plot the **Silhouette Scores** for all of our data points.

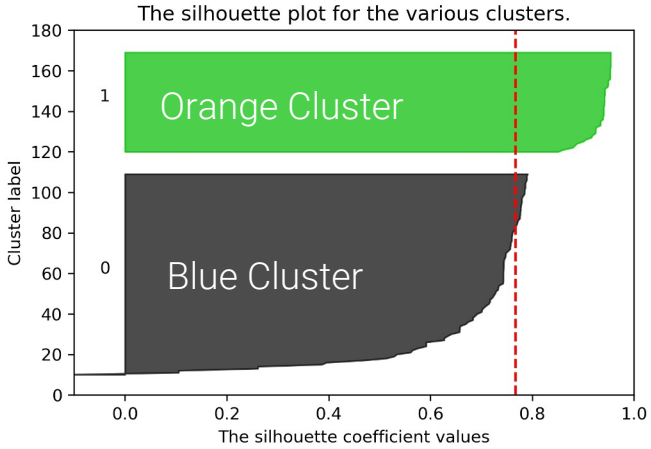
- Points with large silhouette widths are deeply embedded in their cluster.
- Red dotted line shows the average.

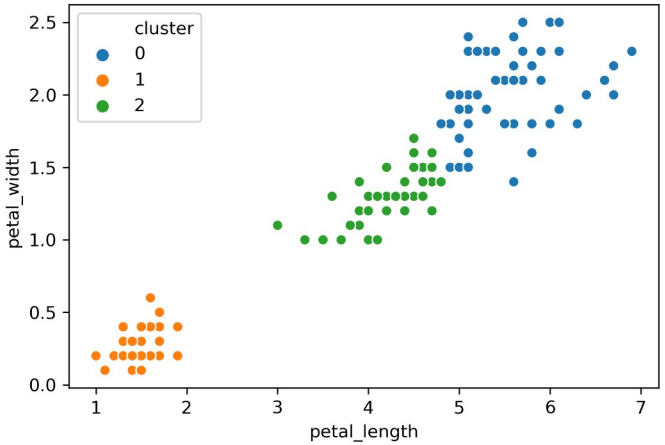


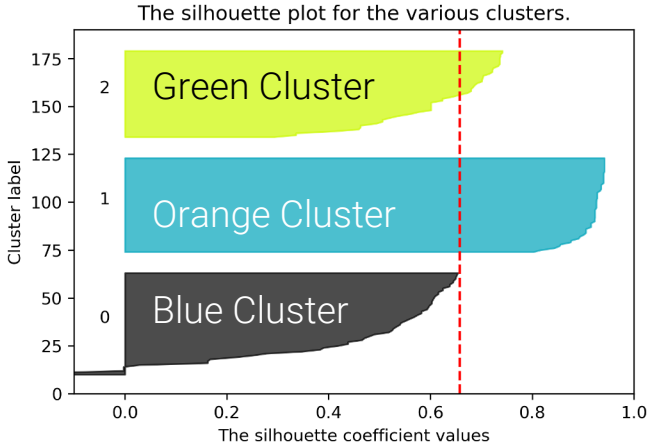


Silhouette Scores, K = 2 vs. K = 3









Average silhouette score is lower.

Picking K: Real World Metrics

Sometimes you can rely on real world metrics to guide your choice of K.

Perform 2 clusterings:

- Cluster heights and weights of customers with K = 3 to design Small, Medium, and Large shirts.
- Cluster heights and weights of customers with K = 5 to design XS, S, M, L, and XL shirts.

To pick K:

- Consider projected costs and sales for the 2 different K's.
- Pick the one that maximizes profit.

Summary

Today we discussed a new machine learning goal: Clustering.

Saw two solutions:

- **K-Means**
  - Tries to optimize a loss function called inertia -- no known algorithm to find the optimal answer in an efficient manner.
- **Hierarchical Agglomerative**

Our version of these algorithms required a hyperparameter k.

- 4 ways to pick k: Intuitively, elbow method, silhouette scores, harnessing real world metrics.