Hands-on Machine Learning

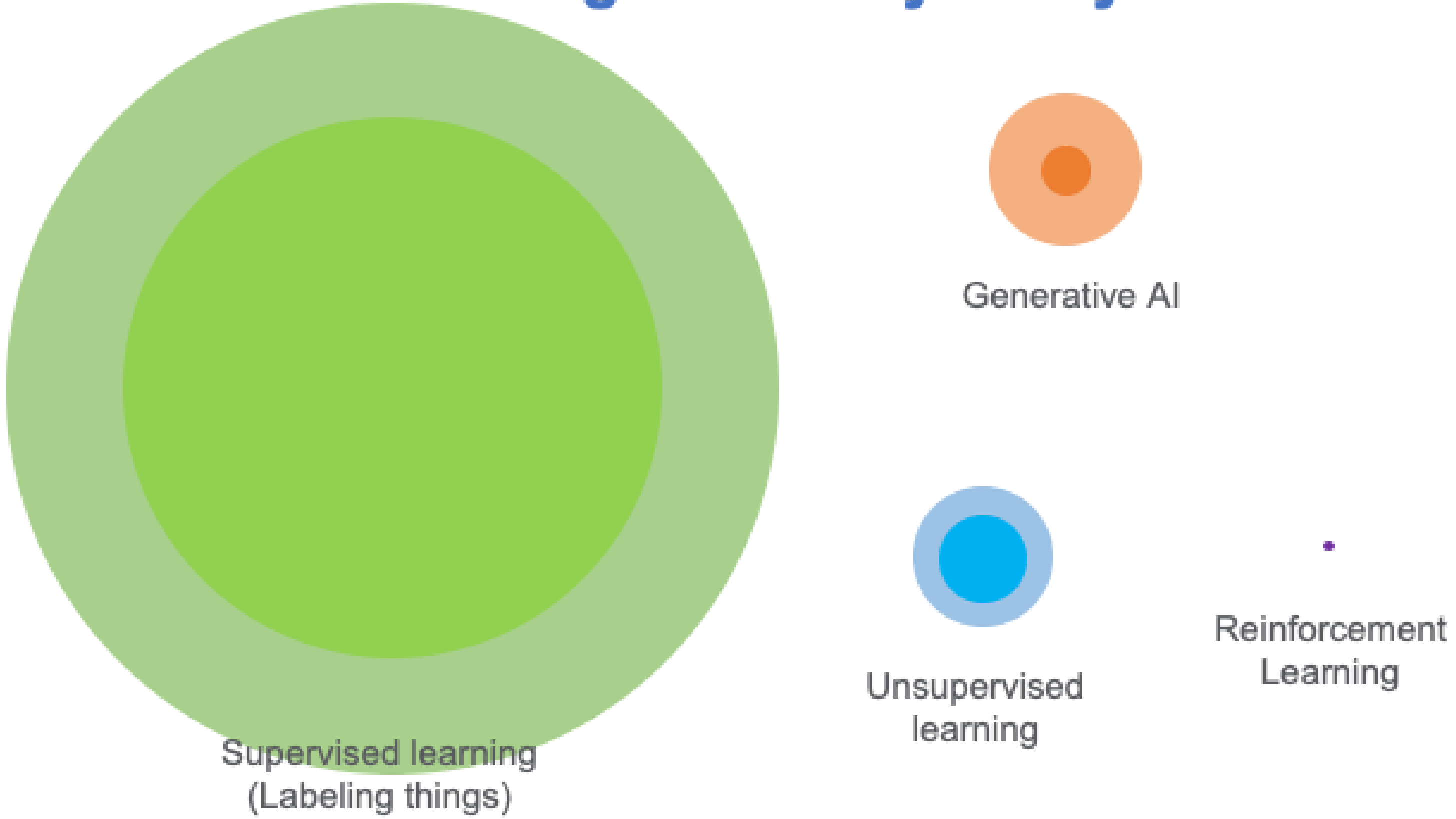
9. Unsupervised Learning

Unsupervised Learning

- Most of the applications of machine learning today are based on supervised learning, but the vast majority of the available data is unlabeled.

- Common unsupervised learning task:
  - *Clustering:* group similar instances together into *clusters.*
  - *Anomaly detection (outlier detection):* learn what "normal" data looks like, and then use that to detect abnormal instances.
  - *Density estimation:* estimating the *probability density function* (PDF) of the random process that generated the dataset.

Value from AI technologies: Today → 3 years

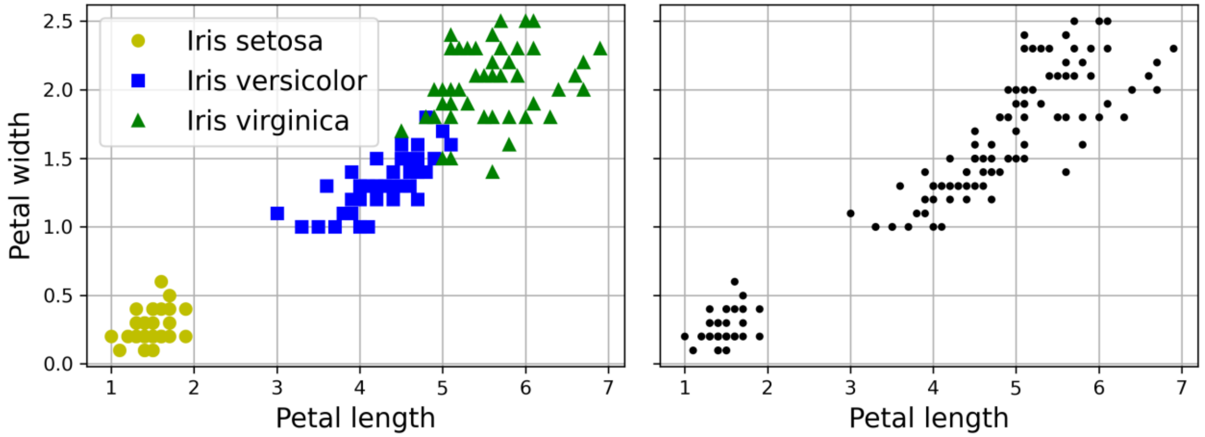


Andrew Ng

1.
Clustering

Clustering

- *Clustering*: the task of identifying similar instances and assigning them to *clusters*, or groups of similar instances.
- Similar to classification, each instance gets assigned to a group. But, unlike classification, clustering is an unsupervised task.



Applications of Clustering

- *Customer segmentation:* cluster customers based on their activity to adapt your products and marketing campaigns to each segment.
- *Data analysis:* when you analyze a new dataset, it can be helpful to run a clustering algorithm, and then analyze each cluster separately.
- *Dimensionality reduction:* each instance's feature vector $\mathbf{x}$ can be replaced with the vector of its cluster affinities.
  - affinity is any measure of how well an instance fits into a cluster.
- *Feature engineering:* the cluster affinities can often be useful as extra features.
- *Anomaly detection:* any instance that has a low affinity to all the clusters is likely to be an anomaly.

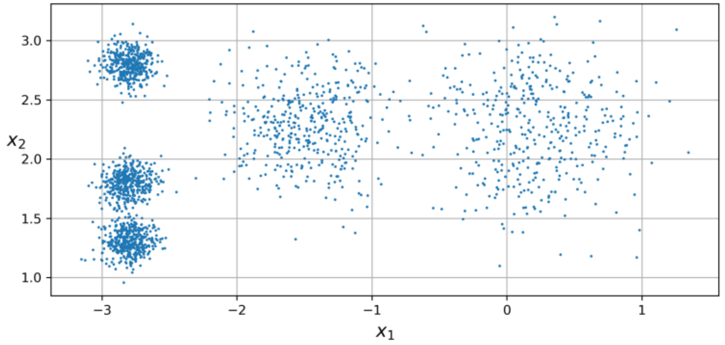
Applications of Clustering

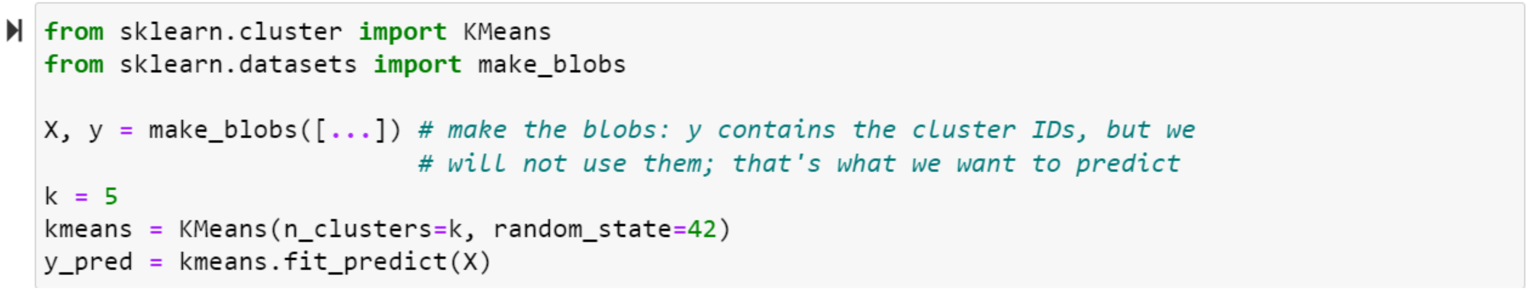
- *Semi-supervised learning:* if you only have a few labels, you could perform clustering and propagate the labels to all the instances in the same cluster.
- *Search engines:* to search for images that are similar to a reference image, apply a clustering algorithm to all the images in your database; and return all the images from the cluster of the searched image.
- *Image segmentation:* cluster pixels according to their color, then replace each pixel’s color with the mean color of its cluster.
  - Image segmentation is used in many object detection and tracking systems, as it makes it easier to detect the contour of each object.

2.
K-means

K-means

- k-means is a simple algorithm capable of clustering many datasets quickly and efficiently.
  - We have to specify the number of clusters k that the algorithm must find.

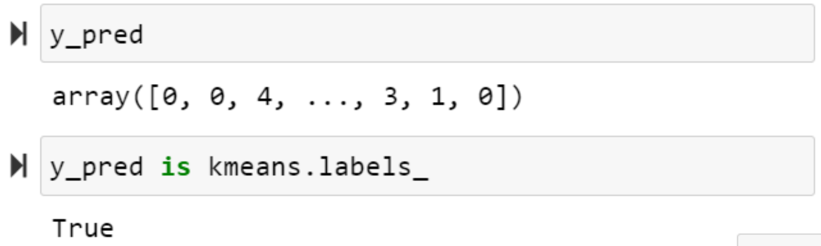




```
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs

X, y = make_blobs([...]) # make the blobs: y contains the cluster IDs, but we
                         # will not use them; that's what we want to predict
k = 5
kmeans = KMeans(n_clusters=k, random_state=42)
y_pred = kmeans.fit_predict(X)
```

K-means

- Each instance will be assigned to one of the five clusters.
  - An instance’s *label* is the index of its cluster.
- `KMeans` instance preserves the predicted labels of the instances it was trained on, available via the `labels_` instance variable:



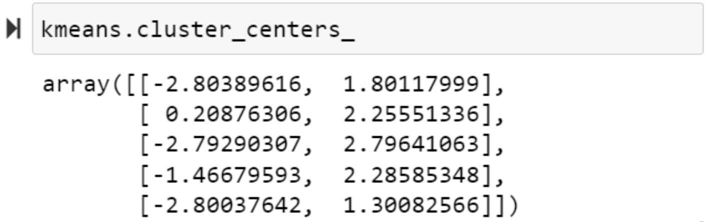
```
y_pred
```

```
array([0, 0, 4, ..., 3, 1, 0])
```

```
y_pred is kmeans.labels_
```

```
True
```

- The centroids that the algorithm found:

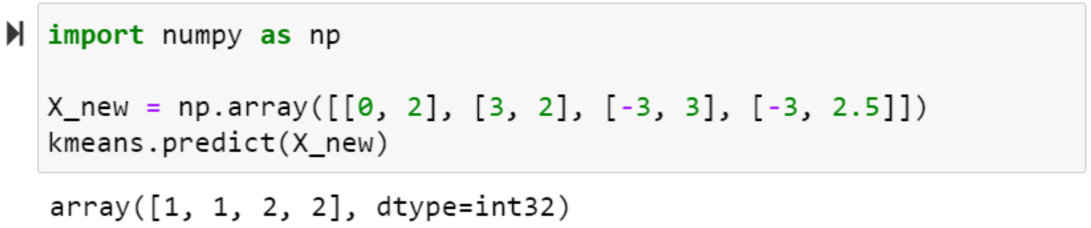


```
kmeans.cluster_centers_
```

```
array([[-2.80389616,  1.80117999],
       [ 0.20876306,  2.25551336],
       [-2.79290307,  2.79641063],
       [-1.46679593,  2.28585348],
       [-2.80037642,  1.30082566]])
```

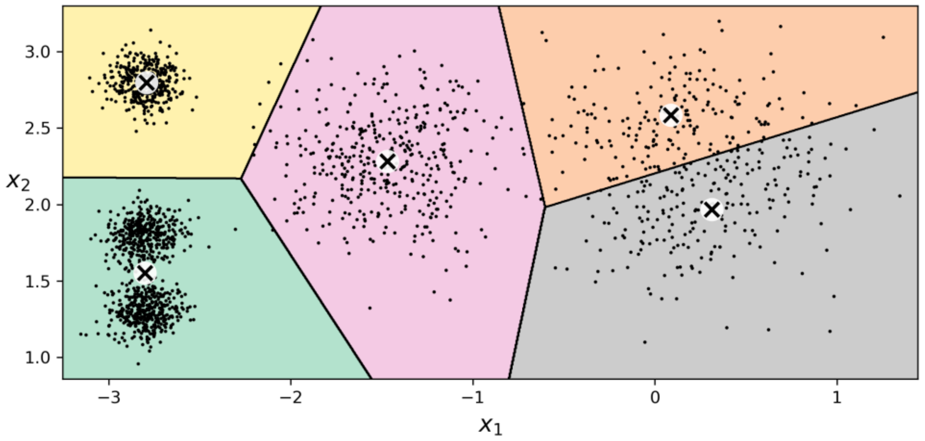
K-means

- New instances get assigned to the cluster whose centroid is closest:



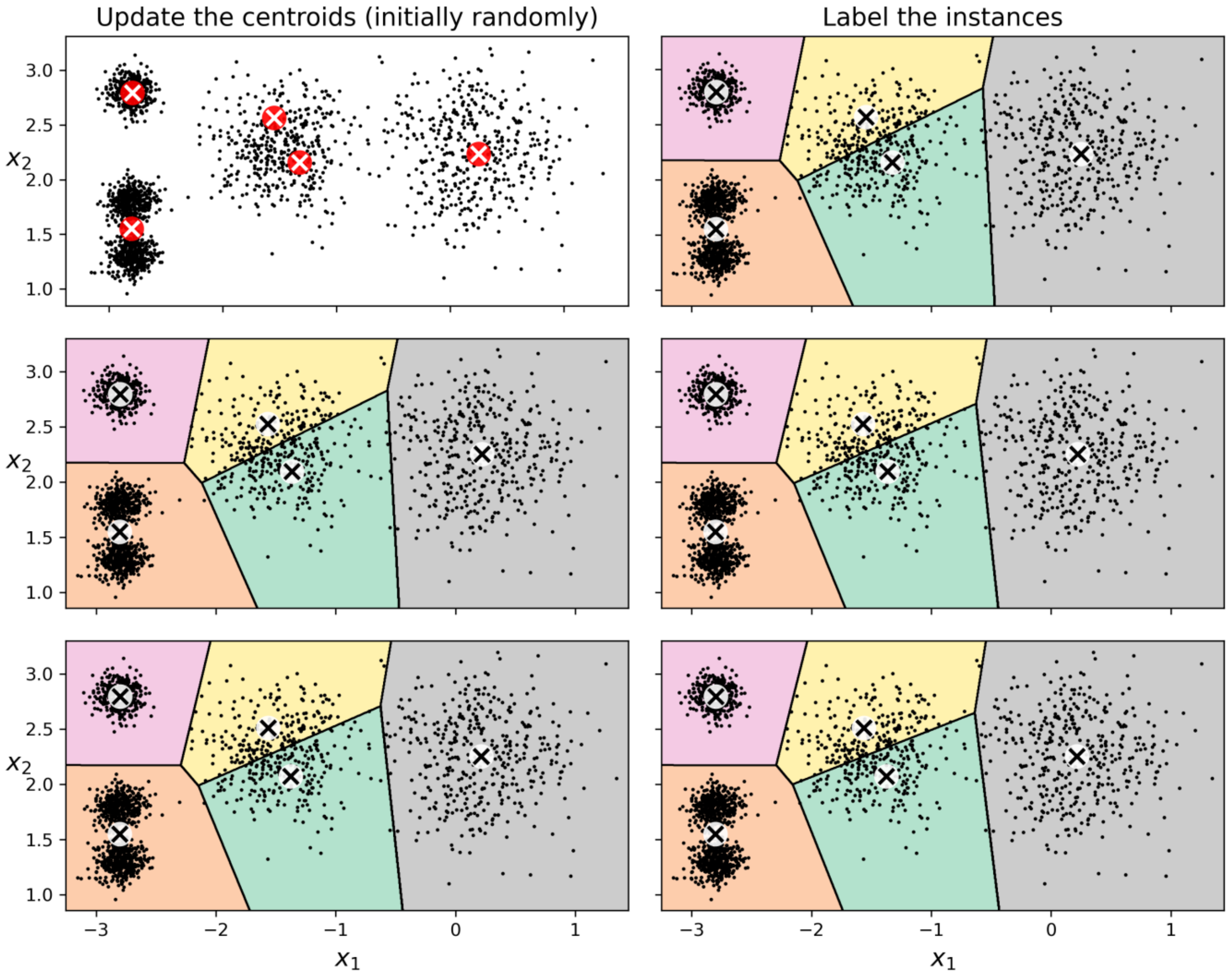
```
import numpy as np

X_new = np.array([[0, 2], [3, 2], [-3, 3], [-3, 2.5]])
kmeans.predict(X_new)
```

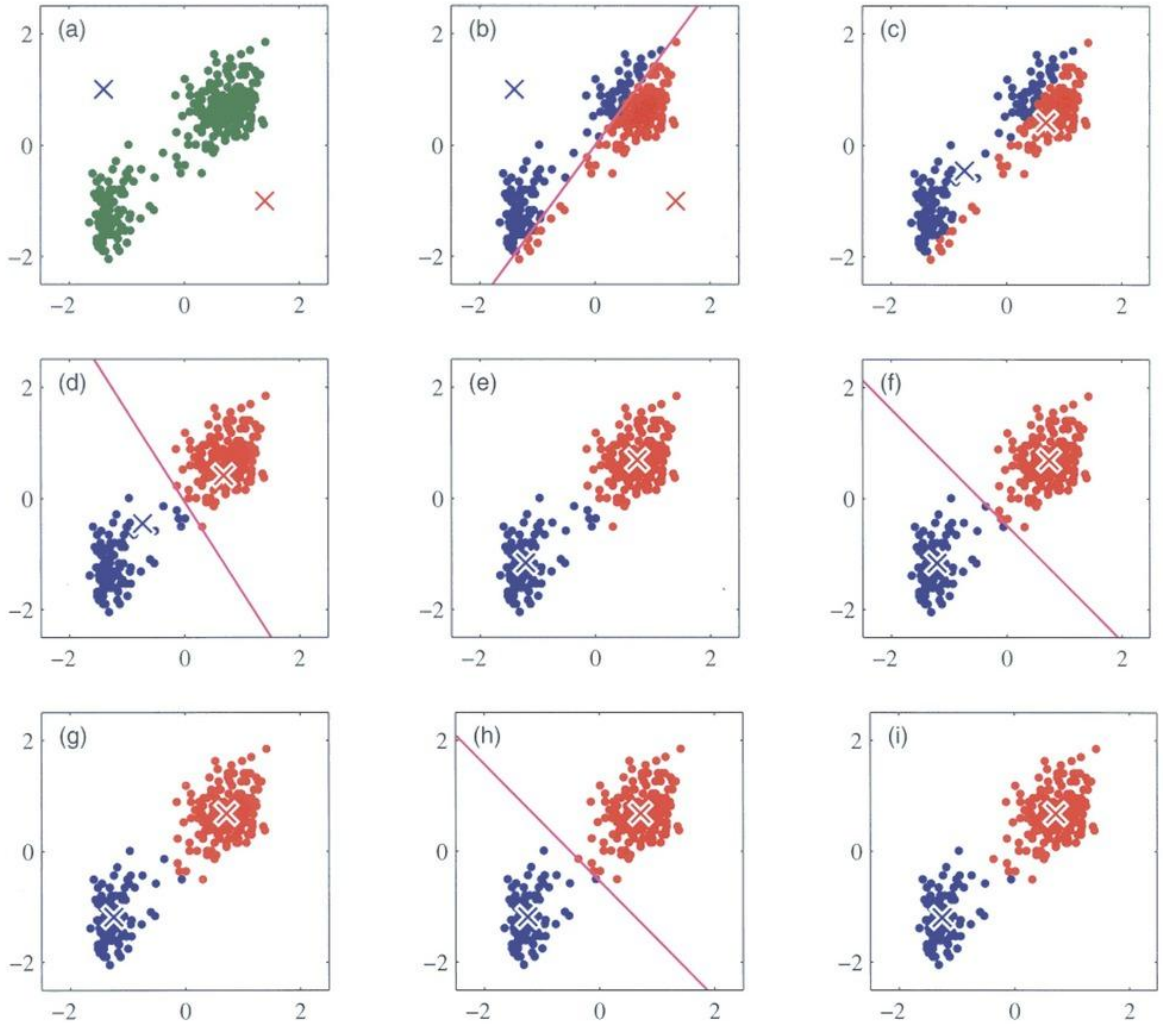
```
array([1, 1, 2, 2], dtype=int32)
```



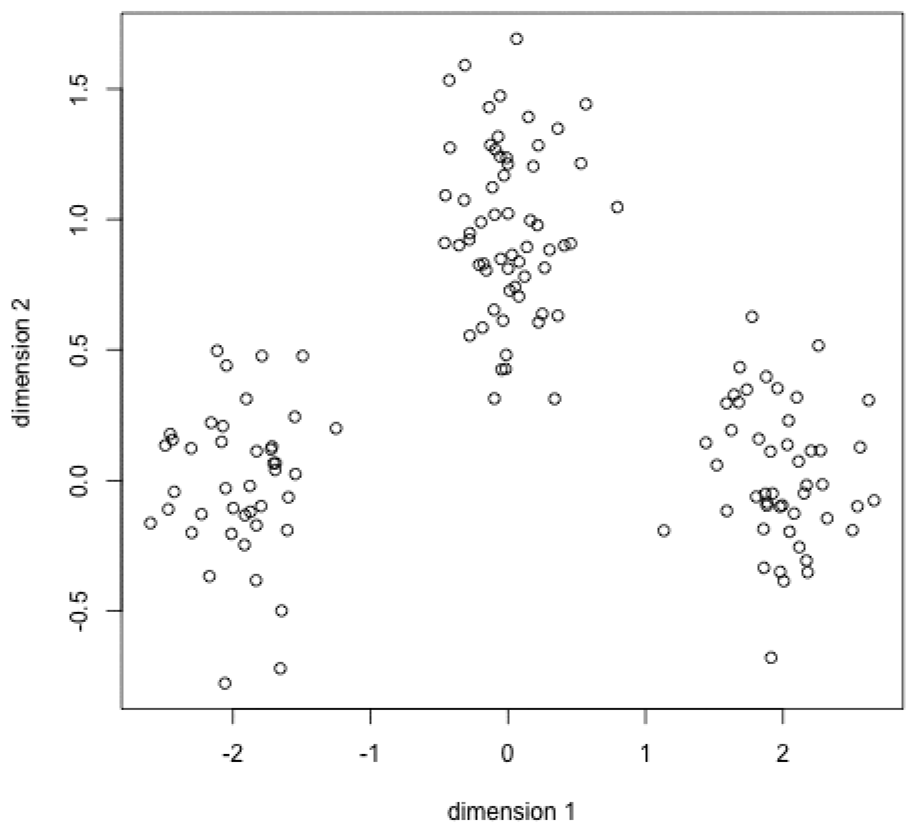
The k-means algorithm

- If you have the centroids, you could label the instances in the dataset by assigning them to the cluster whose centroid is closest.
- If you have all the instance labels, you could locate each cluster’s centroid by computing the mean of the instances in that cluster.
- Start by placing the centroids randomly:
  1) label the instances
  2) update the centroids
  3) repeat (1) and (2) until the centroids stop moving.
- The algorithm is guaranteed to converge in a finite number of steps because the mean squared distance between the instances and their closest centroids can only go down at each step.


Update the centroids (initially randomly)
Label the instances
x_2
x_1
3.0
2.5
2.0
1.5
1.0
−3
−2
−1
0
1

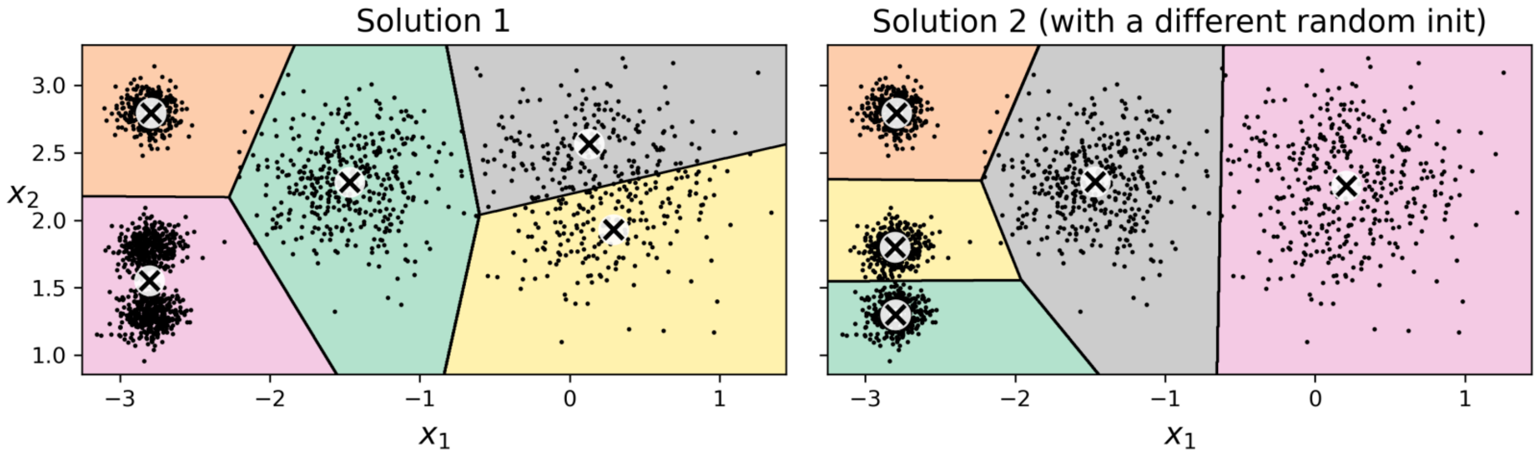

(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
2
0
−2
−2
0
2

step 0



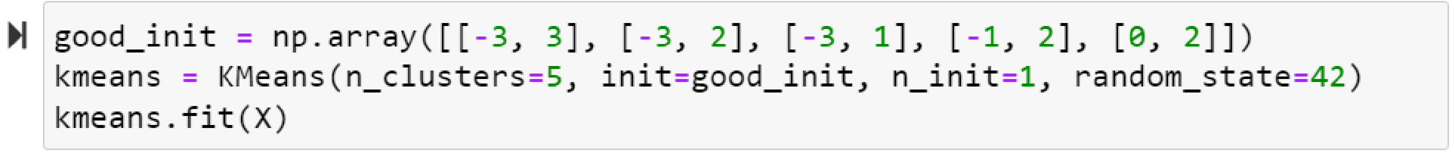
K-means disadvantage

- Although the algorithm is guaranteed to converge, it may not converge to the right solution
  - it may converge to a local optimum
  - whether it does or not depends on the centroid initialization.



Centroid initialization methods

- If you know approximately where the centroids should be (e.g., if you ran another clustering algorithm earlier), then you can set the `init` hyperparameter to a NumPy array containing the list of centroids:

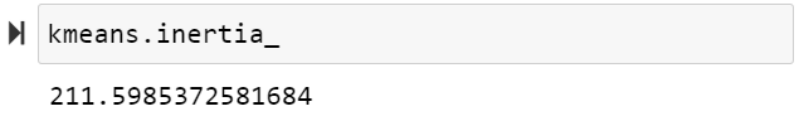


```
good_init = np.array([[-3, 3], [-3, 2], [-3, 1], [-1, 2], [0, 2]])
kmeans = KMeans(n_clusters=5, init=good_init, n_init=1, random_state=42)
kmeans.fit(X)
```

- Another solution is to run the algorithm multiple times with different random initializations and keep the best solution.
  - The number of random initializations is controlled by the `n_init`.
  - The default it is equal to 10.

Performance Metric

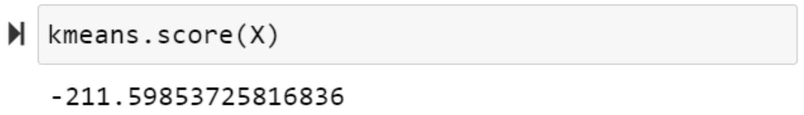
- Model's *inertia*: the sum of the squared distances between the instances and their closest centroids.
- The `KMeans` class runs the algorithm `n_init` times and keeps the model with the lowest inertia.
- A model's inertia is accessible via the `inertia` instance variable:



```
kmeans.inertia_
```

```
211.5985372581684
```

- The `score()` method returns the negative inertia.
  - It is negative because a predictor's `score()` method must always respect Scikit-Learn's "greater is better" rule.



```
kmeans.score(X)
```

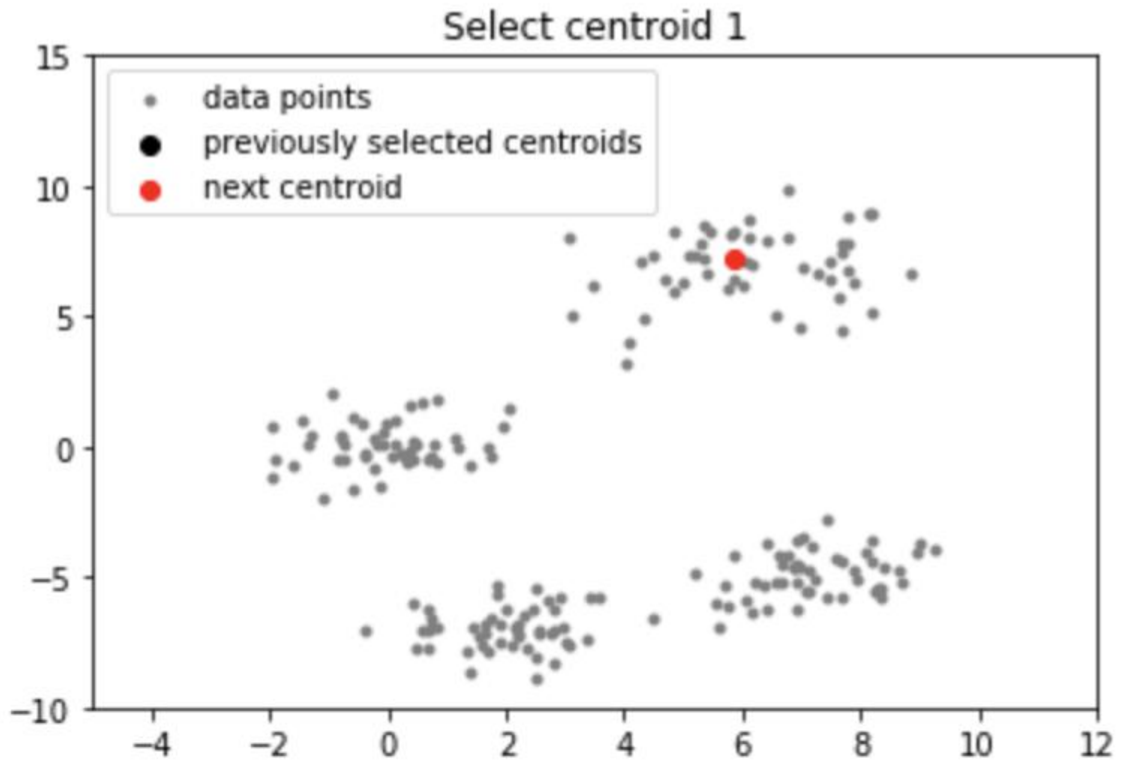
```
-211.59853725816836
```

K-means++

- A smarter initialization step that tends to select centroids that are distant from one another.
  - It makes the k-means algorithm much less likely to converge to a suboptimal solution.

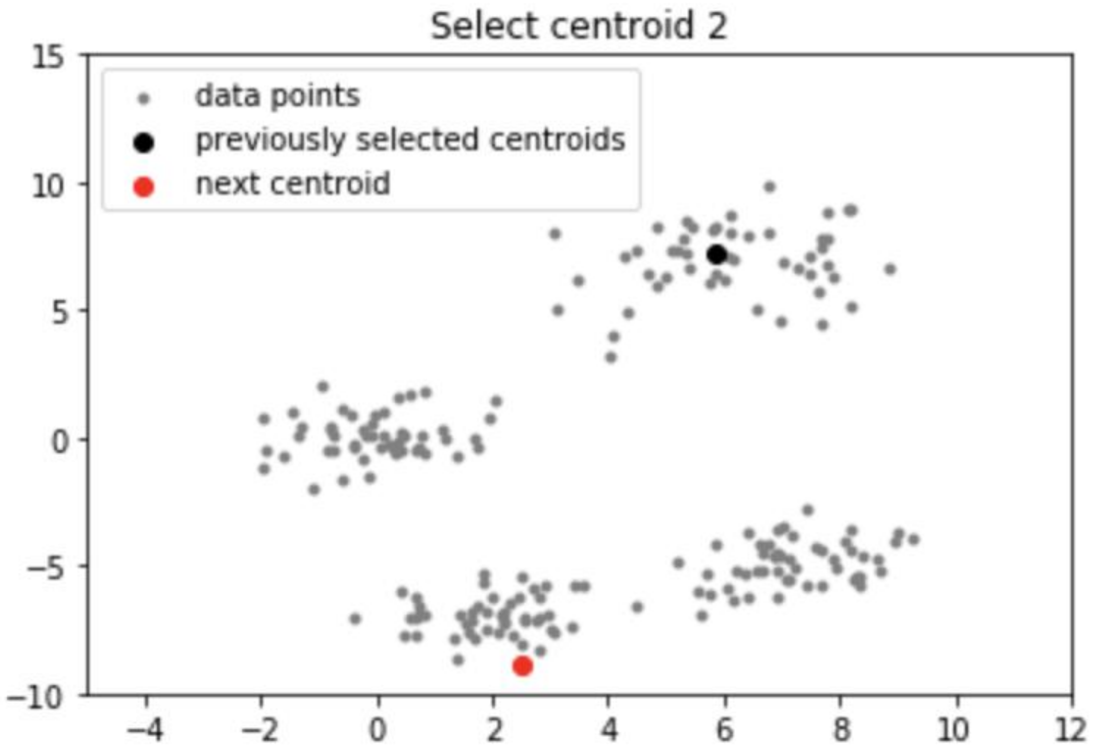
1. Take one centroid $\boldsymbol{c}^{(1)}$, chosen uniformly at random from the dataset.
2. Take a new centroid $\boldsymbol{c}^{(i)}$, choosing an instance $\mathbf{x}^{(i)}$ with probability $\frac{D\left(\mathbf{x}^{(i)}\right)^2}{\sum_{j=1}^{m} D\left(\mathbf{x}^{(j)}\right)^2}$ where $D(\mathbf{x}^{(j)})$ is the distance between the instance $\mathbf{x}^{(j)}$ and the closest centroid that was already chosen.
3. Repeat the previous step until all k centroids have been chosen.

K-means++

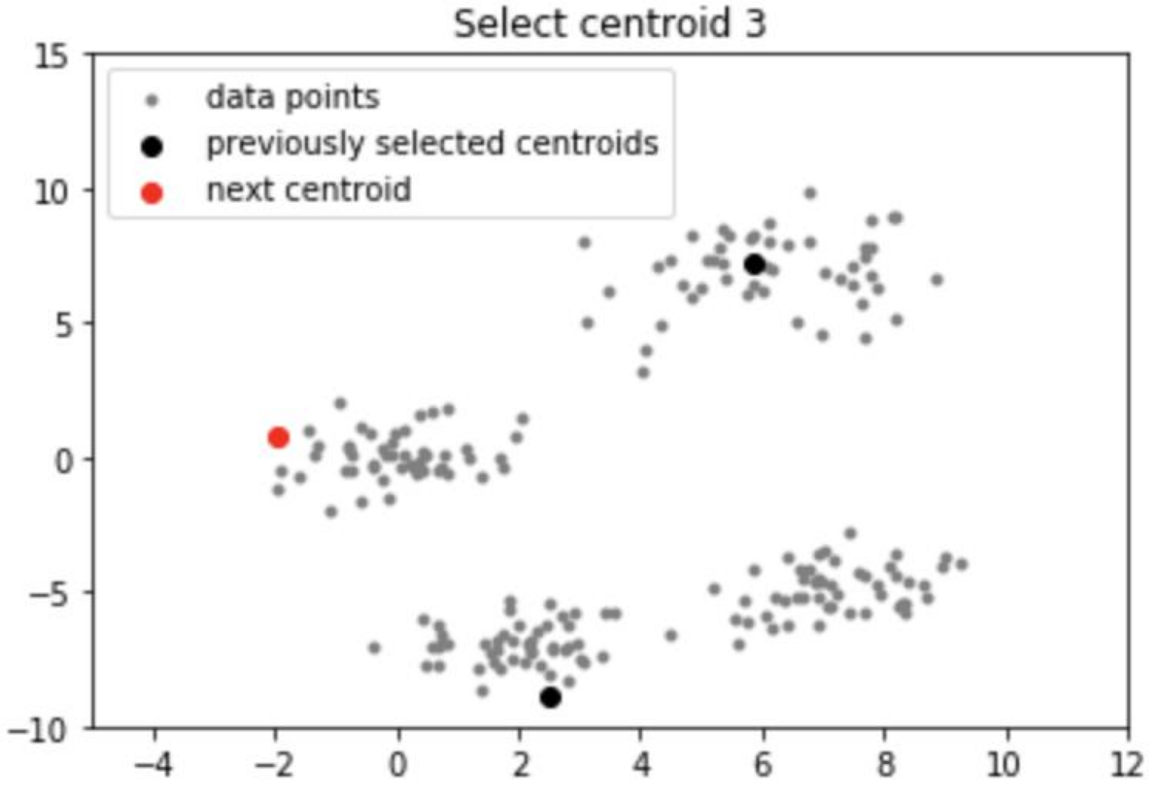


Select centroid 1
data points
previously selected centroids
next centroid
15
10
5
0
−5
−10
−4
−2
0
2
4
6
8
10
12

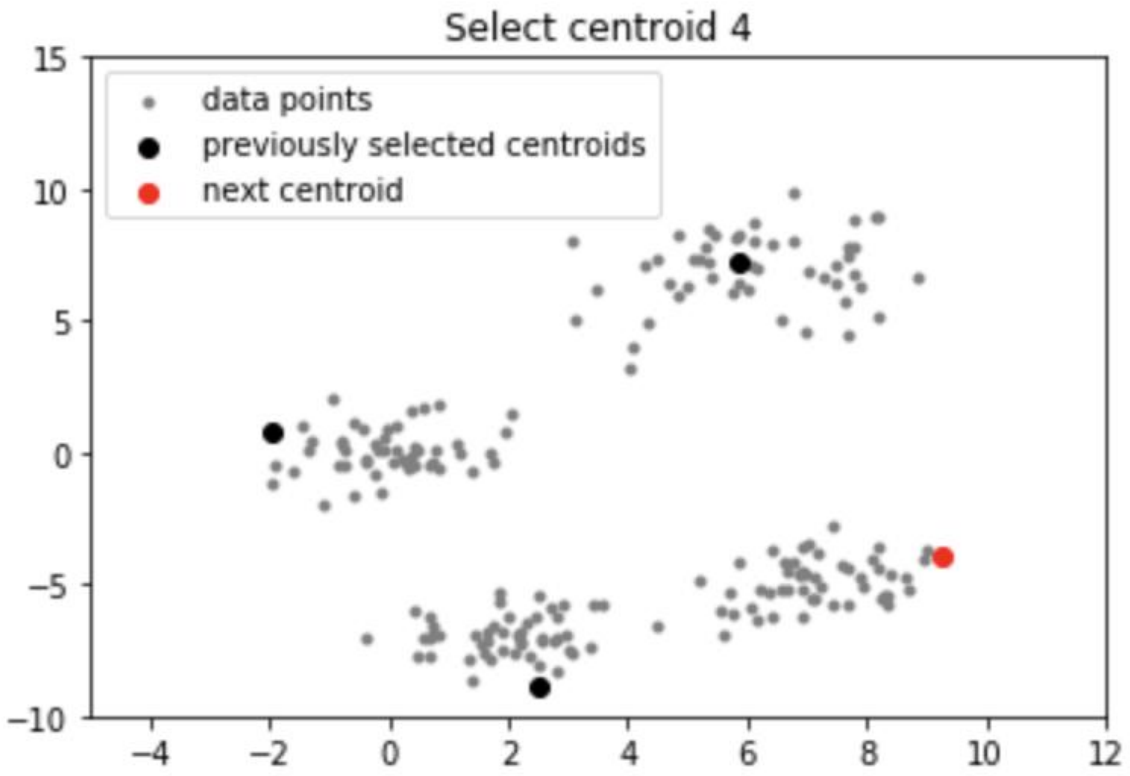
K-means++


Select centroid 2
data points
previously selected centroids
next centroid
15
10
5
0
−5
−10
−4
−2
0
2
4
6
8
10
12

K-means++


Select centroid 3
data points
previously selected centroids
next centroid
15
10
5
0
−5
−10
−4
−2
0
2
4
6
8
10
12

K-means++

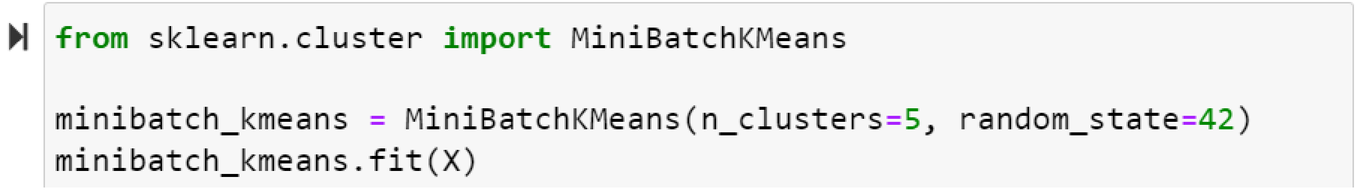

Select centroid 4
data points
previously selected centroids
next centroid
15
10
5
0
−5
−10
−4
−2
0
2
4
6
8
10
12

Accelerated k-means

- Another improvement to the *k*-means algorithm was proposed in a 2003 paper by Charles Elkan.
- On some large datasets with many clusters, the algorithm can be accelerated by avoiding many unnecessary distance calculations.
    - Elkan achieved this by exploiting the triangle inequality and by keeping track of lower and upper bounds for distances between instances and centroids.
- Elkan's algorithm does not always accelerate training, and sometimes it can even slow down training significantly;
    - It depends on the dataset.
    - You can try it by setting `algorithm="elkan"`.

Mini-batch k-means

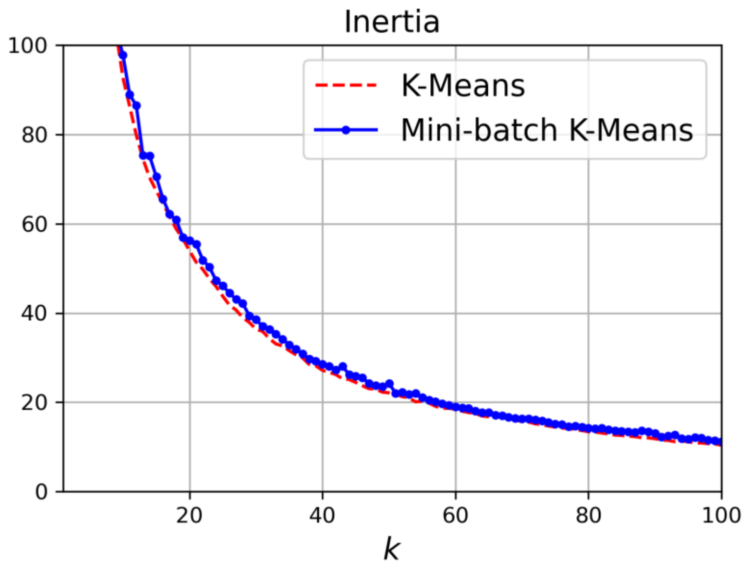
- Mini-batch k-means: instead of using the full dataset at each iteration, the algorithm is capable of using mini-batches, moving the centroids just slightly at each iteration.
- This speeds up the algorithm (typically by a factor of three to four) and makes it possible to cluster huge datasets that do not fit in memory.
- Scikit-Learn implements this algorithm in the `MiniBatchKMeans` class, which you can use just like the `KMeans` class:

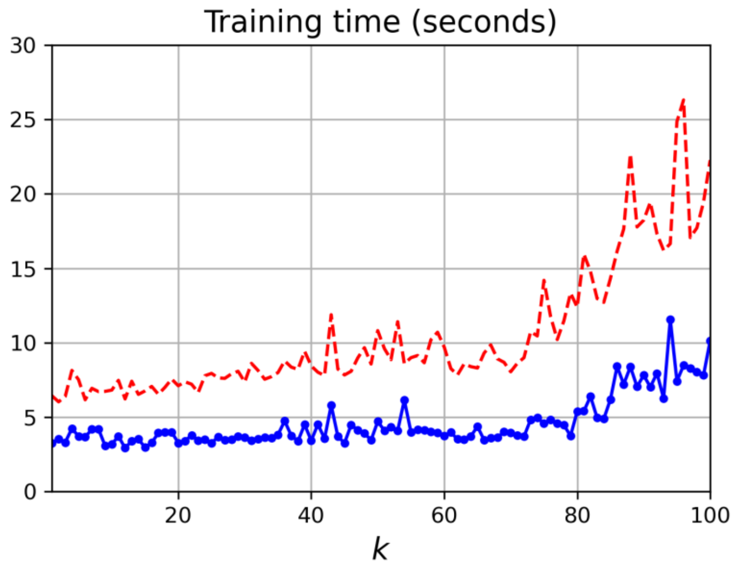


```
from sklearn.cluster import MiniBatchKMeans

minibatch_kmeans = MiniBatchKMeans(n_clusters=5, random_state=42)
minibatch_kmeans.fit(X)
```

Mini-batch k-means

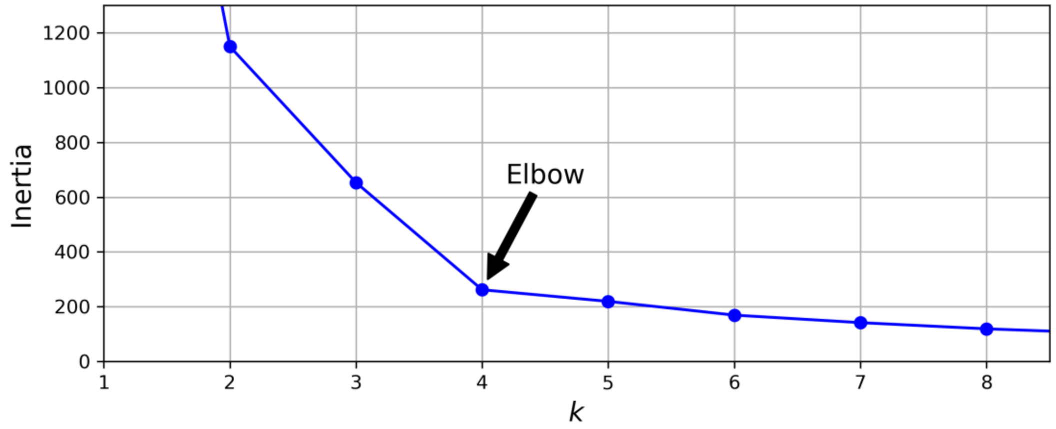
➢ Although the mini-batch k-means algorithm is much faster than the regular k-means algorithm, its inertia is generally slightly worse.





Finding the optimal number of clusters

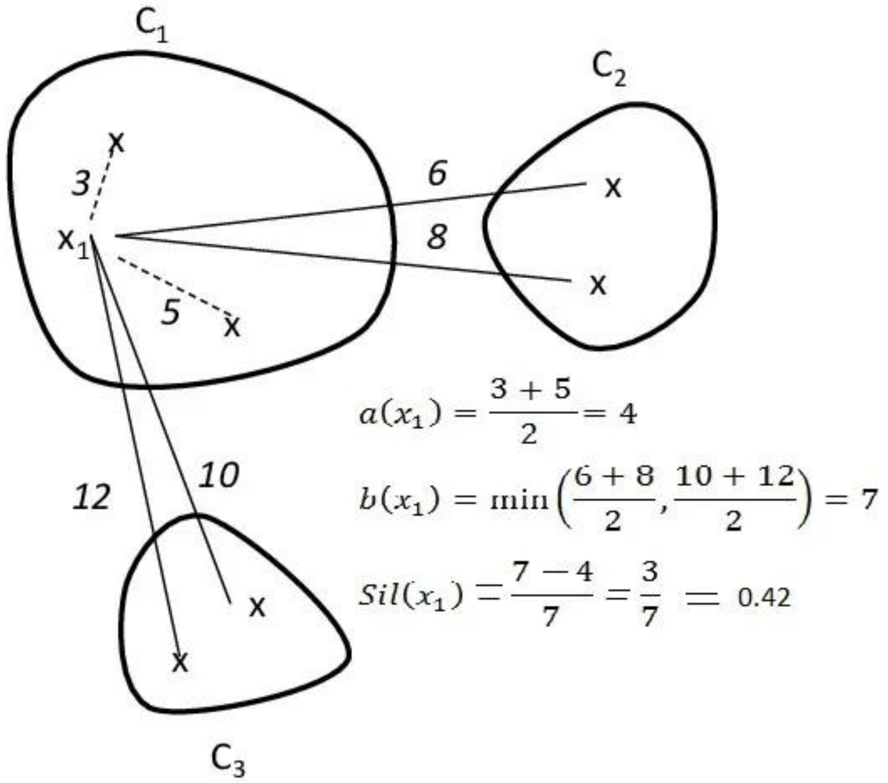
- The inertia is not a good performance metric when trying to choose k because it keeps getting lower as we increase k.
- *Elbow method*: plot the inertia as a function of k, the curve often contains an inflexion point called the *elbow*.



Silhouette Score

- *Silhouette score* is the mean *silhouette coefficient* over all the instances.
- An instance's silhouette coefficient is equal to $\frac{b - a}{\max(a,b)}$
  - a is the mean distance to the other instances in the same cluster (the mean intra-cluster distance).
  - b is the mean nearest-cluster distance.
  - The silhouette coefficient can vary between –1 and +1.
  - A coefficient close to +1 means that the instance is well inside its own cluster and far from other clusters.
  - A coefficient close to 0 means that it is close to a cluster boundary.
  - A coefficient close to –1 means that the instance may have been assigned to the wrong cluster.

Silhouette Coefficient



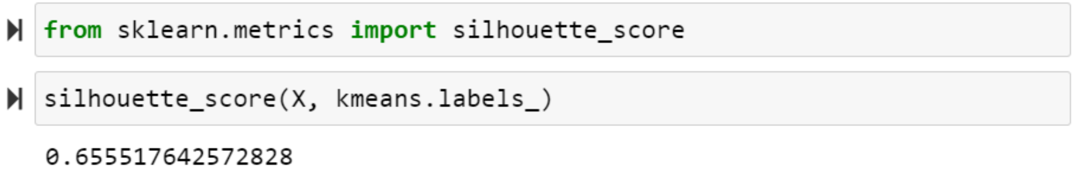
$$a(x_1) = \frac{3+5}{2} = 4$$

$$b(x_1) = \min\left(\frac{6+8}{2}, \frac{10+12}{2}\right) = 7$$

$$Sil(x_1) = \frac{7-4}{7} = \frac{3}{7} = 0.42$$

Silhouette Score

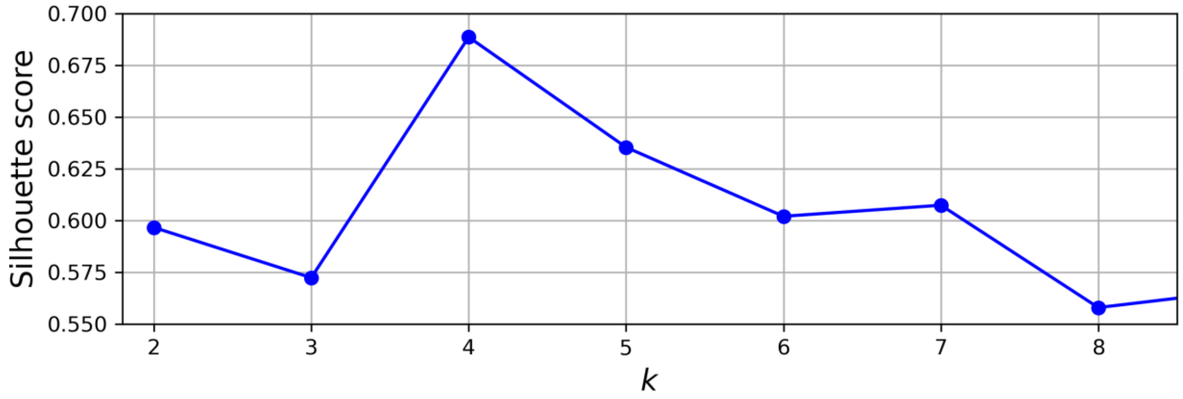
➢ You can use Scikit-Learn's `silhouette_score()` function, giving it all the instances in the dataset and the labels they were assigned:



```
from sklearn.metrics import silhouette_score
```

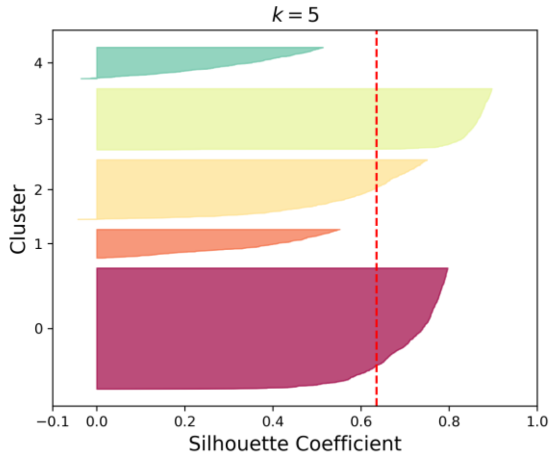
```
silhouette_score(X, kmeans.labels_)
```

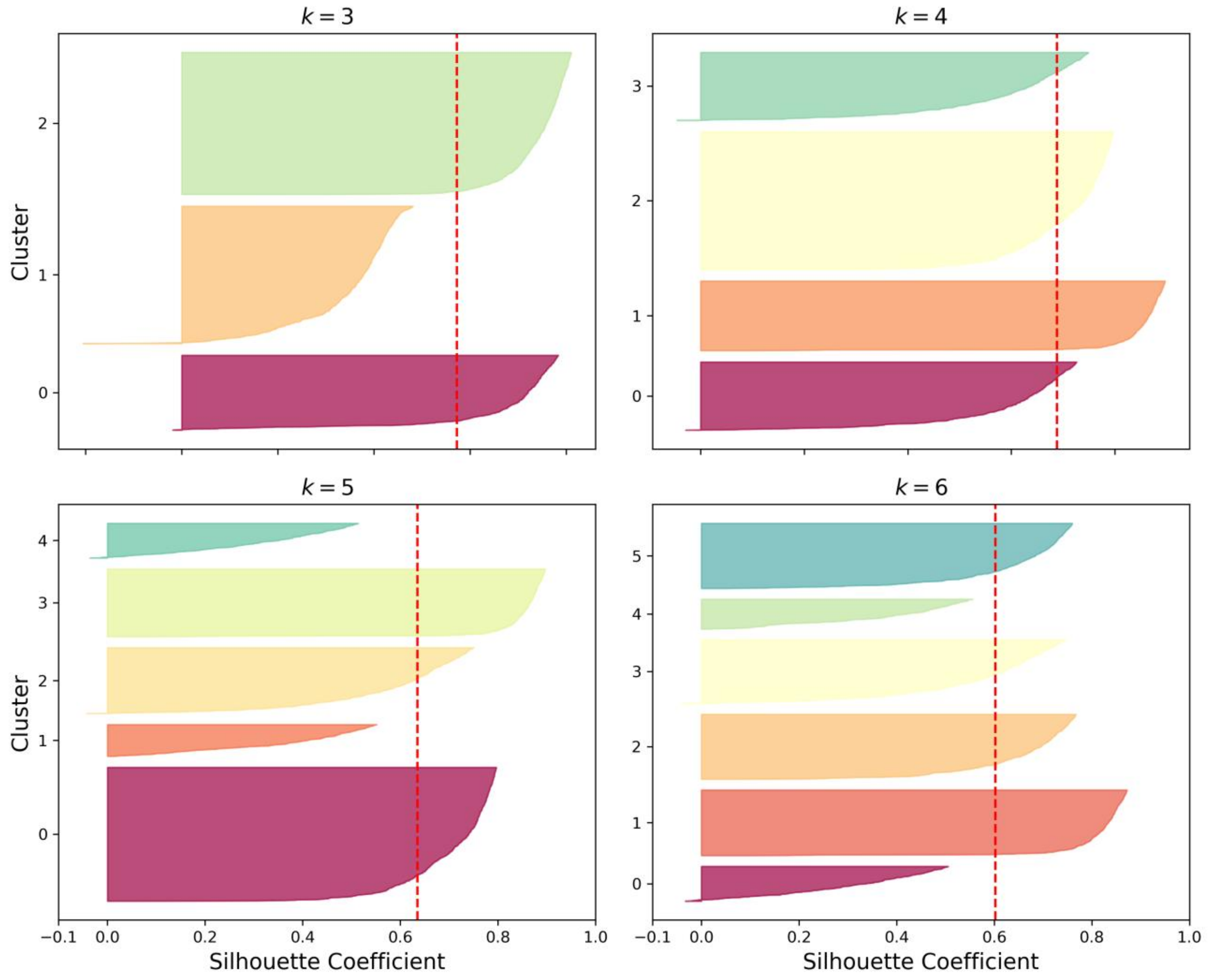
```
0.655517642572828
```



Silhouette Diagram

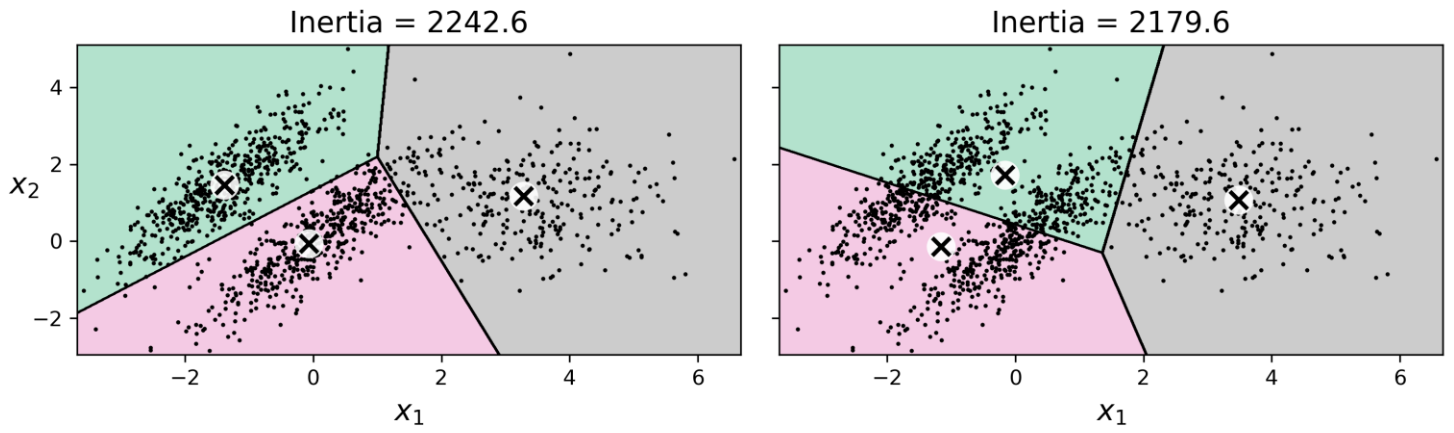
- *Silhouette diagram*: plot every instance's silhouette coefficient, sorted by the clusters they are assigned to and by the value of the coefficient.
- Each diagram contains one knife shape per cluster.
  - The shape's height indicates the number of instances in the cluster
  - Its width represents the sorted silhouette coefficients of the instances in the cluster (wider is better).
- The vertical dashed line is the silhouette score for the clustering.
- When most of the instances in a cluster have a lower coefficient than this score then the cluster is rather bad.




k = 3
k = 4
k = 5
k = 6
Cluster
Cluster
Silhouette Coefficient
Silhouette Coefficient
−0.1
0.0
0.2
0.4
0.6
0.8
1.0

Limits of k-means

- We should run k-means several times to avoid suboptimal solutions.
- You must specify the number of clusters, which can be a problem.
- k-means does not behave very well when the clusters have varying sizes, different densities, or nonspherical shapes.



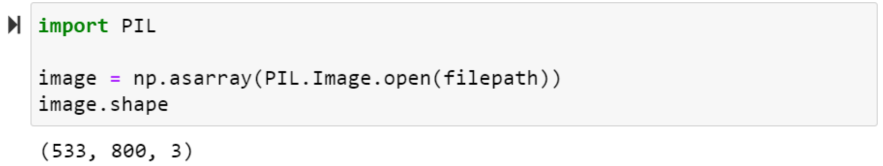
3. Clustering Applications

Using Clustering for Image Segmentation

- *Image segmentation* is the task of partitioning an image into multiple segments:
  - *Color segmentation*: pixels with a similar color get assigned to the same segment.
  - *Semantic segmentation*: all pixels that are part of the same object type get assigned to the same segment.
  - *Instance segmentation*: all pixels that are part of the same individual object are assigned to the same segment.
- The state of the art in semantic or instance segmentation today is achieved using complex architectures based on convolutional neural networks.

Color Segmentation using k-means

- Import the Pillow package (successor to the Python Imaging Library, PIL), and load the *ladybug.png*, assuming it's located at `filepath`:



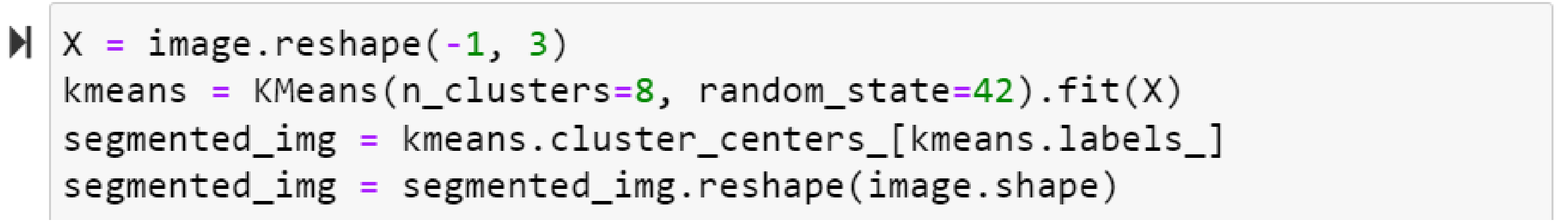
```
import PIL

image = np.asarray(PIL.Image.open(filepath))
image.shape
```

```
(533, 800, 3)
```

- The image is represented as a 3D array.
  - The first dimension's size is the height
  - The second is the width
  - The third is the number of color channels: red, green, and blue (RGB).
- For each pixel there is a 3D vector containing the intensities of red, green, and blue as unsigned 8-bit integers between 0 and 255.

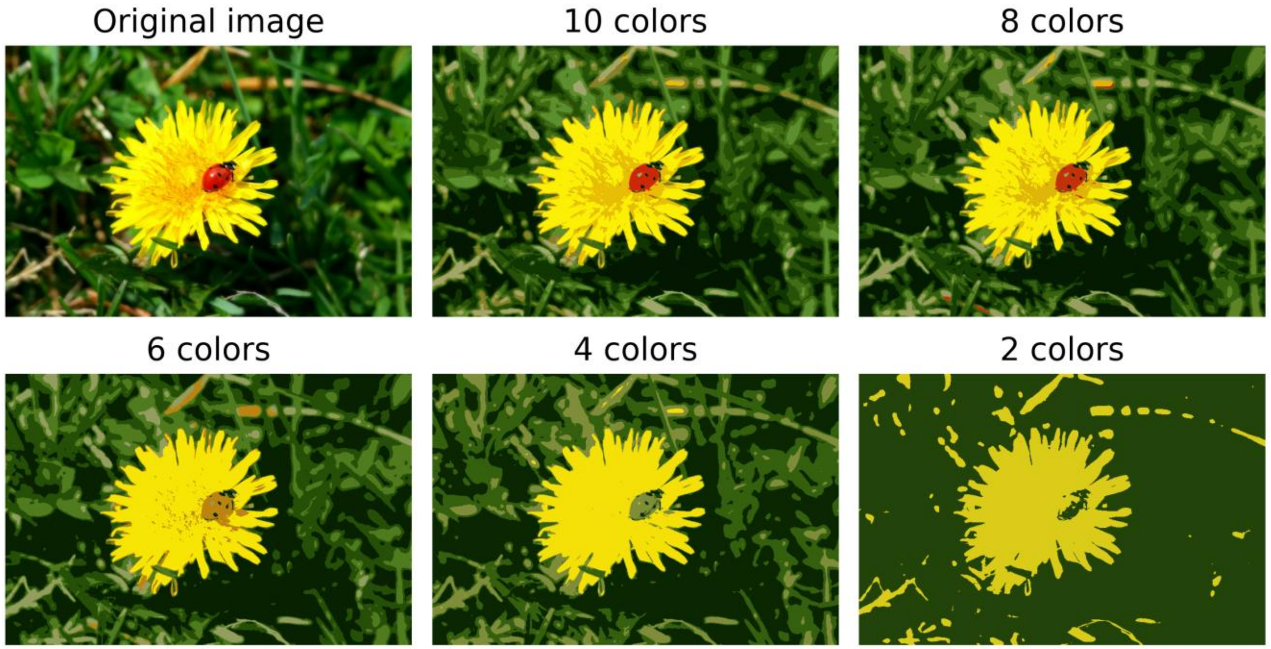
Color Segmentation using k-means

- The following code:
  - reshapes the array to get a long list of RGB colors
  - clusters these colors using k-means with eight clusters
  - creates a `segmented_img` array containing the nearest cluster center for each pixel
  - reshapes this array to the original image shape.



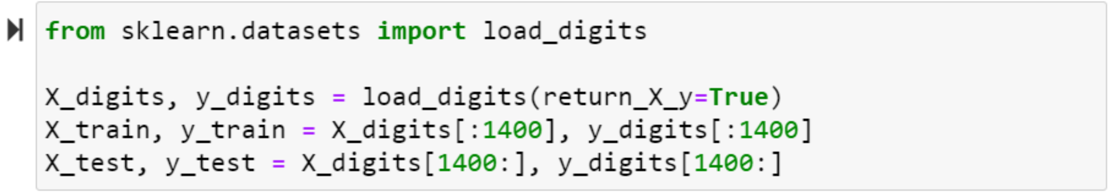
```
X = image.reshape(-1, 3)
kmeans = KMeans(n_clusters=8, random_state=42).fit(X)
segmented_img = kmeans.cluster_centers_[kmeans.labels_]
segmented_img = segmented_img.reshape(image.shape)
```

Color Segmentation using k-means



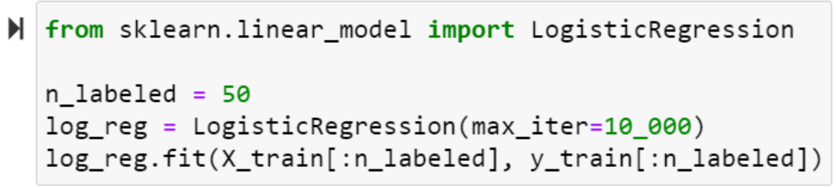
Using Clustering for Semi-Supervised Learning

- In semi-supervised learning, we have plenty of unlabeled instances and very few labeled instances.
- The *digits* dataset is a simple MNIST-like dataset containing 1797 grayscale 8×8 images representing the digits 0 to 9.



```python
from sklearn.datasets import load_digits

X_digits, y_digits = load_digits(return_X_y=True)
X_train, y_train = X_digits[:1400], y_digits[:1400]
X_test, y_test = X_digits[1400:], y_digits[1400:]
```

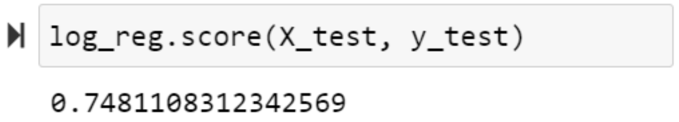
- We pretend we only have labels for 50 instances. To get a baseline, train a logistic regression model on these 50 labeled instances:



```python
from sklearn.linear_model import LogisticRegression

n_labeled = 50
log_reg = LogisticRegression(max_iter=10_000)
log_reg.fit(X_train[:n_labeled], y_train[:n_labeled])
```

Using Clustering for Semi-Supervised Learning

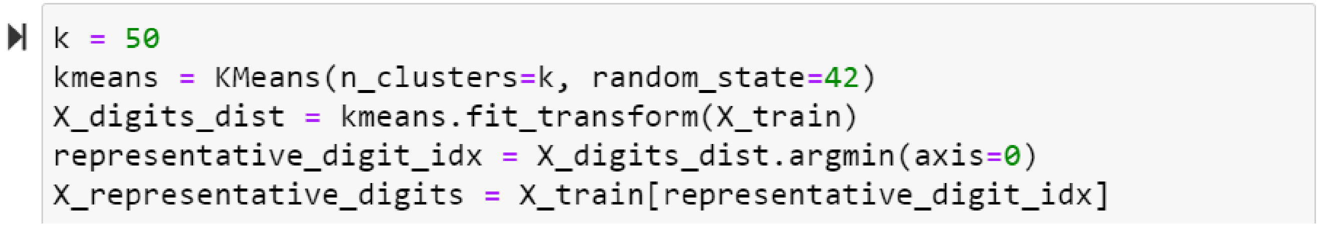
- Measure the accuracy of the baseline model on the test set:



```
log_reg.score(X_test, y_test)
```

```
0.7481108312342569
```

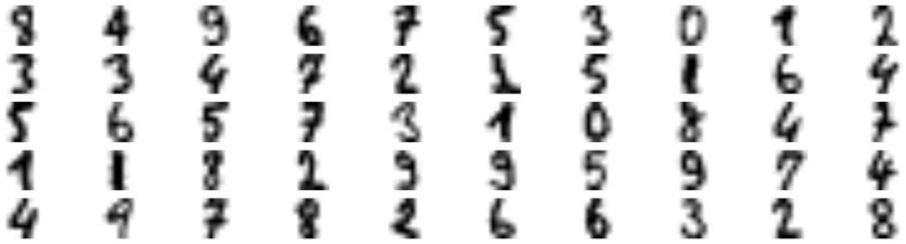
- First, cluster the training set into 50 clusters.
- Then, for each cluster, find the image closest to the centroid.
  - We’ll call these images the *representative images*:



```
k = 50
kmeans = KMeans(n_clusters=k, random_state=42)
X_digits_dist = kmeans.fit_transform(X_train)
representative_digit_idx = X_digits_dist.argmin(axis=0)
X_representative_digits = X_train[representative_digit_idx]
```

Using Clustering for Semi-Supervised Learning

- The 50 representative images:



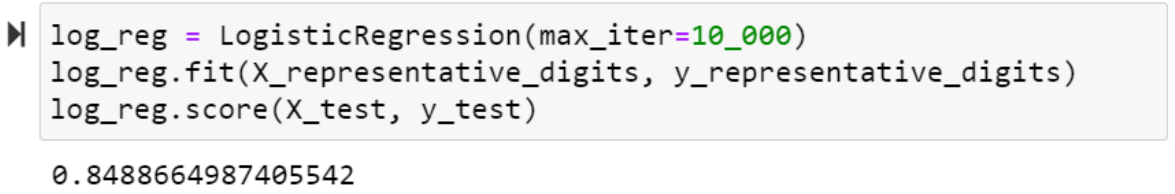
- Look at each image and manually label them:

```
y_representative_digits = np.array([1, 3, 6, 0, 7, 9, 2, ..., 5, 1, 9, 9, 3, 7])
```

- We have a dataset with just 50 labeled instances, but instead of being random instances, each of them is a representative image of its cluster.

Using Clustering for Semi-Supervised Learning

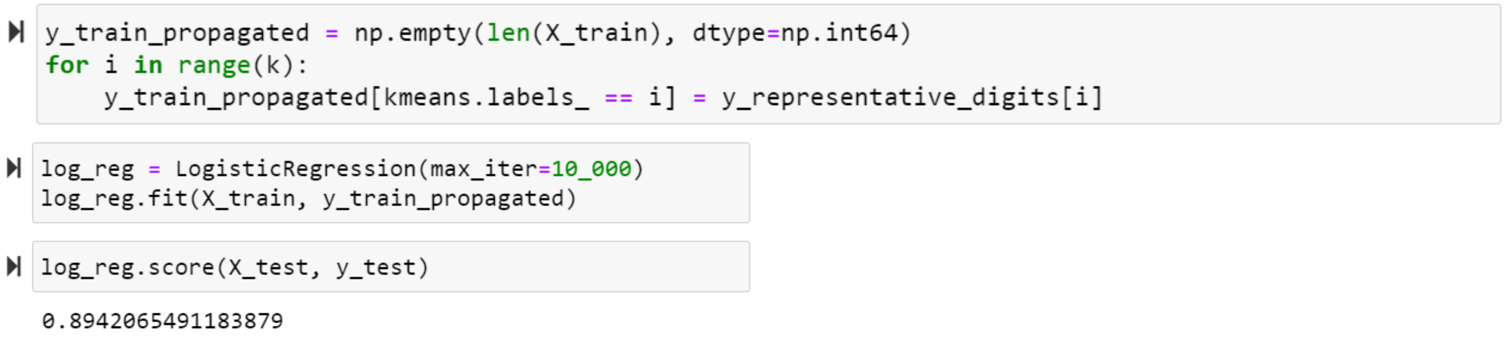
- The performance jumps from 74.8% accuracy to 84.9%:



```
log_reg = LogisticRegression(max_iter=10_000)
log_reg.fit(X_representative_digits, y_representative_digits)
log_reg.score(X_test, y_test)
```

```
0.8488664987405542
```

- *Label propagation:* propagate the labels to all the other instances in the same cluster.



```
y_train_propagated = np.empty(len(X_train), dtype=np.int64)
for i in range(k):
    y_train_propagated[kmeans.labels_ == i] = y_representative_digits[i]
```

```
log_reg = LogisticRegression(max_iter=10_000)
log_reg.fit(X_train, y_train_propagated)
```

```
log_reg.score(X_test, y_test)
```

```
0.8942065491183879
```

Using Clustering for Semi-Supervised Learning

- Ignore the 1% of instances that are farthest from their cluster center.
  - This should eliminate some outliers.

```
percentile_closest = 99

X_cluster_dist = X_digits_dist[np.arange(len(X_train)), kmeans.labels_]
for i in range(k):
    in_cluster = (kmeans.labels_ == i)
    cluster_dist = X_cluster_dist[in_cluster]
    cutoff_distance = np.percentile(cluster_dist, percentile_closest)
    above_cutoff = (X_cluster_dist > cutoff_distance)
    X_cluster_dist[in_cluster & above_cutoff] = -1

partially_propagated = (X_cluster_dist != -1)
X_train_partially_propagated = X_train[partially_propagated]
y_train_partially_propagated = y_train_propagated[partially_propagated]
```

```
log_reg = LogisticRegression(max_iter=10_000)
log_reg.fit(X_train_partially_propagated, y_train_partially_propagated)
log_reg.score(X_test, y_test)
```

```
0.9093198992443325
```

Label Propagation in Scikit-Learn

- Scikit-Learn have two classes in the `sklearn.semi_supervised` package that can propagate labels automatically:
  - `LabelSpreading`
  - `LabelPropagation`
- They construct a similarity matrix between instances, and iteratively propagate labels from labeled instances to similar unlabeled instances.
- `SelfTrainingClassifier`: another class in the same package
  - You give it a base classifier (e.g. `RandomForest`) and it trains it on the labeled instances, then uses it to predict labels for the unlabeled samples.
  - It then updates the training set with the labels it is most confident about, and repeats this process of training and labeling until it cannot add labels anymore.

Active Learning

- *Active learning*: when a human expert provides labels for specific instances when the learning algorithm requests them.
- *Uncertainty sampling*: the most common strategy for active learning
  1. The model is trained on the labeled instances gathered so far, and this model is used to make predictions on all the unlabeled instances.
  2. The instances for which the model is most uncertain (i.e., where its estimated probability is lowest) are given to the expert for labeling.
  3. You iterate this process until the performance improvement stops being worth the labeling effort.
- Other strategies include labeling the instances that would result in the largest model change or the largest drop in the model's validation error, or the instances that different models disagree on.