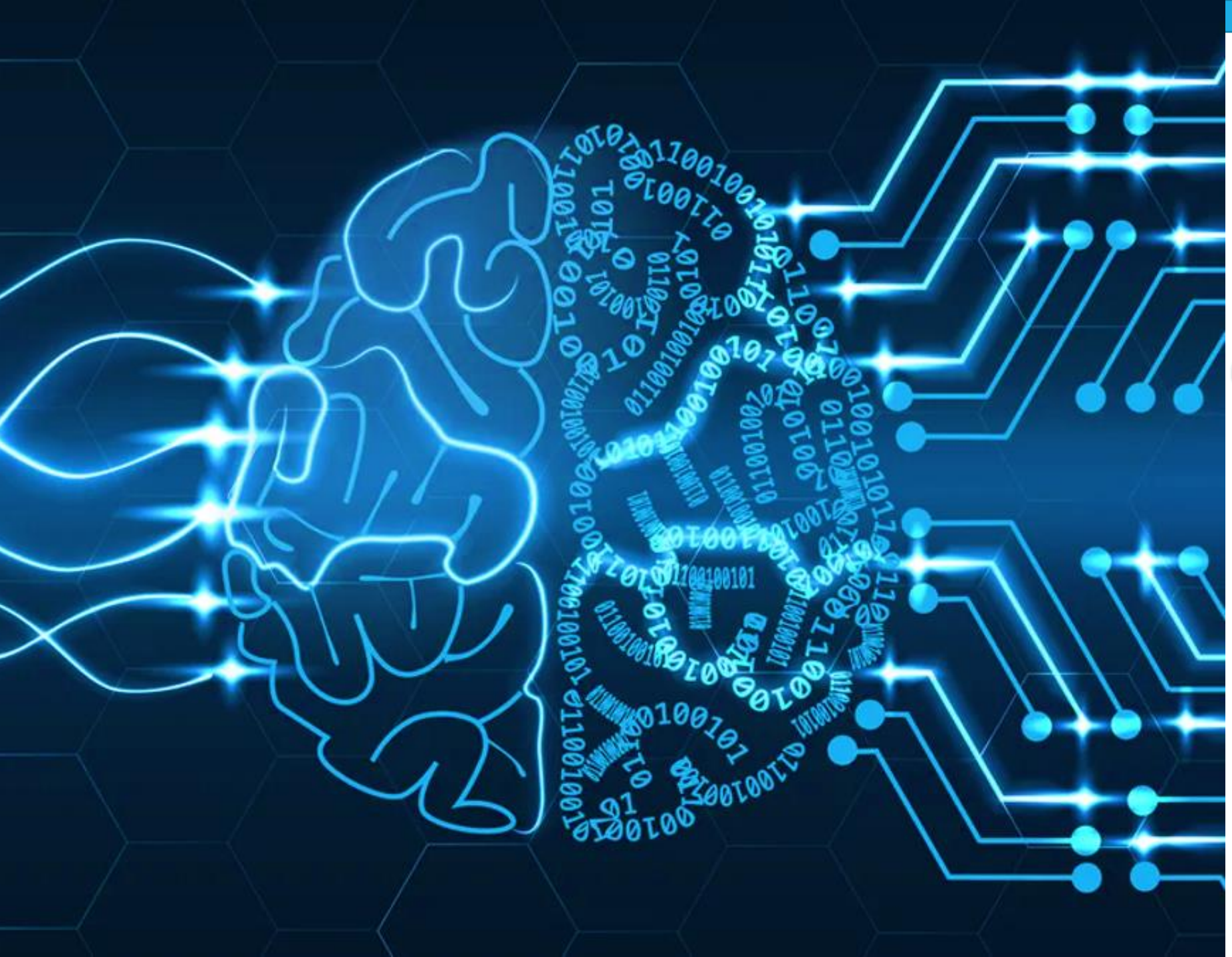


یادگیری بدون نظارت

اردیبهشت ۱۴۰۲

دانشکده مهندسی صنایع

دانشگاه صنعتی شریف

دکتر مهدی شریف‌زاده

رضا الوندی


بسم الله الرحمن الرحیم

Unsupervised Learning

Although most of the applications of Machine Learning today are based on supervised learning (and as a result, this is where most of the investments go to), the vast majority of the available data is unlabeled: we have the input features X, but we do not have the labels y. The computer scientist **Yann LeCun** famously said that “if intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake.” In other words, there is a huge potential in unsupervised learning that we have only barely started to sink our teeth into.

Unsupervised Learning

Say you want to create a system that will take a few pictures of each item on a **manufacturing production** line and detect which items are **defective**. You can fairly easily create a system that will take pictures automatically, and this might give you thousands of pictures every day. You can then build a reasonably large dataset in just a few weeks. But wait, there are no labels! If you want to train a regular binary classifier that will predict whether an item is defective or not, you will need to label every single picture as “defective” or “normal.” This will generally require human experts to sit down and manually go through all the pictures. This is a **long, costly, and tedious task**, so it will usually only be done on a small subset of the available pictures.

Unsupervised Learning

As a result, the labeled dataset will be quite small, and the classifier's performance will be disappointing. Moreover, every time the company **makes any change to** its products, the whole process will need to be started over from scratch. Wouldn't it be great if the algorithm could just exploit the unlabeled data without needing humans to label every picture? Enter unsupervised learning.

Unsupervised Learning

In Chapter 8 we looked at the most common unsupervised learning task: **dimensionality reduction**. In this chapter we will look at a few more unsupervised learning tasks and algorithms:

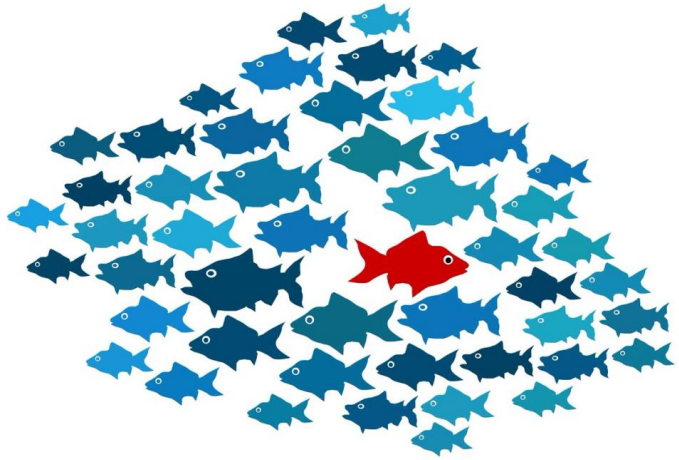
Clustering

The goal is to **group similar instances together** into clusters. Clustering is a great tool for **data analysis, customer segmentation, recommender systems, search engines, image segmentation, semi-supervised learning, dimensionality reduction**, and more.

Unsupervised Learning

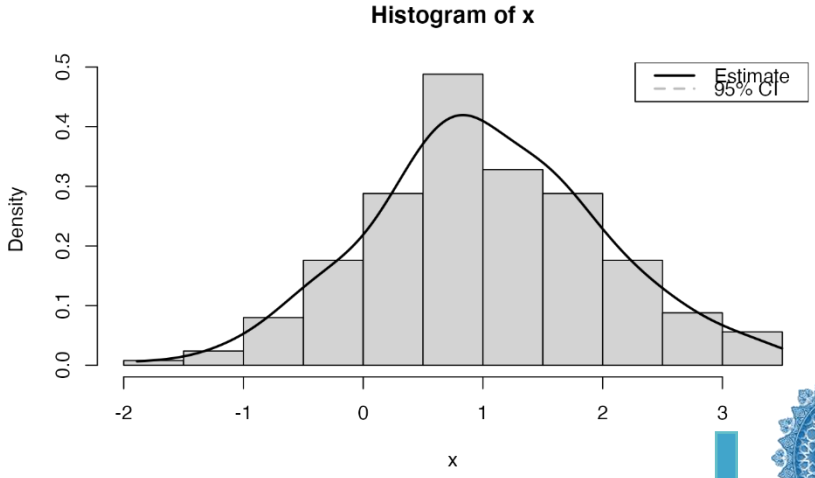
Anomaly detection

The objective is to learn what **“normal”** data looks like, and then use that to detect **abnormal** instances, such as defective items on a production line or a new trend in a time series.



Density estimation

This is the task of estimating the probability density function (PDF) of the random process that generated the dataset. Density estimation is commonly used for **anomaly detection**: instances located in very low-density regions are likely to be anomalies. It is also useful for data analysis and visualization.



Clustering

As you enjoy a hike in the mountains, you **stumble upon a plant** you have never seen before. You look around and you **notice a few more**. They are **not identical**, yet they are **sufficiently similar** for you to know that they most likely belong to the same species (or at least the same genus). You may need a botanist to tell you what species that is, but you certainly don't need an expert to identify groups of similar-looking objects. This is called **clustering:** it is the task of identifying similar instances and assigning them to clusters, or groups of similar instances.

Clustering

Just like in classification, each instance gets assigned to a group. However, unlike classification, clustering is an unsupervised task. Consider Figure 9-1: on the left is the iris dataset (introduced in Chapter 4), where each instance's species (i.e., its class) is represented with a different marker. It is a labeled dataset, for which classification algorithms such as Logistic Regression, SVMs, or Random Forest classifiers are well suited. On the right is the same dataset, but without the labels, so you cannot use a classification algorithm anymore.

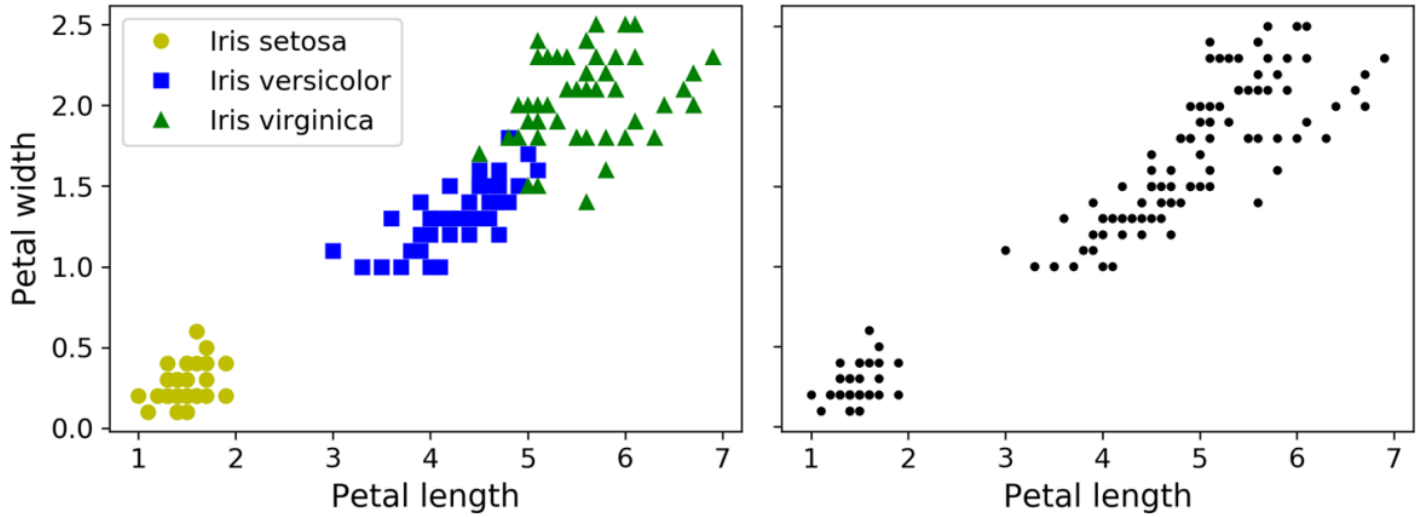


Figure 9-1. Classification (left) versus clustering (right)

Clustering

This is where clustering algorithms step in: many of them can easily detect the lower-left cluster. It is also quite easy to see with our own eyes, but it is not so obvious that the upper-right cluster is composed of two distinct sub-clusters. That said, the dataset has two additional features (sepal length and width), not represented here, and clustering algorithms can make good use of all features, so in fact they identify the three clusters fairly well (e.g., using a Gaussian mixture model, only 5 instances out of 150 are assigned to the wrong cluster).

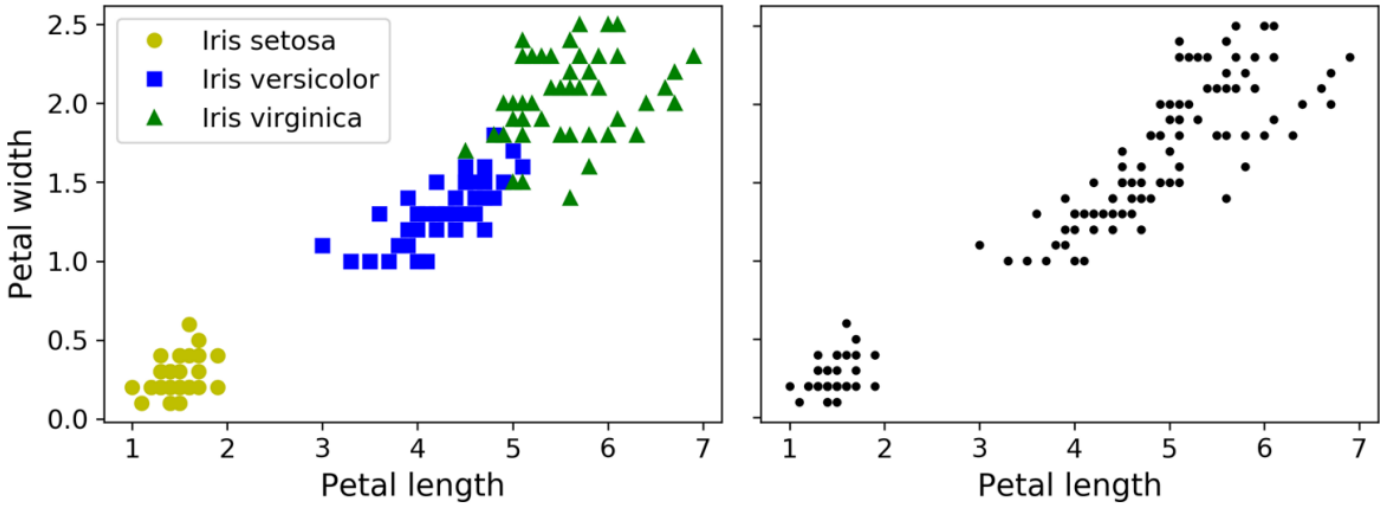


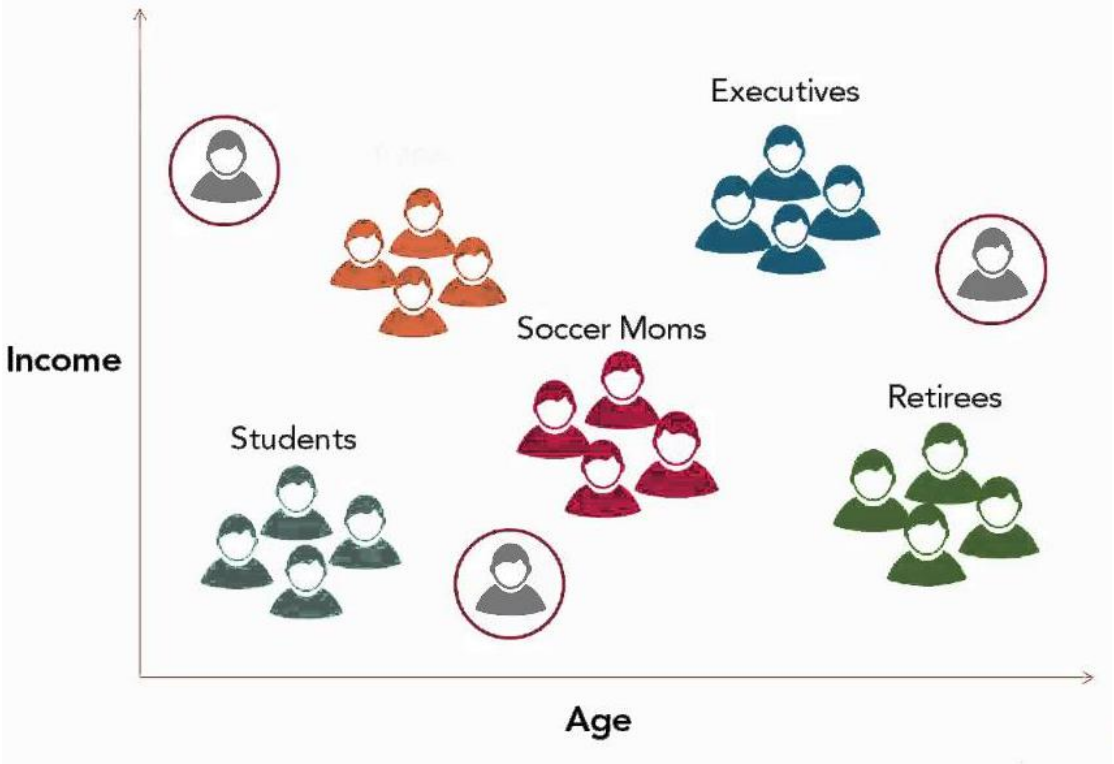
Figure 9-1. Classification (left) versus clustering (right)

Clustering usage

Clustering is used in a wide variety of applications, including these:

For customer segmentation

You can cluster your customers based on their purchases and their activity on your website. This is useful to understand who your customers are and what they need, so you can adapt your products and marketing campaigns to each segment. For example, customer segmentation can be useful in **recommender systems** to suggest content that other users in the same cluster enjoyed.



Clustering usage

For data analysis

When you analyze a new dataset, it can be helpful to run a clustering algorithm, and then analyze each cluster separately.

As a dimensionality reduction technique

Once a dataset has been clustered, it is usually possible to measure each **instance's affinity** with each cluster (affinity is any measure of how well an instance fits into a cluster). Each instance's feature vector x can then be replaced with the **vector of its cluster affinities**. If there are k clusters, then this vector is k-dimensional. This vector is typically much lower-dimensional than the original feature vector, but it can preserve enough information for further processing.

Clustering usage

For 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. This technique can greatly increase the number of labels available for a subsequent supervised learning algorithm, and thus improve its performance.

For anomaly detection (also called outlier detection)

Any instance that has a low affinity to all the clusters is likely to be an **anomaly**. For example, if you have clustered the users of your website based on their behavior, you can detect users with unusual behavior, such as an unusual number of requests per second. Anomaly detection is particularly useful in detecting defects in manufacturing, or for fraud detection.

Clustering usage

For search engines

Some search engines let you search for images that are similar to a reference image. To build such a system, you would first apply a clustering algorithm to all the images in your database; similar images would end up in the same cluster. Then when a user provides a reference image, all you need to do is use the trained clustering model to find this image's cluster, and you can then simply return all the images from this cluster.

To segment an image

By clustering pixels according to their color, then replacing each pixel's color with the mean color of its cluster, it is possible to considerably reduce the number of different colors in the image. **Image segmentation** is used in many object detection and tracking systems, as it makes it easier to detect the contour of each object.

Clustering usage

There is no universal definition of what a cluster is: it really depends on the context, and different algorithms will capture different kinds of clusters. Some algorithms look for instances **centered around a particular point**, called **a centroid**. Others look for **continuous regions of densely packed instances**: these clusters can take on any shape. Some algorithms are hierarchical, looking for clusters of clusters. And the list goes on. In this section, we will look at two popular clustering algorithms, **KMeans** and **DBSCAN,** and explore some of their applications, such as nonlinear dimensionality reduction, semi-supervised learning, and anomaly detection.

K-Means

Consider the unlabeled dataset represented in Figure 9-2: you can clearly see five blobs of instances. The K-Means algorithm is a simple algorithm capable of clustering this kind of dataset very quickly and efficiently, often in just a few iterations. It was proposed by **Stuart Lloyd** at **Bell Labs** in 1957 as a technique for pulse-code modulation, but it was only published outside of the company in 1982. In 1965, Edward W. Forgy had published virtually the same algorithm, so K-Means is sometimes referred to as **Lloyd–Forgy**.

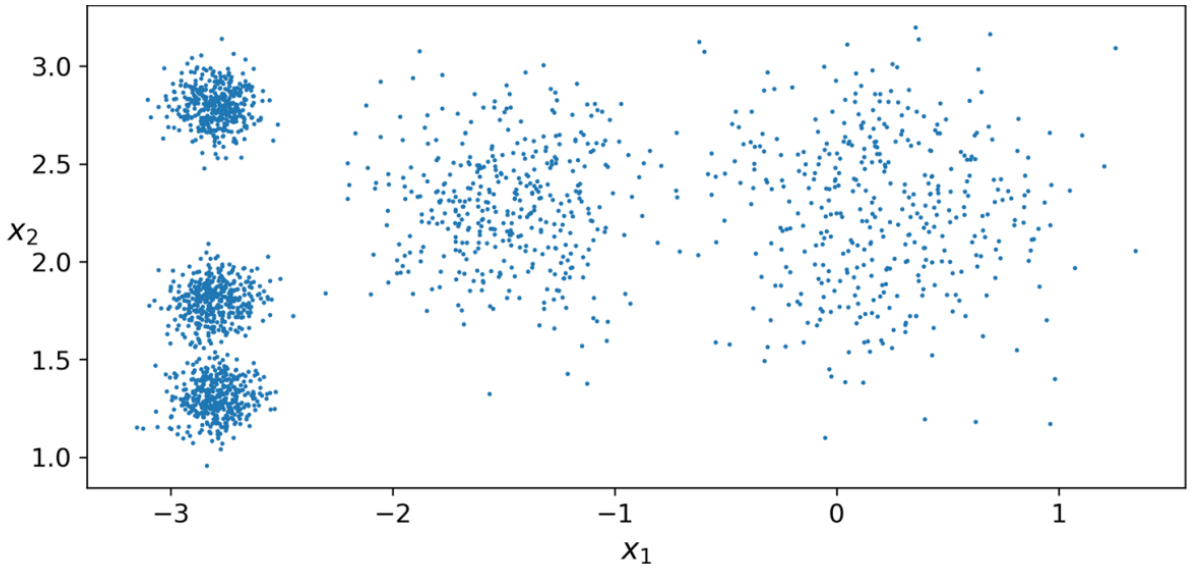


Figure 9-2. An unlabeled dataset composed of five blobs of instances

K-Means

Let’s train a K-Means clusterer on this dataset. It will try to find each blob’s center and assign each instance to the closest blob:

```
from sklearn.cluster import KMeans
k = 5
kmeans = KMeans(n_clusters=k)
y_pred = kmeans.fit_predict(X)
```

Note that you have to specify the number of clusters k that the algorithm must find. In this example, it is pretty obvious from looking at the data that k should be set to 5, but in general it is not that easy. We will discuss this shortly.

K-Means

Each instance was assigned to one of the five clusters. In the context of clustering, an instance's label is the index of the cluster that this instance gets assigned to by the algorithm: this is not to be confused with the class labels in classification (remember that clustering is an unsupervised learning task). The KMeans instance preserves a copy of the labels of the instances it was trained on, available via the labels_ instance variable:

```
>>> y_pred
array([4, 0, 1, ..., 2, 1, 0], dtype=int32)
>>> y_pred is kmeans.labels_
True
```

K-Means

We can also take a look at the five 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]])
```

You can easily assign new instances to the cluster whose centroid is closest:

```
>>> X_new = np.array([[0, 2], [3, 2], [-3, 3], [-3, 2.5]])
>>> kmeans.predict(X_new)
array([1, 1, 2, 2], dtype=int32)
```

K-Means

If you plot the cluster's decision boundaries, you get a Voronoi tessellation (see Figure 9-3, where each centroid is represented with an X).

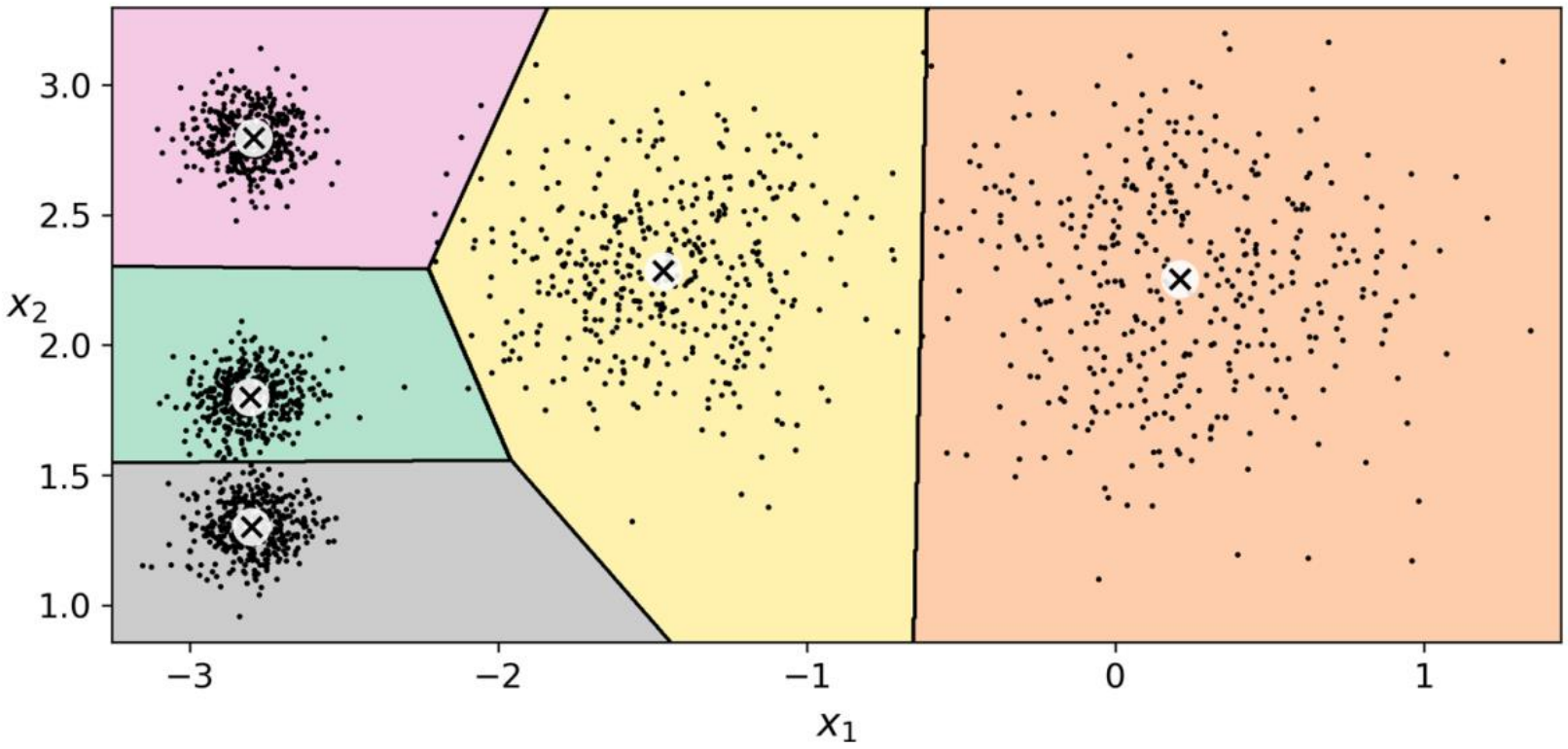


Figure 9-3. K-Means decision boundaries (Voronoi tessellation)

K-Means

The vast majority of the instances were clearly assigned to the appropriate cluster, but a few instances were probably mislabeled (especially near the boundary between the top-left cluster and the central cluster). Indeed, the K-Means algorithm does not behave very well when the blobs have very different diameters because all it cares about when assigning an instance to a cluster is the distance to the centroid.

Instead of assigning each instance to a single cluster, which is called **hard clustering,** it can be useful to give each instance a score per cluster, which is called **soft clustering**. The score can be the distance between the instance and the centroid; conversely, it can be a similarity score (or affinity), such as the Gaussian Radial Basis Function (introduced in Chapter 5). In the KMeans class, the transform() method measures the distance from each instance to every centroid:

K-Means

```
>>> kmeans.transform(X_new)
array([[2.81093633, 0.32995317, 2.9042344 , 1.49439034, 2.88633901],
       [5.80730058, 2.80290755, 5.84739223, 4.4759332 , 5.84236351],
       [1.21475352, 3.29399768, 0.29040966, 1.69136631, 1.71086031],
       [0.72581411, 3.21806371, 0.36159148, 1.54808703, 1.21567622]])
```

In this example, the first instance in **X_new** is located at a distance of 2.81 from the first centroid, 0.33 from the second centroid, 2.90 from the third centroid, 1.49 from the fourth centroid, and 2.89 from the fifth centroid. If you have a high-dimensional dataset and you transform it this way, you end up with a k-dimensional dataset: this transformation can be a very efficient **nonlinear dimensionality reduction technique**.

The K-Means algorithm

So, how does the algorithm work? Well, suppose you were given the centroids. You could easily label all the instances in the dataset by assigning each of them to the cluster whose centroid is closest. Conversely, if you were given all the instance labels, you could easily locate all the centroids by computing the mean of the instances for each cluster. But you are given neither the labels nor the centroids, so how can you proceed? Well, just start by placing the centroids randomly (e.g., by picking k instances at random and using their locations as centroids). Then label the instances, update the centroids, label the instances, update the centroids, and so on until the centroids stop moving. The algorithm is guaranteed to converge in a finite number of steps (usually quite small); it will not oscillate forever.

The K-Means algorithm

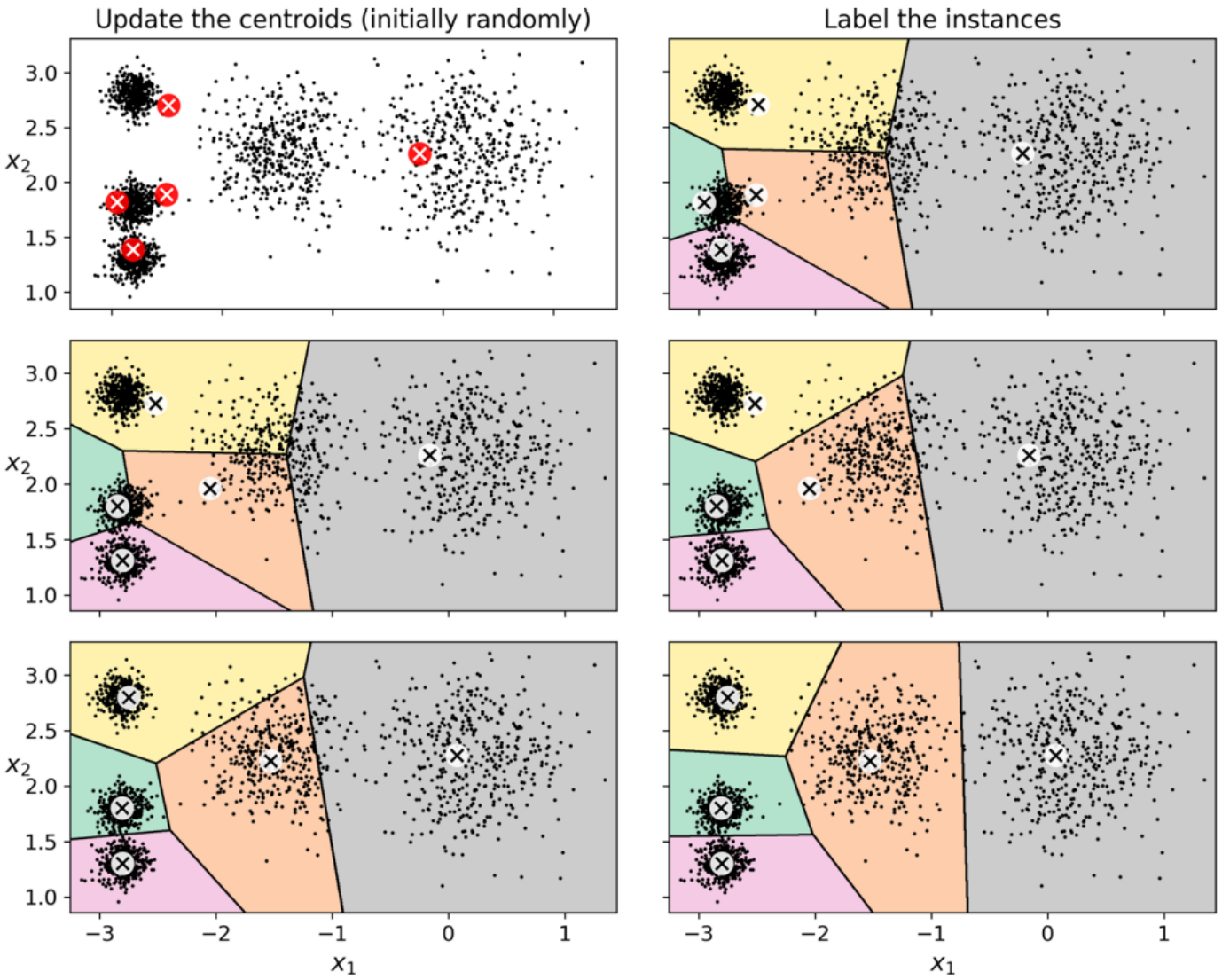
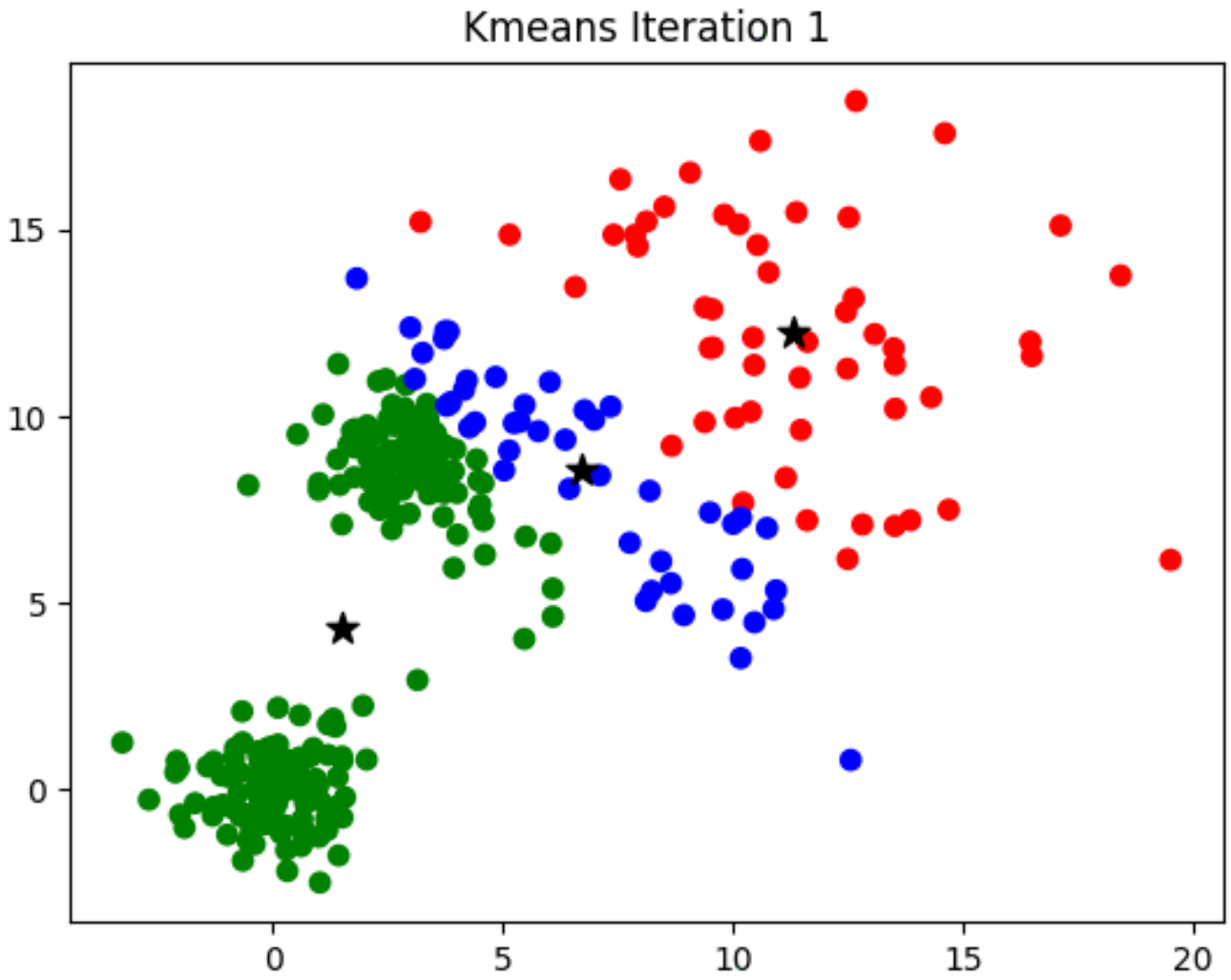


Figure 9-4. The K-Means algorithm

You can see the algorithm in action in Figure 9-4: the centroids are initialized randomly (top left), then the instances are labeled (top right), then the centroids are updated (center left), the instances are relabeled (center right), and so on. As you can see, in just **three iterations**, the algorithm has reached a clustering that seems close to optimal.

The K-Means algorithm



The K-Means algorithm

Although the algorithm is guaranteed to converge, it may not converge to the right solution (i.e., it may converge to a local optimum): whether it does or not depends on the **centroid initialization**. Figure 9-5 shows two suboptimal solutions that the algorithm can converge to if you are not lucky with the random initialization step.

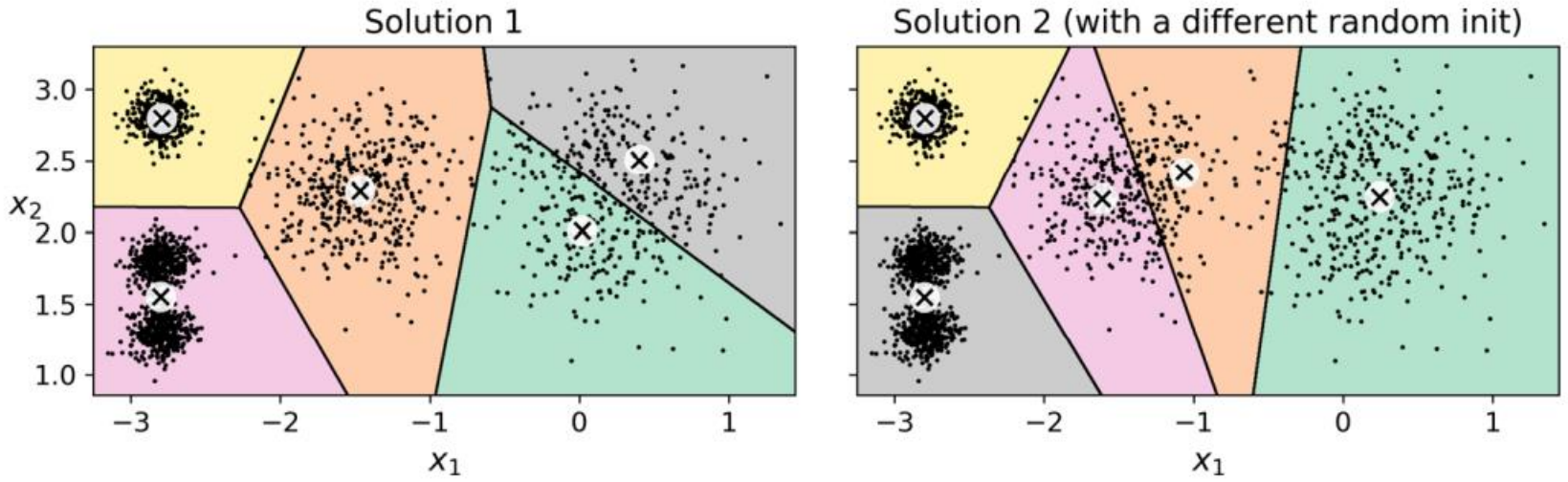


Figure 9-5. Suboptimal solutions due to unlucky centroid initializations

Centroid initialization methods

Let's look at a few ways you can mitigate this risk by improving the centroid initialization.

If you happen to **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, and set n_init to 1:

```
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)
```

Centroid initialization methods

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** hyperparameter: by default, it is equal to 10, which means that the whole algorithm described earlier runs 10 times when you call **fit()**, and Scikit-Learn keeps the best solution.

But how exactly does it know which solution is the best? It uses a performance metric! That metric is called the model's **inertia**, which is the **mean squared distance** between each instance and its closest centroid. It is roughly equal to 223.3 for the model on the left in Figure 9-5, 237.5 for the model on the right in Figure 9-5, and 211.6 for the model in Figure 9- 3.

Centroid initialization methods

The KMeans class runs the algorithm **n_init** times and keeps the model with the lowest inertia. In this example, the model in Figure 9-3 will be selected (unless we are very unlucky with **n_init** consecutive random initializations). If you are curious, a model's inertia is accessible via the **inertia_** instance variable:

```
>>> kmeans.inertia_
211.59853725816856
```

Centroid initialization methods

An important improvement to the K-Means algorithm, **K-Means++,** was proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii. They introduced a smarter initialization step that tends to select centroids that are distant from one another, and this improvement makes the K-Means algorithm much less likely to converge to a suboptimal solution. They showed that the additional computation required for the smarter initialization step is well worth it because it makes it possible to drastically reduce the number of times the algorithm needs to be run to find the optimal solution. Next slide shows the K-Means++ initialization algorithm:

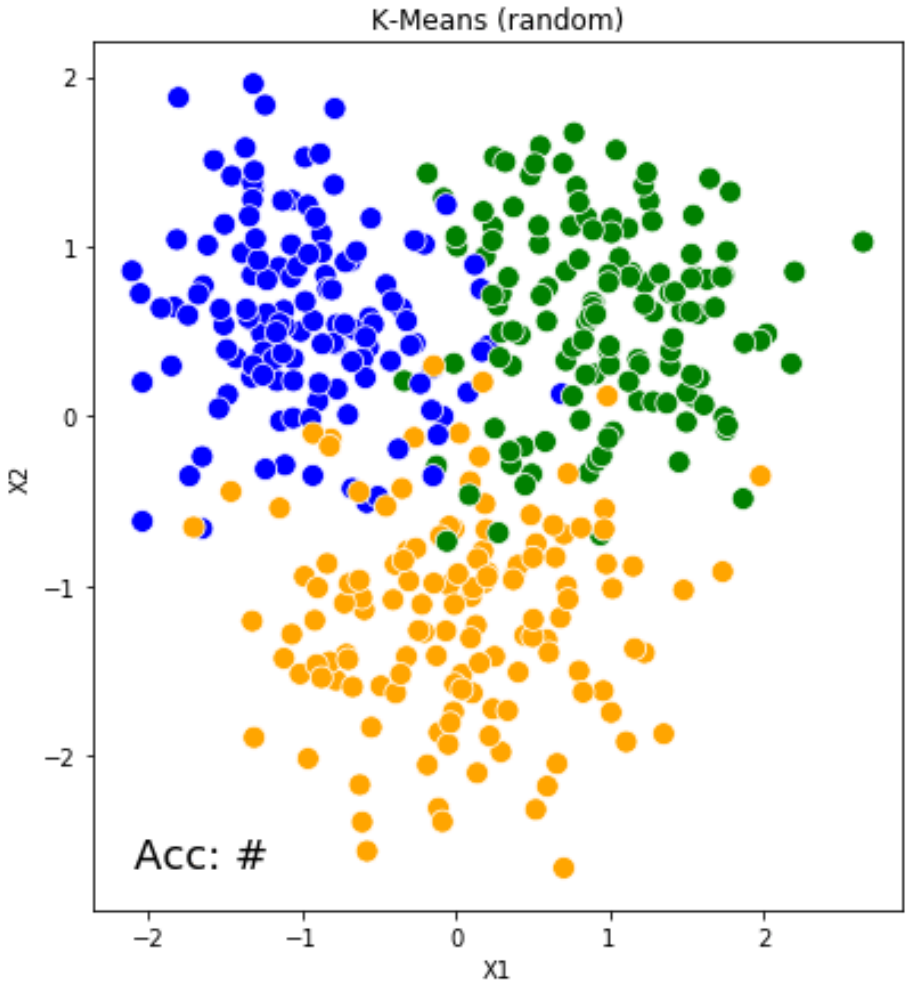
Centroid initialization methods

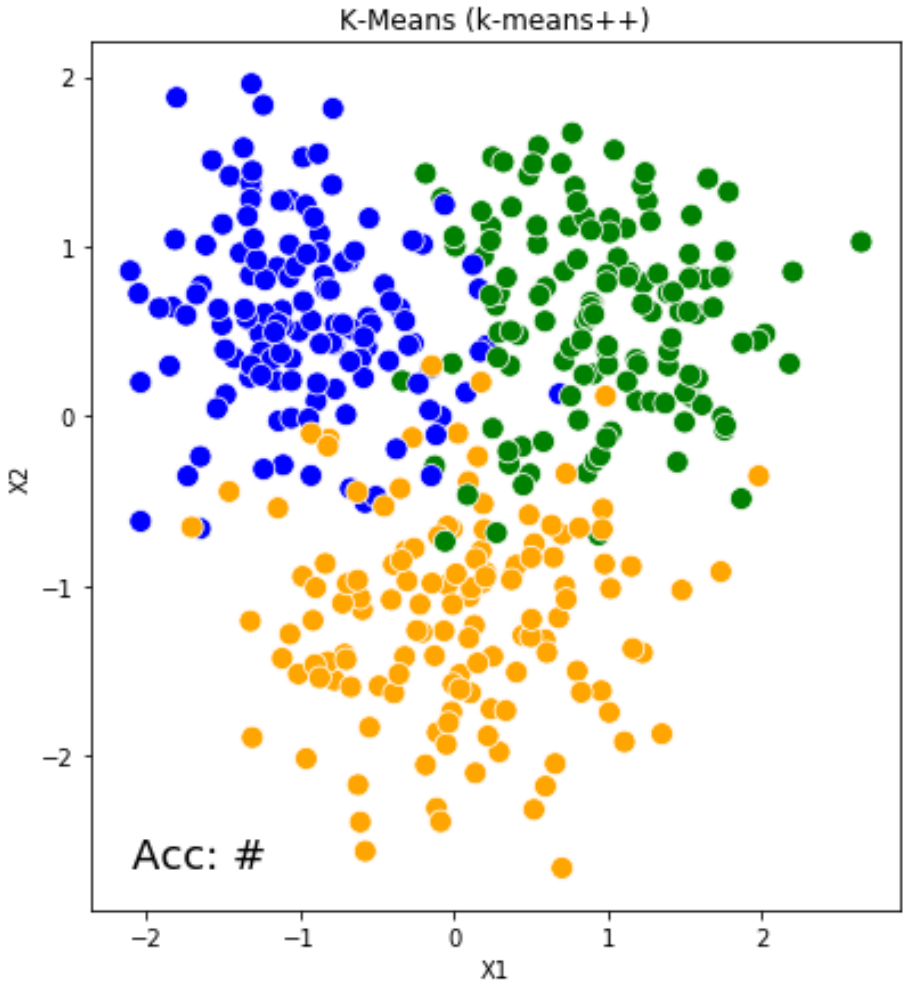
1. Take one centroid $\mathbf{c}^{(1)}$, chosen uniformly at random from the dataset.

2. Take a new centroid $\mathbf{c}^{(i)}$, choosing an instance $\mathbf{x}^{(i)}$ with probability $D\left(\mathbf{x}^{(i)}\right)^2 / \sum_{j=1}^{m} D\left(\mathbf{x}^{(j)}\right)^2$, where $D(\mathbf{x}^{(i)})$ is the distance between the instance $\mathbf{x}^{(i)}$ and the closest centroid that was already chosen. This probability distribution ensures that instances farther away from already chosen centroids are much more likely be selected as centroids.

3. Repeat the previous step until all k centroids have been chosen.

Centroid initialization methods





Centroid initialization methods

The KMeans class uses this initialization method by default. If you want to force it to use the original method (i.e., picking k instances randomly to define the initial centroids), then you can set the **init** hyperparameter to "random". You will rarely need to do this.

Accelerated K-Means and mini-batch K-Means

Another important improvement to the K-Means algorithm was proposed in a 2003 paper by Charles Elkan. It considerably accelerates the algorithm by avoiding many unnecessary distance calculations. Elkan achieved this by exploiting the **triangle inequality** (i.e., that a straight line is always the shortest distance between two points) and by keeping track of lower and upper bounds for distances between instances and centroids. This is the algorithm the KMeans class uses by default (you can force it to use the original algorithm by setting the algorithm hyperparameter to "full", although you probably will never need to).

Accelerated K-Means and mini-batch K-Means

Yet another important variant of the K-Means algorithm was proposed in a 2010 paper by David Sculley. 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 or four and makes it possible to cluster huge datasets that do not fit in memory. Scikit-Learn implements this algorithm in the **MiniBatchKMeans** class. You can just use this class like the KMeans class:

```
from sklearn.cluster import MiniBatchKMeans

minibatch_kmeans = MiniBatchKMeans(n_clusters=5)
minibatch_kmeans.fit(X)
```

Accelerated K-Means and mini-batch K-Means

If the dataset does not fit in memory, the simplest option is to use the **memmap** class, as we did for incremental PCA in Chapter 8. Alternatively, you can pass one mini-batch at a time to the **partial_fit()** method, but this will require much more work, since you will need to perform multiple initializations and select the best one yourself (see the mini-batch KMeans section of the notebook for an example).
Although the Mini-batch K-Means algorithm is much faster than the regular K-Means algorithm, its inertia is generally slightly worse, especially as the number of clusters increases. You can see this in Figure 9-6: the plot on the left compares the inertias of Mini-batch KMeans and regular K-Means models trained on the previous dataset using 4 5 6 various numbers of clusters k.

Accelerated K-Means and mini-batch K-Means

The difference between the two curves remains fairly constant, but this difference becomes more and more significant as k increases, since the inertia becomes smaller and smaller. In the plot on the right, you can see that Mini-batch K-Means is much faster than regular K-Means, and this difference increases with k.

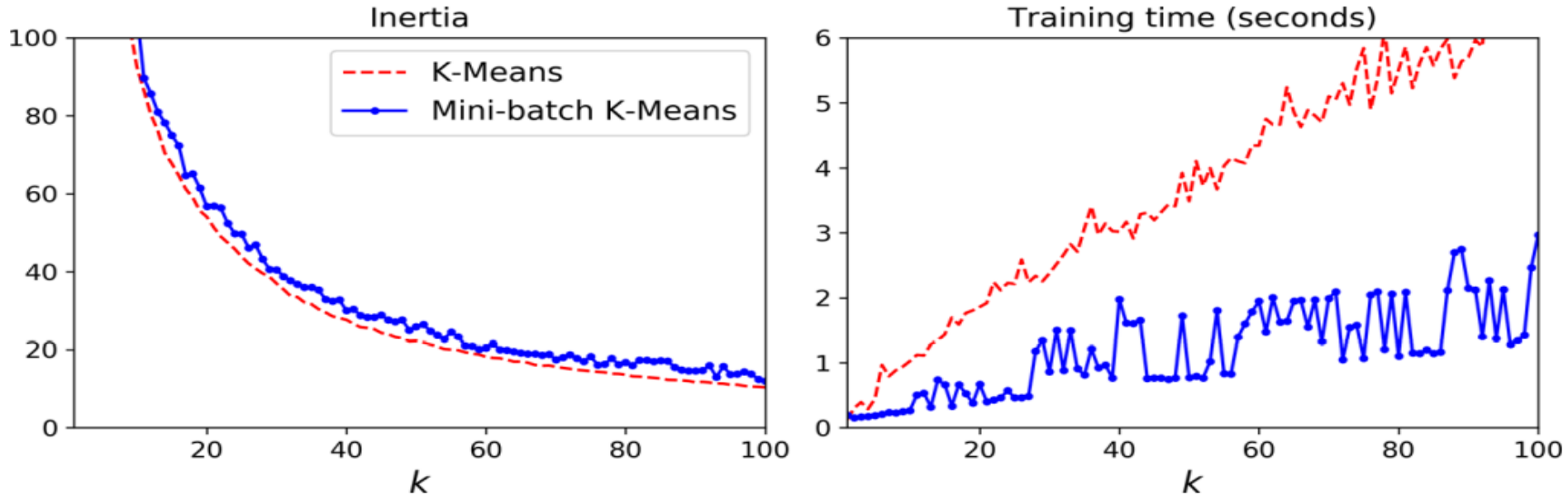


Figure 9-6. Mini-batch K-Means has a higher inertia than K-Means (left) but it is much faster (right), especially as k increases

Finding the optimal number of clusters

So far, we have set the number of clusters k to 5 because it was obvious by looking at the data that this was the correct number of clusters. But in general, it will not be so easy to know how to set k, and the result might be quite bad if you set it to the wrong value. As you can see in Figure 9-7, setting k to 3 or 8 results in fairly bad models.

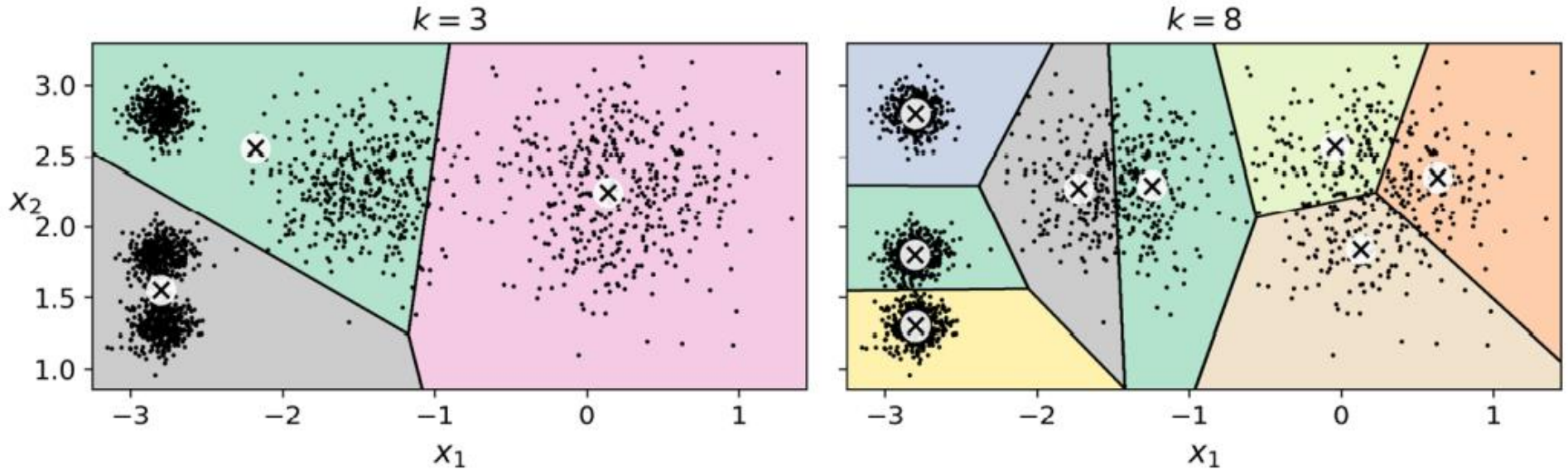


Figure 9-7. Bad choices for the number of clusters: when k is too small, separate clusters get merged (left), and when k is too large, some clusters get chopped into multiple pieces (right)

Finding the optimal number of clusters

You might be thinking that we could just pick the model with the lowest inertia, right? Unfortunately, it is not that simple. The inertia for k=3 is 653.2, which is much higher than for k=5 (which was 211.6). But with k=8, the inertia is just 119.1.

The inertia is not a good performance metric when trying to choose k because it keeps getting lower as we increase k. Indeed, the more clusters there are, the closer each instance will be to its closest centroid, and therefore the lower the inertia will be. Let's plot the inertia as a function of k (see Figure 9-8).

Finding the optimal number of clusters

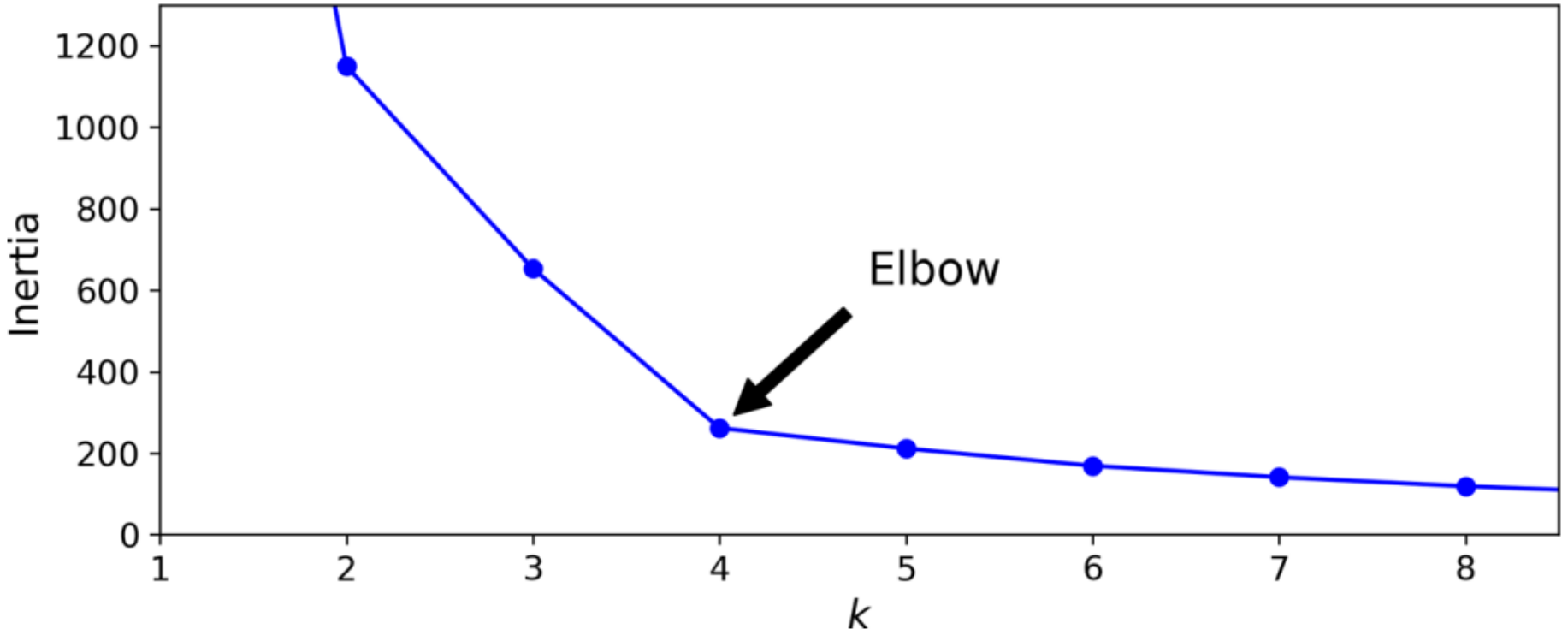


Figure 9-8. When plotting the inertia as a function of the number of clusters k, the curve often contains an inflexion point called the "elbow"

Finding the optimal number of clusters

As you can see, the inertia drops very quickly as we increase k up to 4, but then it decreases much more slowly as we keep increasing k. This curve has roughly the shape of an arm, and there is an **“elbow”** at k = 4. So, if we did not know better, 4 would be a good choice: any lower value would be dramatic, while any higher value would not help much, and we might just be splitting perfectly good clusters in half for no good reason.

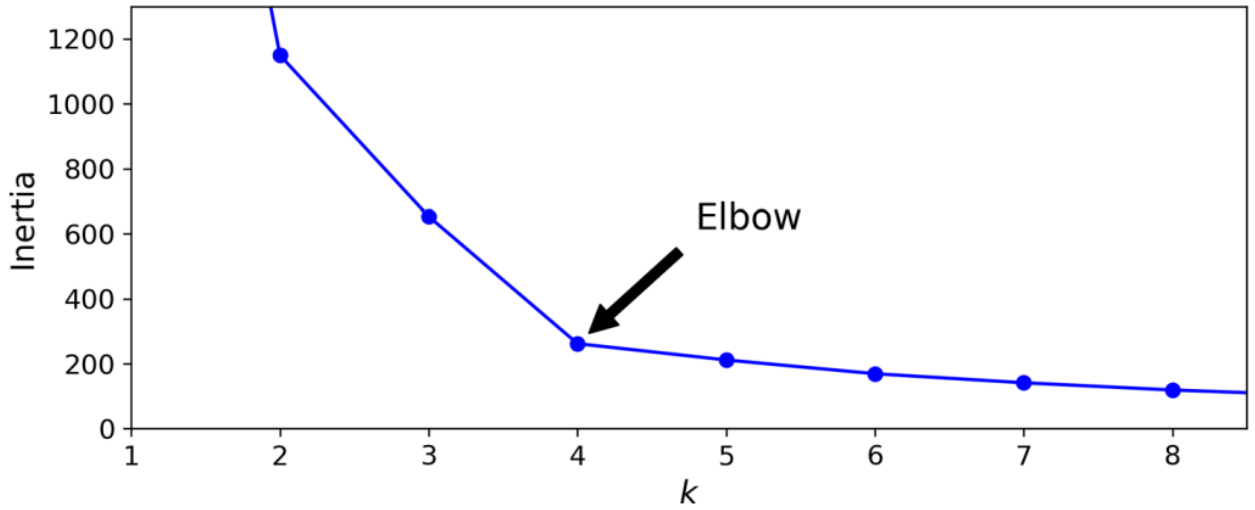


Figure 9-8. When plotting the inertia as a function of the number of clusters k, the curve often contains an inflexion point called the “elbow”

Finding the optimal number of clusters

This technique for choosing the best value for the number of clusters is rather coarse. A more precise approach (but also more computationally expensive) is to use the **silhouette score**, which is the mean silhouette coefficient over all the instances. An instance's silhouette coefficient is equal to $\frac{b-a}{\max(a,b)}$ where a is the mean distance to the other instances in the same cluster (i.e., the mean intra-cluster distance) and b is the mean nearest-cluster distance (i.e., the mean distance to the instances of the next closest cluster, defined as the one that minimizes b, excluding the instance's own cluster). 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, while a coefficient close to 0 means that it is close to a cluster boundary, and finally a coefficient close to –1 means that the instance may have been assigned to the wrong cluster.

Finding the optimal number of clusters

To compute the 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
```

Let's compare the silhouette scores for different numbers of clusters (see Figure 9-9).

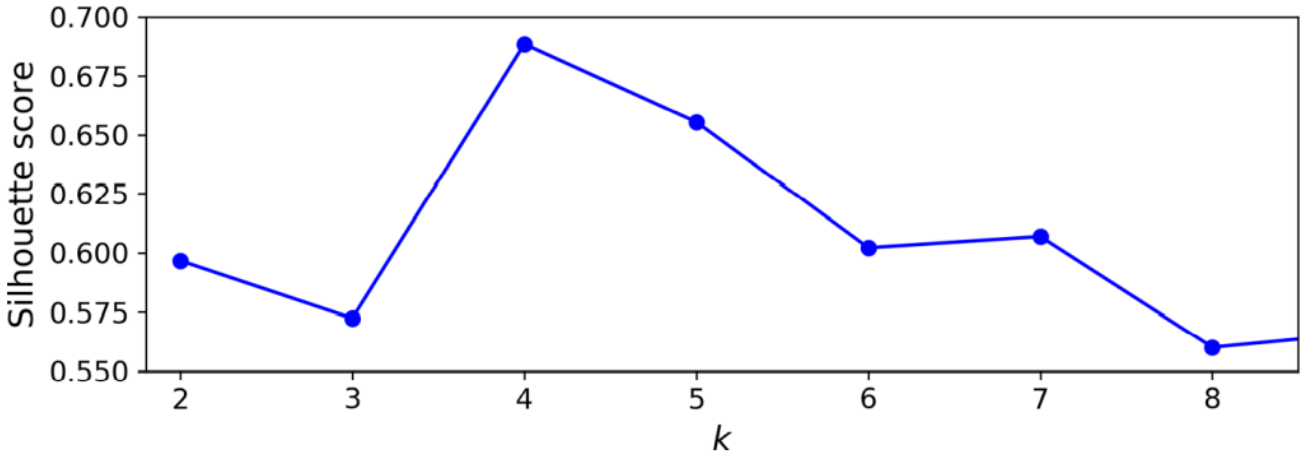


Figure 9-9. Selecting the number of clusters k using the silhouette score

Finding the optimal number of clusters

As you can see, this visualization is much richer than the previous one: although it confirms that k = 4 is a very good choice, it also underlines the fact that k = 5 is quite good as well, and much better than k = 6 or 7. This was not visible when comparing inertias.

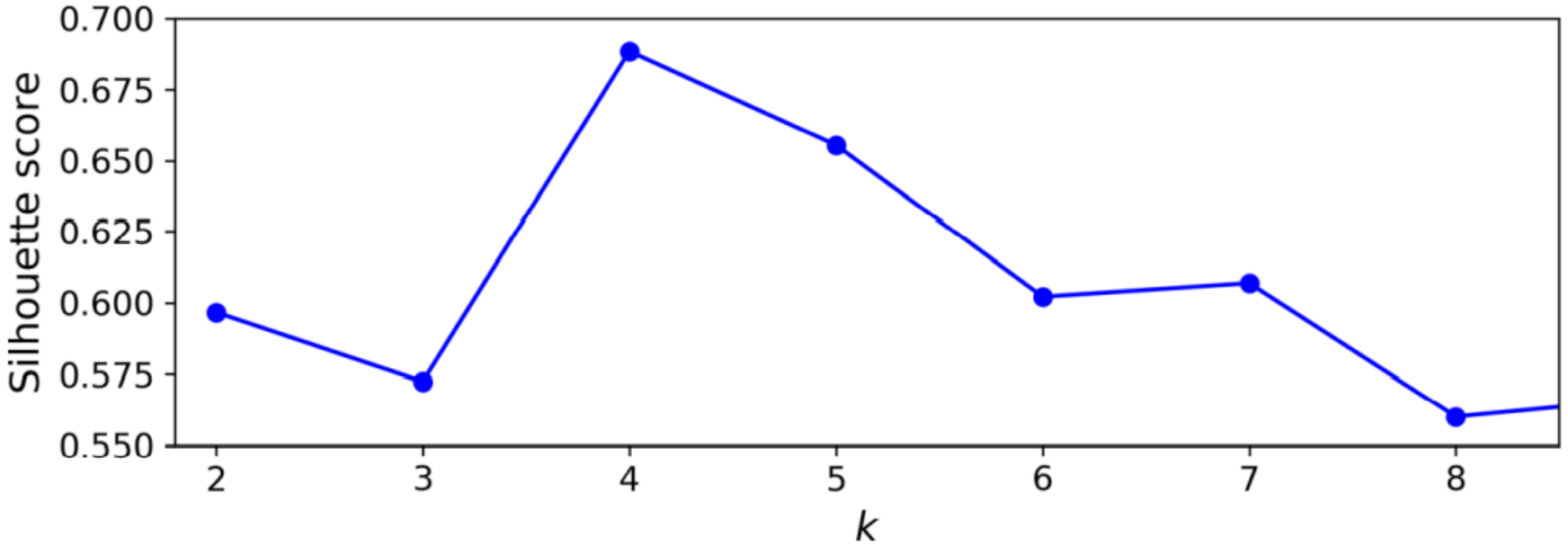


Figure 9-9. Selecting the number of clusters k using the silhouette score

Finding the optimal number of clusters

The vertical dashed lines represent the **silhouette score** for each number of clusters. When most of the instances in a cluster have a lower coefficient than this score (i.e., if many of the instances stop short of the dashed line, ending to the left of it), then the cluster is rather bad since this means its instances are much too close to other clusters. We can see that when k = 3 and when k = 6, we get bad clusters. But when k = 4 or k = 5, the clusters look pretty good: most instances extend beyond the dashed line, to the right and closer to 1.0. When k = 4, the cluster at index 1 (the third from the top) is rather big. When k = 5, all clusters have similar sizes. So, even though the overall silhouette score from k = 4 is slightly greater than for k = 5, it seems like a good idea to use k = 5 to get clusters of similar sizes.

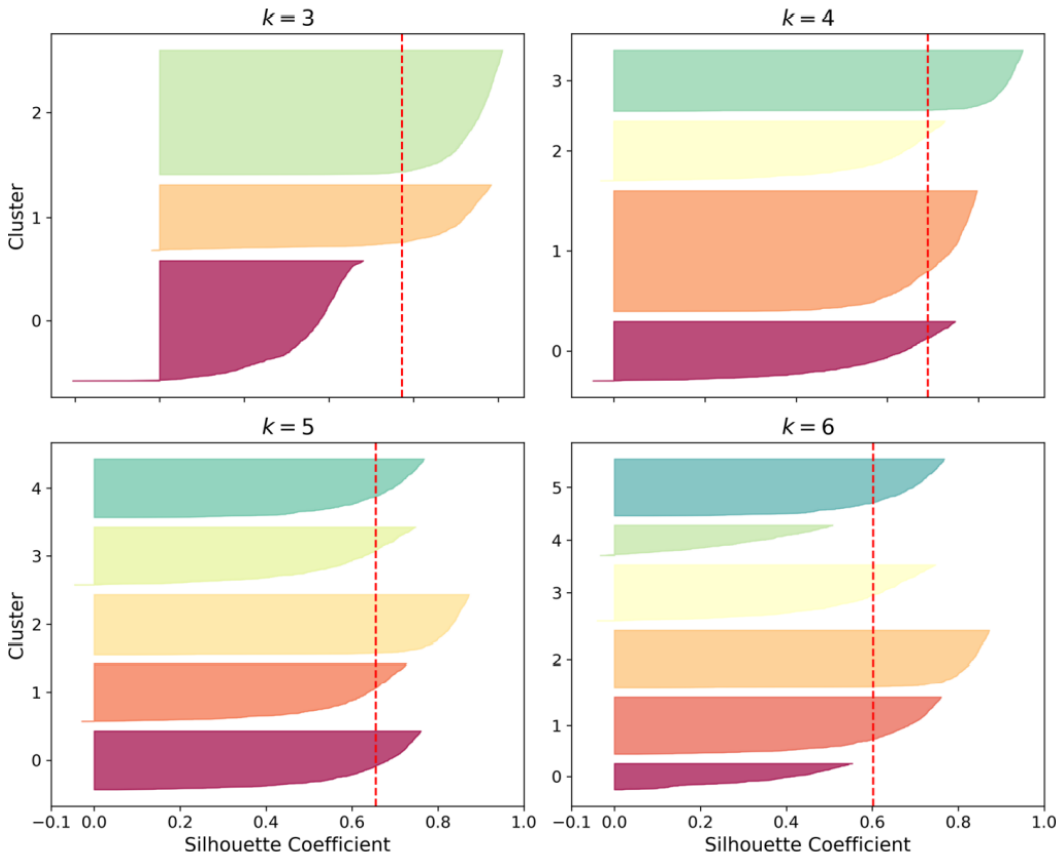


Figure 9-10. Analyzing the silhouette diagrams for various values of k

Limits of K-Means

Despite its many merits, most notably **being fast and scalable,** K-Means is not perfect. As we saw, it is necessary to run the algorithm **several times** to avoid suboptimal solutions, plus you need to specify the number of clusters, which can be quite a hassle. Moreover, K-Means does not behave very well when the clusters **have varying sizes**, **different densities, or non-spherical shapes**. For example, Figure 9-11 shows how K-Means clusters a dataset containing three ellipsoidal clusters of different dimensions, densities, and orientations.

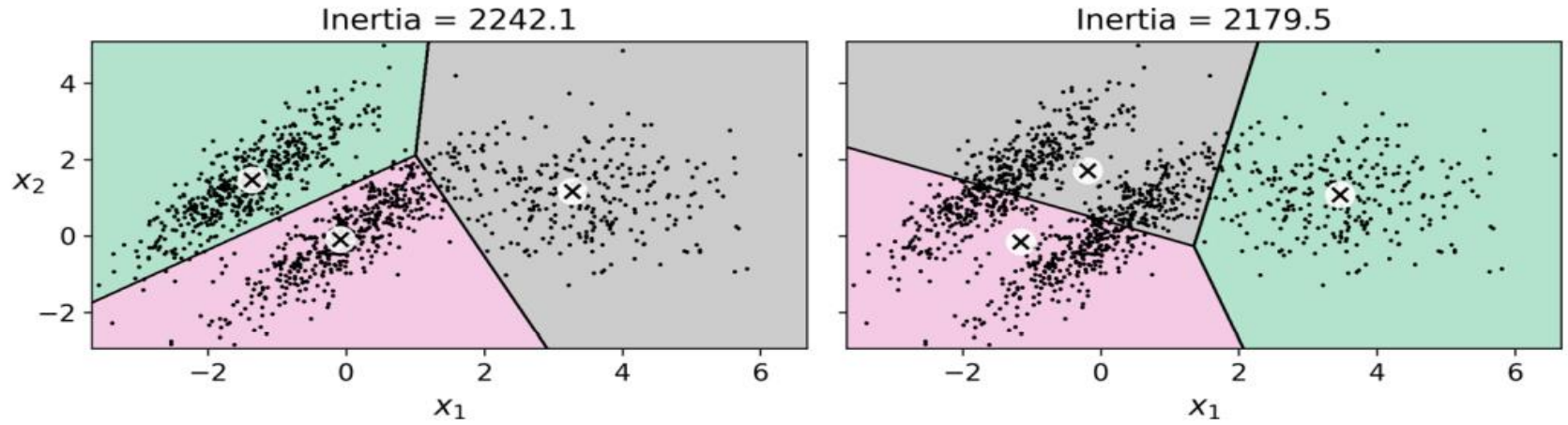


Figure 9-11. K-Means fails to cluster these ellipsoidal blobs properly

Limits of K-Means

As you can see, neither of these solutions is any good. The solution on the left is better, but it still chops off 25% of the middle cluster and assigns it to the cluster on the right. The solution on the right is just terrible, even though its inertia is lower. So, depending on the data, different clustering algorithms may perform better. On these types of elliptical clusters, Gaussian mixture models work great.

TIP:

It is important to scale the input features before you run K-Means, or the clusters may be very stretched and K-Means will perform poorly. Scaling the features does not guarantee that all the clusters will be nice and spherical, but it generally improves things.

Using Clustering for Image Segmentation

Now let’s look at a few ways we can benefit from clustering. We will use K-Means, but feel free to experiment with other clustering algorithms.

Using Clustering for Image Segmentation

Image segmentation is the task of partitioning an image into multiple segments. In **semantic segmentation**, all pixels that are part of the same object type get assigned to the same segment. For example, in a self-driving car's vision system, all pixels that are part of a pedestrian's image might be assigned to the "pedestrian" segment (there would be one segment containing all the pedestrians). In **instance segmentation,** all pixels that are part of the same individual object are assigned to the same segment. In this case there would be a different segment for each pedestrian.

Using Clustering for Image Segmentation

The state of the art in semantic or instance segmentation today is achieved using complex architectures based on convolutional neural networks. Here, we are going to do something much simpler: color segmentation. We will simply assign pixels to the same segment if they have a similar color. In some applications, this may be sufficient. For example, if you want to analyze satellite images to measure how much total forest area there is in a region, color segmentation may be just fine.

Using Clustering for Image Segmentation

First, use Matplotlib's **imread()** function to load the image (see the upper-left image in Figure 9-12):

```
>>> from matplotlib.image import imread  # or `from imageio import
imread`
>>> image =
imread(os.path.join("images","unsupervised_learning","ladybug.png"))

>>> 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; and the third is the number of color channels, in this case red, green, and blue (RGB).

Figure 9-12. Image segmentation using K-Means with various numbers of color clusters

Using Clustering for Image Segmentation

In other words, for each pixel there is a 3D vector containing the intensities of red, green, and blue, each between 0.0 and 1.0 (or between 0 and 255, if you use **imageio.imread()**). Some images may have fewer channels, such as grayscale images (one channel). And some images may have more channels, such as images with an additional alpha channel for transparency or satellite images, which often contain channels for many light frequencies (e.g., infrared).

The following code reshapes the array to get a long list of RGB colors, then it clusters these colors using K-Means:

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

Using Clustering for Image Segmentation

For example, it may identify a color cluster for all shades of green. Next, for each color (e.g., dark green), it looks for the mean color of the pixel's color cluster. For example, all shades of green may be replaced with the same light green color (assuming the mean color of the green cluster is light green). Finally, it reshapes this long list of colors to get the same shape as the original image. And we're done!

This outputs the image shown in the upper right of Figure 9-12(Next Slide). You can experiment with various numbers of clusters, as shown in the figure. When you use fewer than eight clusters, notice that the ladybug's flashy red color fails to get a cluster of its own: it gets merged with colors from the environment. This is because K-Means prefers **clusters of similar sizes**. The ladybug is small—much smaller than the rest of the image—so even though its color is flashy, K-Means fails to dedicate a cluster to it.

Using Clustering for Image Segmentation

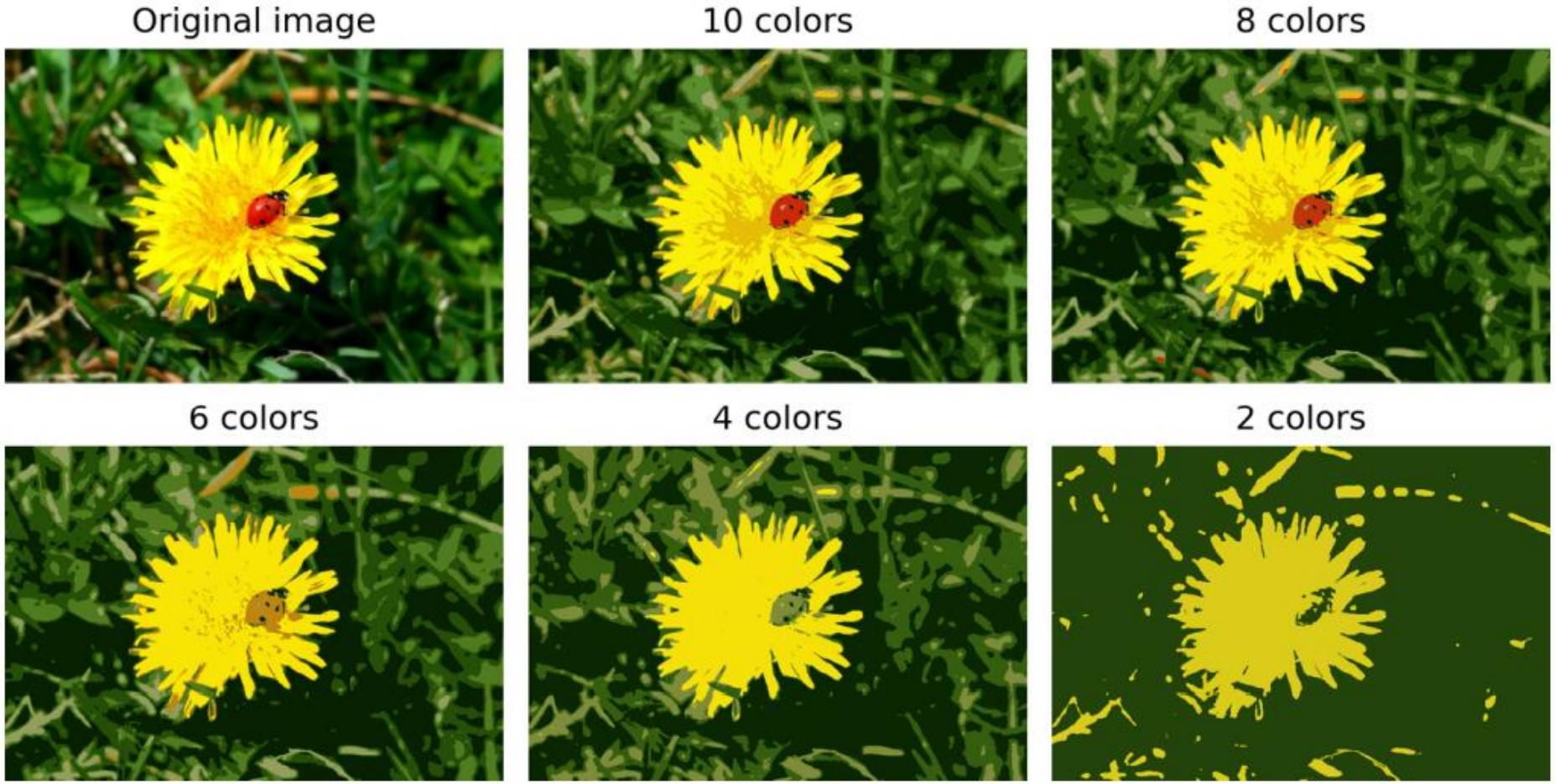
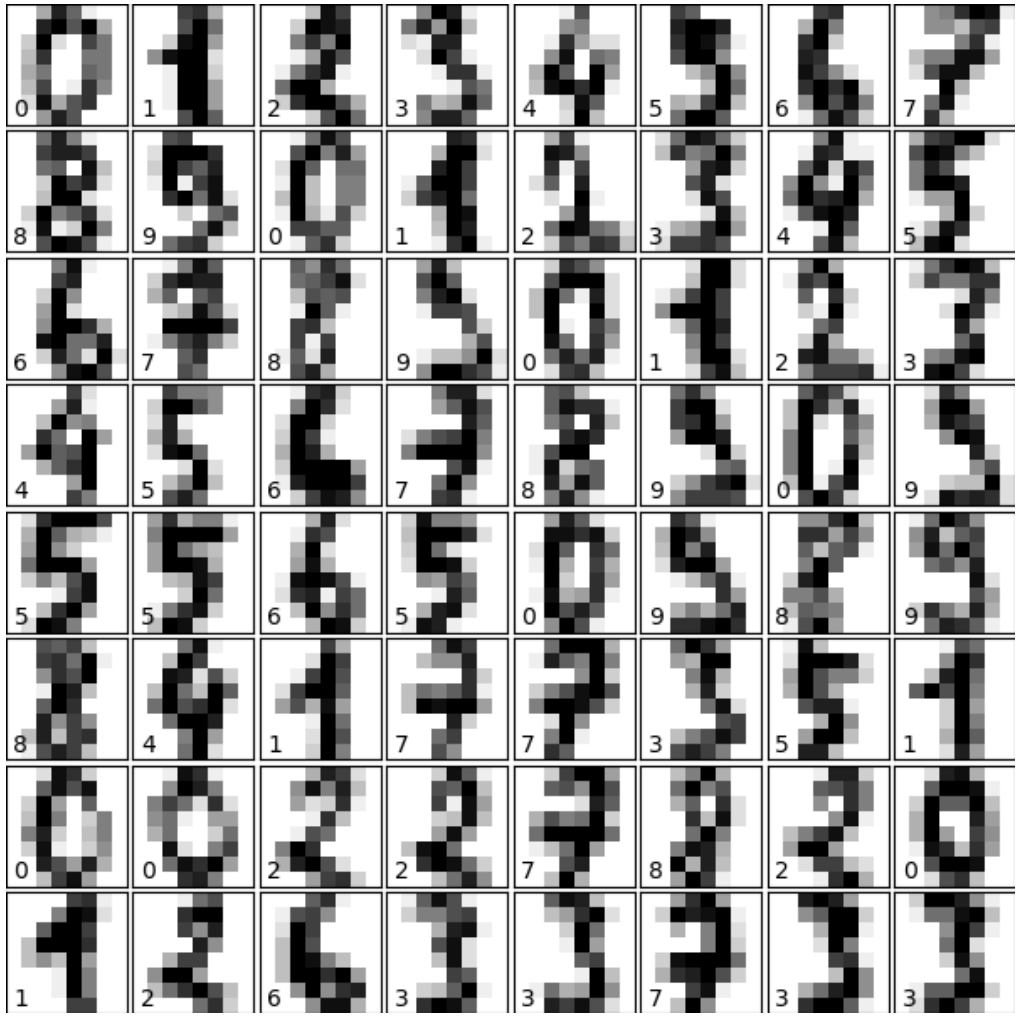


Figure 9-12. Image segmentation using K-Means with various numbers of color clusters

Using Clustering for Preprocessing

Clustering can be an efficient approach to dimensionality reduction, in particular as a **preprocessing step before** a supervised learning algorithm. As an example of using clustering for dimensionality reduction, let's tackle the digits dataset, which is a simple MNIST-like dataset containing 1,797 grayscale 8 × 8 images representing the digits 0 to 9.



Using Clustering for Preprocessing

First, load the dataset:

```
from sklearn.datasets import load_digits

X_digits, y_digits = load_digits(return_X_y=True)
```

Now, split it into a training set and a test set:

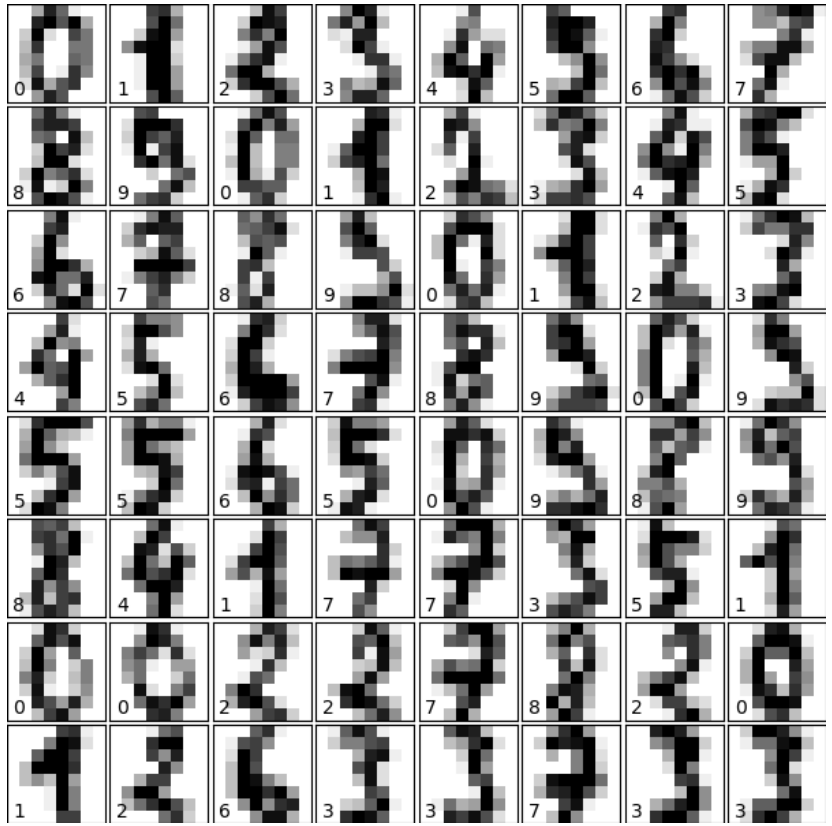
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X_digits, y_digits)
```

Next, fit a Logistic Regression model:

```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression()
log_reg.fit(X_train, y_train)
```



Using Clustering for Preprocessing

Let’s evaluate its accuracy on the test set:

```
>>> log_reg.score(X_test, y_test)
0.9688888888888889
```

OK, **that’s our baseline**: 96.9% accuracy. Let’s see if we can do better by using K-Means as a preprocessing step. We will create a pipeline that will first cluster the training set **into 50 clusters** and replace the images with their distances to these 50 clusters, then apply a Logistic Regression model:

Using Clustering for Preprocessing

```
from sklearn.pipeline import Pipeline

pipeline = Pipeline([
    ("kmeans", KMeans(n_clusters=50)),
    ("log_reg", LogisticRegression()),
])
pipeline.fit(X_train, y_train)
```

WARNING

Since there are 10 different digits, it is tempting to set the number of clusters to 10. However, each digit can be written several different ways, so it is preferable to use a larger number of clusters, such as 50.

Using Clustering for Preprocessing

Now let's evaluate this classification pipeline:

```
>>> pipeline.score(X_test, y_test)
0.9777777777777777
```

How about that? We reduced the error rate by almost 30% (from about 3.1% to about 2.2%)!

But we chose the number of clusters k arbitrarily; we can surely do better. Since K-Means is just a preprocessing step in a classification pipeline, finding a good value for k is much simpler than earlier. There's no need to perform silhouette analysis or minimize the inertia; the best value of k is simply the one that results in the best classification performance during cross-validation. We can use **GridSearchCV** to find the optimal number of clusters:

Using Clustering for Preprocessing

```
from sklearn.model_selection import GridSearchCV

param_grid = dict(kmeans__n_clusters=range(2, 100))
grid_clf = GridSearchCV(pipeline, param_grid, cv=3, verbose=2)
grid_clf.fit(X_train, y_train)
```

Let's look at the best value for k and the performance of the resulting pipeline:

```
>>> grid_clf.best_params_
{'kmeans__n_clusters': 99}
>>> grid_clf.score(X_test, y_test)
0.9822222222222222
```

With k = 99 clusters, we get a significant accuracy boost, reaching **98.22% accuracy** on the test set. Cool! You may want to keep exploring higher values for k, since 99 was the largest value in the range we explored.

Using Clustering for Semi-Supervised Learning

Another use case for clustering is in **semi-supervised learning**, when we have plenty of unlabeled instances and very few labeled instances.
Let's train a Logistic Regression model on a sample of 50 labeled instances from the digits dataset:

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

What is the performance of this model on the test set?

```
>>> log_reg.score(X_test, y_test)
0.8333333333333334
```

Using Clustering for Semi-Supervised Learning

The accuracy is just 83.3%. It should come as no surprise that this is much lower than earlier, when we trained the model on the full training set. Let's see how we can do better. First, let's cluster the training set into 50 clusters. Then for each cluster, let's find the image **closest to the centroid**. We will call these images the **representative images**:

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

Figure 9-13 shows these 50 representative images.

Using Clustering for Semi-Supervised Learning

Figure 9-13. Fifty representative digit images (one per cluster)

Let’s look at each image and manually label it:

```
y_representative_digits = np.array([4, 8, 0, 6, 8, 3, ..., 7, 6, 2, 3, 1,
1])
```

Now 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. Let’s see if the performance is any better:

Using Clustering for Semi-Supervised Learning

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_representative_digits, y_representative_digits)
>>> log_reg.score(X_test, y_test)
0.9222222222222223
```

Wow! We jumped from 83.3% accuracy to 92.2%, although we are still only training the model on 50 instances. Since it is often costly and painful to label instances, especially when it has to be done manually by experts, it is a good idea to label representative instances rather than just random instances.

But perhaps we can go one step further: what if **we propagated** the labels to all the other instances in the same cluster? This is called **label propagation**:

Using Clustering for Semi-Supervised Learning

```
y_train_propagated = np.empty(len(X_train), dtype=np.int32)
for i in range(k):
    y_train_propagated[kmeans.labels_==i] = y_representative_digits[i]
```

Now let's train the model again and look at its performance:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_train, y_train_propagated)
>>> log_reg.score(X_test, y_test)
0.9333333333333333
```

We got a reasonable accuracy boost, but nothing absolutely astounding. The problem is that we propagated each representative instance's label to all the instances in the same cluster, including the instances located close to the cluster boundaries, which are more likely to be mislabeled. Let's see what happens if we only propagate the labels to the 20% of the instances that are closest to the centroids:

Using Clustering for Semi-Supervised Learning

```
percentile_closest = 20

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]
```

Now let's train the model again on this partially propagated dataset:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_train_partially_propagated,
y_train_partially_propagated)
>>> log_reg.score(X_test, y_test)
0.94
```

Using Clustering for Semi-Supervised Learning

Nice! With just 50 labeled instances (only 5 examples per class on average!), we got 94.0% accuracy, which is pretty close to the performance of Logistic Regression on the fully labeled digits dataset (which was 96.9%). This good performance is due to the fact that the propagated labels are actually pretty good—their accuracy is very close to 99%, as the following code shows:

```
>>> np.mean(y_train_partially_propagated ==
y_train[partially_propagated])
0.9896907216494846
```

Using Clustering for Semi-Supervised Learning

ACTIVE LEARNING - To continue improving your model and your training set, the next step could be to do a few rounds of active learning, which is when a human expert interacts with the learning algorithm, providing labels for specific instances when the algorithm requests them. There are many different strategies for active learning, but one of the most common ones is called uncertainty sampling. Here is how it works:

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., when its estimated probability is lowest) are given to the expert to be labeled.
3. You iterate this process until the performance improvement stops being worth the labeling effort.

Using Clustering for Semi-Supervised Learning

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 (e.g., an SVM or a Random Forest).

Before we move on to **Gaussian mixture models**, let's take a look at DBSCAN, another popular clustering algorithm that illustrates a very different approach based on local density estimation. This approach allows the algorithm to identify **clusters of arbitrary shapes**.

Density-based spatial clustering of applications with noise (DBSCAN)

This algorithm defines clusters as continuous regions of high density. Here is how it works:

- For each instance, the algorithm counts how many instances are located within a small distance ε (epsilon) from it. This region is called the instance's ε-neighborhood.
- If an instance has at least $\min\_samples$ instances in its ε-neighborhood (including itself), then it is considered a core instance. In other words, core instances are those that are located in dense regions.
- All instances in the neighborhood of a core instance belong to the same cluster. This neighborhood may include other core instances; therefore, a long sequence of neighboring core instances forms a single cluster.
- Any instance that is not a core instance and does not have one in its neighborhood is considered an anomaly.

Density-based spatial clustering of applications with noise (DBSCAN)

This algorithm works well if all the clusters are dense enough and if they are well separated by low-density regions. The DBSCAN class in Scikit-Learn is as simple to use as you might expect. Let's test it on the moons dataset, introduced in Chapter 5:

```
from sklearn.cluster import DBSCAN
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=1000, noise=0.05)
dbscan = DBSCAN(eps=0.05, min_samples=5)
dbscan.fit(X)
```

The labels of all the instances are now available in the labels_ instance variable:

```
>>> dbscan.labels_
array([ 0,  2, -1, -1,  1,  0,  0,  0, ...,  3,  2,  3,  3,  4,  2,  6,
3])
```

Density-based spatial clustering of applications with noise (DBSCAN)

Notice that some instances have a cluster index equal to –1, which means that they are considered as anomalies by the algorithm. The indices of the core instances are available in the **core_sample_indices_** instance variable, and the core instances themselves are available in the **components_** instance variable:

```
>>> len(dbscan.core_sample_indices_)
808
>>> dbscan.core_sample_indices_
array([ 0,  4,  5,  6,  7,  8, 10, 11, ..., 992, 993, 995, 997, 998,
999])
>>> dbscan.components_
array([[-0.02137124,  0.40618608],
       [-0.84192557,  0.53058695],
                  ...
       [-0.94355873,  0.3278936 ],
       [ 0.79419406,  0.60777171]])
```

Density-based spatial clustering of applications with noise (DBSCAN)

This clustering is represented in the lefthand plot of Figure 9-14. As you can see, it identified quite a lot of anomalies, plus seven different clusters. How disappointing! Fortunately, if we widen each instance's neighborhood by increasing eps to 0.2, we get the clustering on the right, which looks perfect. Let's continue with this model.

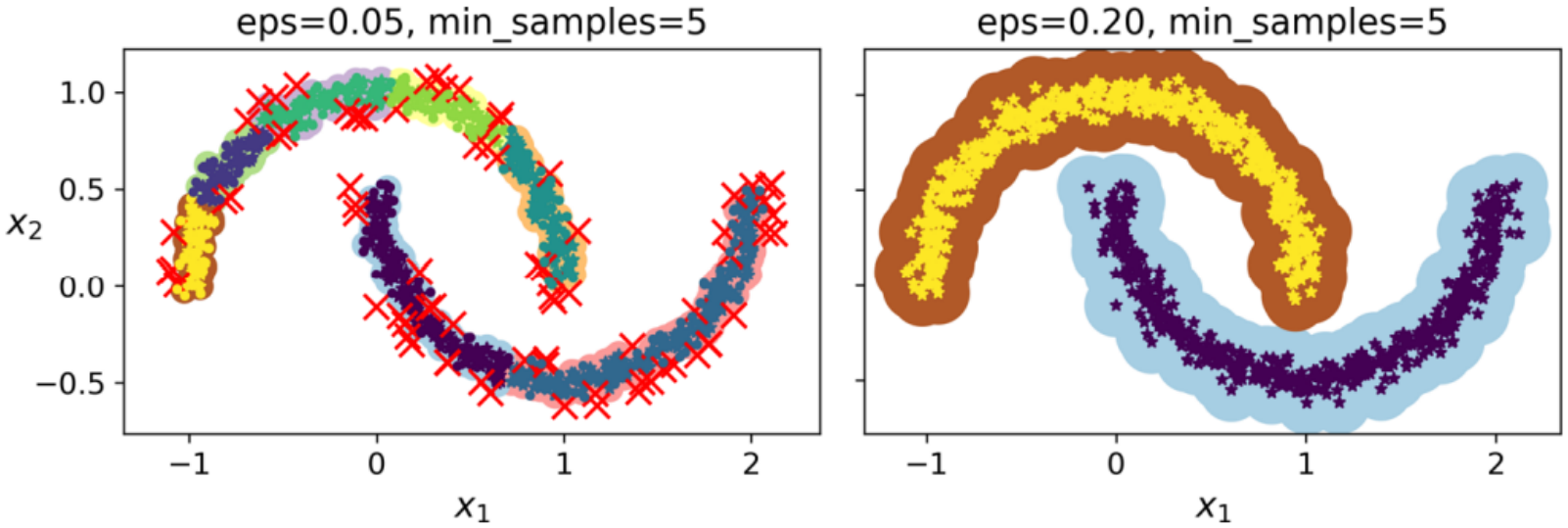


Figure 9-14. DBSCAN clustering using two different neighborhood radiuses

Density-based spatial clustering of applications with noise (DBSCAN)

Somewhat surprisingly, the DBSCAN class does not have a **predict()** method, although it has a **fit_predict()** method. In other words, it cannot predict which cluster a new instance belongs to. This implementation decision was made because different classification algorithms can be better for different tasks, so the authors decided to let the user choose which one to use. Moreover, it's not hard to implement. For example, let's train a **KNeighborsClassifier**:

```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors=50)
knn.fit(dbscan.components_, dbscan.labels_[dbscan.core_sample_indices_])
```

Now, given a few new instances, we can predict which cluster they most likely belong to and even estimate a probability for each cluster:

Density-based spatial clustering of applications with noise (DBSCAN)

```
>>> X_new = np.array([[-0.5, 0], [0, 0.5], [1, -0.1], [2, 1]])
>>> knn.predict(X_new)
array([1, 0, 1, 0])
>>> knn.predict_proba(X_new)
array([[0.18, 0.82],
       [1.  , 0.  ],
       [0.12, 0.88],
       [1.  , 0.  ]])
```

Note that we only trained the classifier on the core instances, but we could also have chosen to train it on all the instances, or all but the anomalies: this choice depends on the final task.

Density-based spatial clustering of applications with noise (DBSCAN)

The decision boundary is represented in Figure 9-15 (the crosses represent the four instances in **X_new**). Notice that since there is no anomaly in the training set, the classifier always chooses a cluster, even when that cluster is far away. It is fairly straightforward to introduce a maximum distance, in which case the two instances that are far away from both clusters are classified as anomalies. To do this, use the **kneighbors()** method of the **KNeighborsClassifier**. Given a set of instances, it returns the distances and the indices of the k nearest neighbors in the training set (two matrices, each with k columns):

```
>>> y_dist, y_pred_idx = knn.kneighbors(X_new, n_neighbors=1)
>>> y_pred = dbscan.labels_[dbscan.core_sample_indices_][y_pred_idx]
>>> y_pred[y_dist > 0.2] = -1
>>> y_pred.ravel()
array([-1,  0,  1, -1])
```

Density-based spatial clustering of applications with noise (DBSCAN)

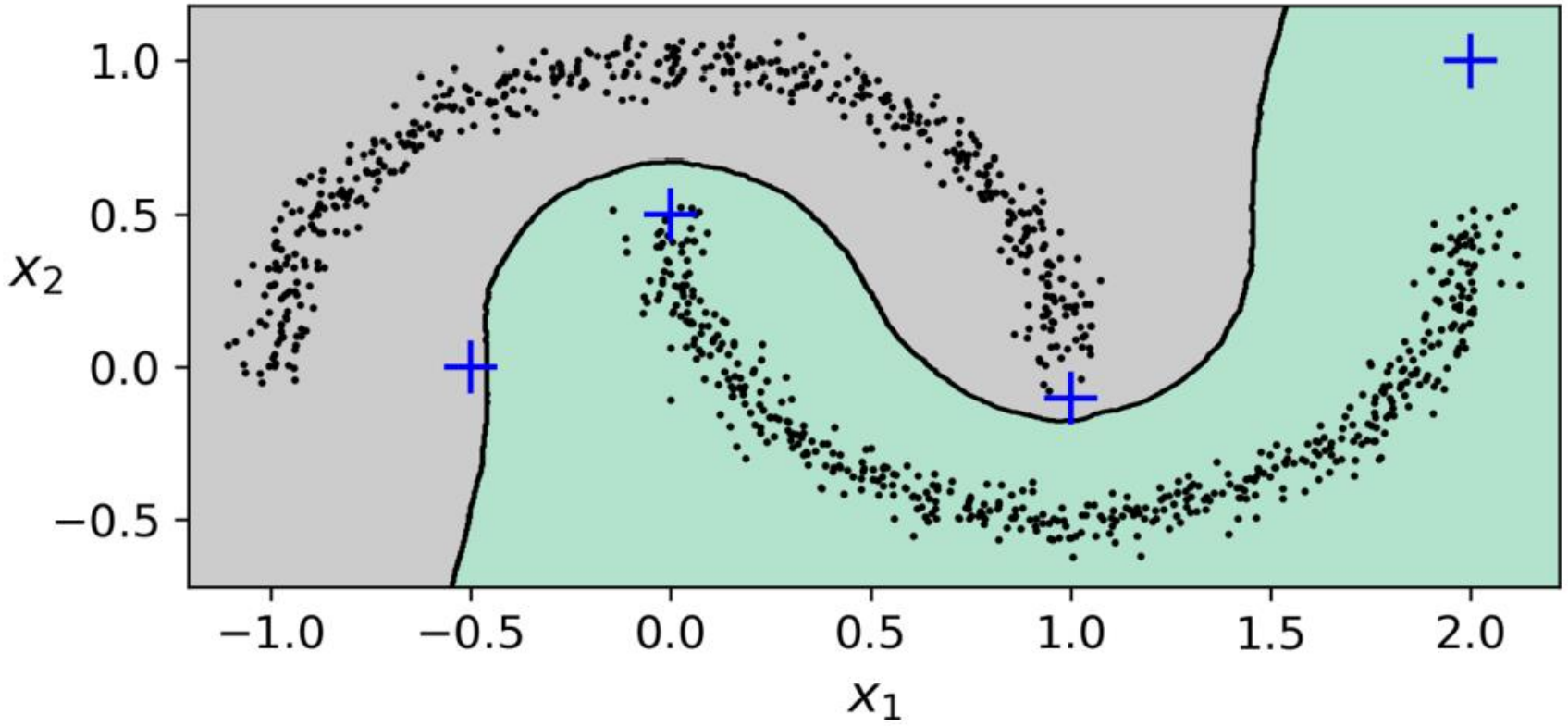


Figure 9-15. Decision boundary between two clusters

Density-based spatial clustering of applications with noise (DBSCAN)

In short, DBSCAN is a very simple yet powerful algorithm capable of identifying any number of clusters of any shape. It is robust to outliers, and it has just two hyperparameters (**eps** and **min_samples**). If the density varies significantly across the clusters, however, it can be impossible for it to capture all the clusters properly. Its computational complexity is roughly $O(m \log m)$, making it pretty close to linear with regard to the number of instances, but Scikit-Learn's implementation can require up to $O(m^2)$ memory if eps is large.

Gaussian Mixtures

A Gaussian mixture model (GMM) is a probabilistic model that assumes that the instances were generated from a mixture of several Gaussian distributions whose parameters are unknown. All the instances generated from a single Gaussian distribution form a cluster that typically looks like an ellipsoid. Each cluster can have a different ellipsoidal shape, size, density, and orientation, just like in Figure 9-11. When you observe an instance, you know it was generated from one of the Gaussian distributions, but you are not told which one, and you do not know what the parameters of these distributions are.

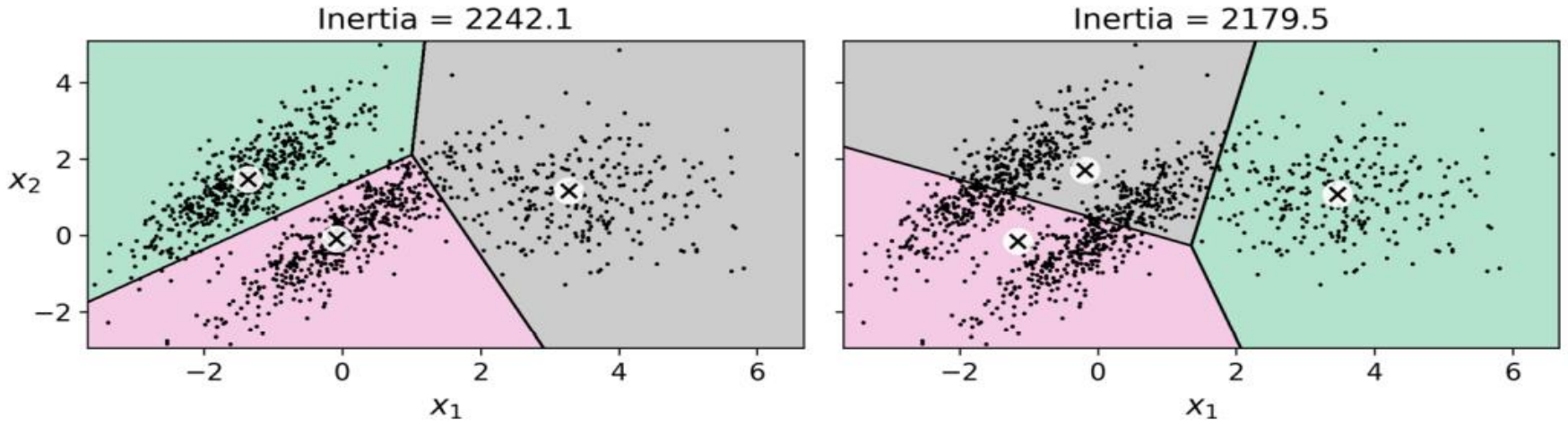


Figure 9-11. K-Means fails to cluster these ellipsoidal blobs properly

Gaussian Mixtures

There are several GMM variants. In the simplest variant, implemented in the **GaussianMixture** class, you must know in advance the number k of Gaussian distributions. The dataset X is assumed to have been generated through the following probabilistic process:

- For each instance, a cluster is picked randomly from among k clusters. The probability of choosing the j^{th} cluster is defined by the cluster's weight, $\phi(j)$. The index of the cluster chosen for the i^{th} instance is noted $z^{(i)}$.
- If $z^{(i)} = j$, meaning the i^{th} instance has been assigned to the j^{th} cluster, the location $\boldsymbol{x}^{(i)}$ of this instance is sampled randomly from the Gaussian distribution with mean $\boldsymbol{\mu}^{(j)}$ and covariance matrix $\Sigma^{(j)}$. This is noted $\boldsymbol{x}^{(i)} \sim \mathcal{N}(\boldsymbol{\mu}^{(j)}, \Sigma^{(j)})$.

Gaussian Mixtures

This generative process can be represented as a graphical model. Figure 9- 16 represents the structure of the conditional dependencies between random variables.

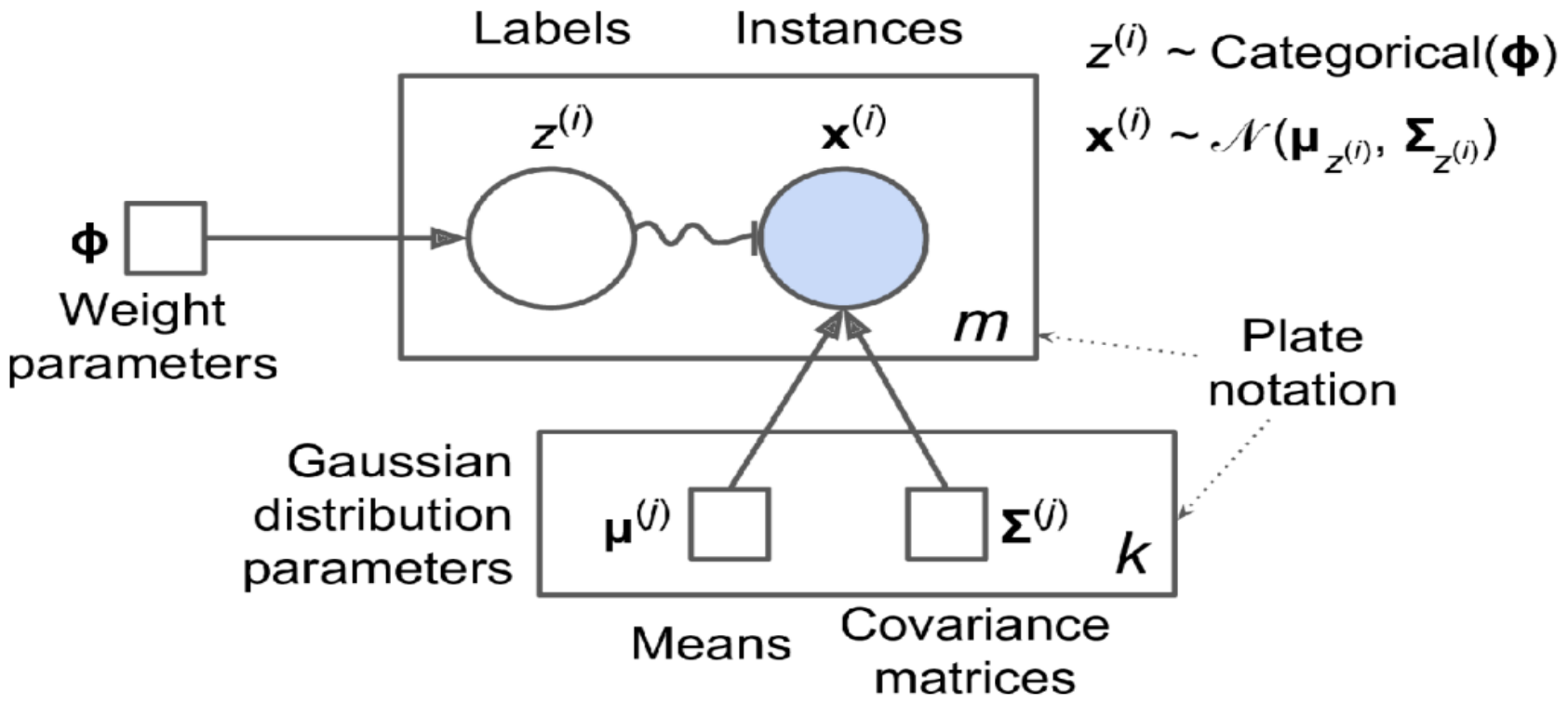


Figure 9-16. A graphical representation of a Gaussian mixture model, including its parameters (squares), random variables (circles), and their conditional dependencies (solid arrows)

Gaussian Mixtures

Here is how to interpret the figure:

- The circles represent random variables.
- The squares represent fixed values (i.e., parameters of the model).
- The large rectangles are called plates. They indicate that their content is repeated several times.
- The number at the bottom right of each plate indicates how many times its content is repeated. So, there are m random variables $z^{(i)}$ (from $z^{(1)}$ to $z^{(m)}$) and m random variables $\boldsymbol{x}^{(i)}$. There are also k means $\mu^{(j)}$ and k covariance matrices $\Sigma^{(j)}$. Lastly, there is just one weight vector ϕ (containing all the weights $\phi^{(1)}$ to $\phi^{(k)}$).

Gaussian Mixtures

- Each variable $z^{(i)}$ is drawn from the categorical distribution with weights ϕ. Each variable $\boldsymbol{x}^{(i)}$ is drawn from the normal distribution, with the mean and covariance matrix defined by its cluster $z^{(i)}$.
- The solid arrows represent conditional dependencies. For example, the probability distribution for each random variable $z^{(i)}$ depends on the weight vector ϕ. Note that when an arrow crosses a plate boundary, it means that it applies to all the repetitions of that plate. For example, the weight vector ϕ conditions the probability distributions of all the random variables $\boldsymbol{x}^{(1)}$ to $\boldsymbol{x}^{(m)}$.

Gaussian Mixtures

- The squiggly arrow from $z^{(i)}$ to $\boldsymbol{x}^{(i)}$ represents a switch: depending on the value of $z^{(i)}$, the instance $\boldsymbol{x}^{(i)}$ will be sampled from a different Gaussian distribution. For example, if $z^{(i)} = j$, then $\boldsymbol{x}^{(i)} \sim \mathcal{N}(\boldsymbol{\mu}^{(j)}, \Sigma^{(j)})$.
- Shaded nodes indicate that the value is known. So, in this case, only the random variables $\boldsymbol{x}^{(i)}$ have known values: they are called observed variables. The unknown random variables $z^{(i)}$ are called latent variables.

Gaussian Mixtures

So, what can you do with such a model? Well, given the dataset **X**, you typically want to start by estimating the weights $\boldsymbol{\phi}$ and all the distribution parameters $\boldsymbol{\mu}^{(1)}$ to $\boldsymbol{\mu}^{(k)}$ and $\boldsymbol{\Sigma}^{(1)}$ to $\boldsymbol{\Sigma}^{(k)}$. Scikit-Learn's $GaussianMixture$ class makes this super easy:

```
from sklearn.mixture import GaussianMixture

gm = GaussianMixture(n_components=3, n_init=10)
gm.fit(X)
```

Let's look at the parameters that the algorithm estimated:

Gaussian Mixtures

```
>>> gm.weights_
array([0.20965228, 0.4000662 , 0.39028152])
>>> gm.means_
array([[ 3.39909717,  1.05933727],
       [-1.40763984,  1.42710194],
       [ 0.05135313,  0.07524095]])
>>> gm.covariances_
array([[[ 1.14807234, -0.03270354],
        [-0.03270354,  0.95496237]],

       [[ 0.63478101,  0.72969804],
        [ 0.72969804,  1.1609872 ]],

       [[ 0.68809572,  0.79608475],
        [ 0.79608475,  1.21234145]]])
```

Gaussian Mixtures

Great, it worked fine! Indeed, the weights that were used to generate the data were 0.2, 0.4, and 0.4; and similarly, the means and covariance matrices were very close to those found by the algorithm. But how? This class relies on the Expectation-Maximization (EM) algorithm, which has many similarities with the K-Means algorithm: it also initializes the cluster parameters randomly, then it repeats two steps until convergence, first assigning instances to clusters (this is called the expectation step) and then updating the clusters (this is called the maximization step).

Gaussian Mixtures

Sounds familiar, right? In the context of clustering, you can think of EM as a generalization of K-Means that not only finds the cluster centers ($\boldsymbol{\mu}^{(1)}$ to $\boldsymbol{\mu}^{(k)}$), but also their size, shape, and orientation ($\Sigma^{(1)}$ to $\Sigma^{(k)}$), as well as their relative weights ($\phi^{(1)}$ to $\phi^{(k)}$). Unlike K-Means, though, EM uses soft cluster assignments, not hard assignments. For each instance, during the expectation step, the algorithm estimates the probability that it belongs to each cluster (based on the current cluster parameters). Then, during the maximization step, each cluster is updated using all the instances in the dataset, with each instance weighted by the estimated probability that it belongs to that cluster. These probabilities are called the **responsibilities of the clusters for the instances**. During the maximization step, each cluster's update will mostly be impacted by the instances it is most responsible for.

Gaussian Mixtures

WARNING

Unfortunately, just like K-Means, EM can end up converging to poor solutions, so it needs to be run several times, keeping only the best solution. This is why we set **n_init** to 10. Be careful: by default **n_init** is set to 1.

You can check whether or not the algorithm converged and how many iterations it took:

```
>>> gm.converged_
True
>>> gm.n_iter_
3
```

Gaussian Mixtures

Now that you have an estimate of the location, size, shape, orientation, and relative weight of each cluster, the model can easily assign each instance to the most likely cluster (hard clustering) or estimate the probability that it belongs to a particular cluster (soft clustering). Just use the **predict()** method for hard clustering, or the **predict_proba()** method for soft clustering:

```
>>> gm.predict(X)
array([2, 2, 1, ..., 0, 0, 0])
>>> gm.predict_proba(X)
array([[2.32389467e-02, 6.77397850e-07, 9.76760376e-01],
       [1.64685609e-02, 6.75361303e-04, 9.82856078e-01],
       [2.01535333e-06, 9.99923053e-01, 7.49319577e-05],
       ...,
       [9.99999571e-01, 2.13946075e-26, 4.28788333e-07],
       [1.00000000e+00, 1.46454409e-41, 5.12459171e-16],
       [1.00000000e+00, 8.02006365e-41, 2.27626238e-15]])
```

Gaussian Mixtures

A Gaussian mixture model is a generative model, meaning you can sample new instances from it (note that they are ordered by cluster index):

```
>>> X_new, y_new = gm.sample(6)
>>> X_new
array([[ 2.95400315,  2.63680992],
       [-1.16654575,  1.62792705],
       [-1.39477712, -1.48511338],
       [ 0.27221525,  0.690366  ],
       [ 0.54095936,  0.48591934],
       [ 0.38064009, -0.56240465]])

>>> y_new
array([0, 1, 2, 2, 2, 2])
```

Gaussian Mixtures

It is also possible to estimate the density of the model at any given location. This is achieved using the **score_samples()** method: for each instance it is given, this method estimates the log of the probability density function (PDF) at that location. The greater the score, the higher the density:

```
>>> gm.score_samples(X)
array([-2.60782346, -3.57106041, -3.33003479, ..., -3.51352783,
       -4.39802535, -3.80743859])
```

If you compute the exponential of these scores, you get the value of the PDF at the location of the given instances. These are not probabilities, but probability densities: they can take on any positive value, not just a value between 0 and 1. To estimate the probability that an instance will fall within a particular region, you would have to integrate the PDF over that region (if you do so over the entire space of possible instance locations, the result will be 1).

Gaussian Mixtures

Figure 9-17 shows the cluster means, the decision boundaries (dashed lines), and the density contours of this model.

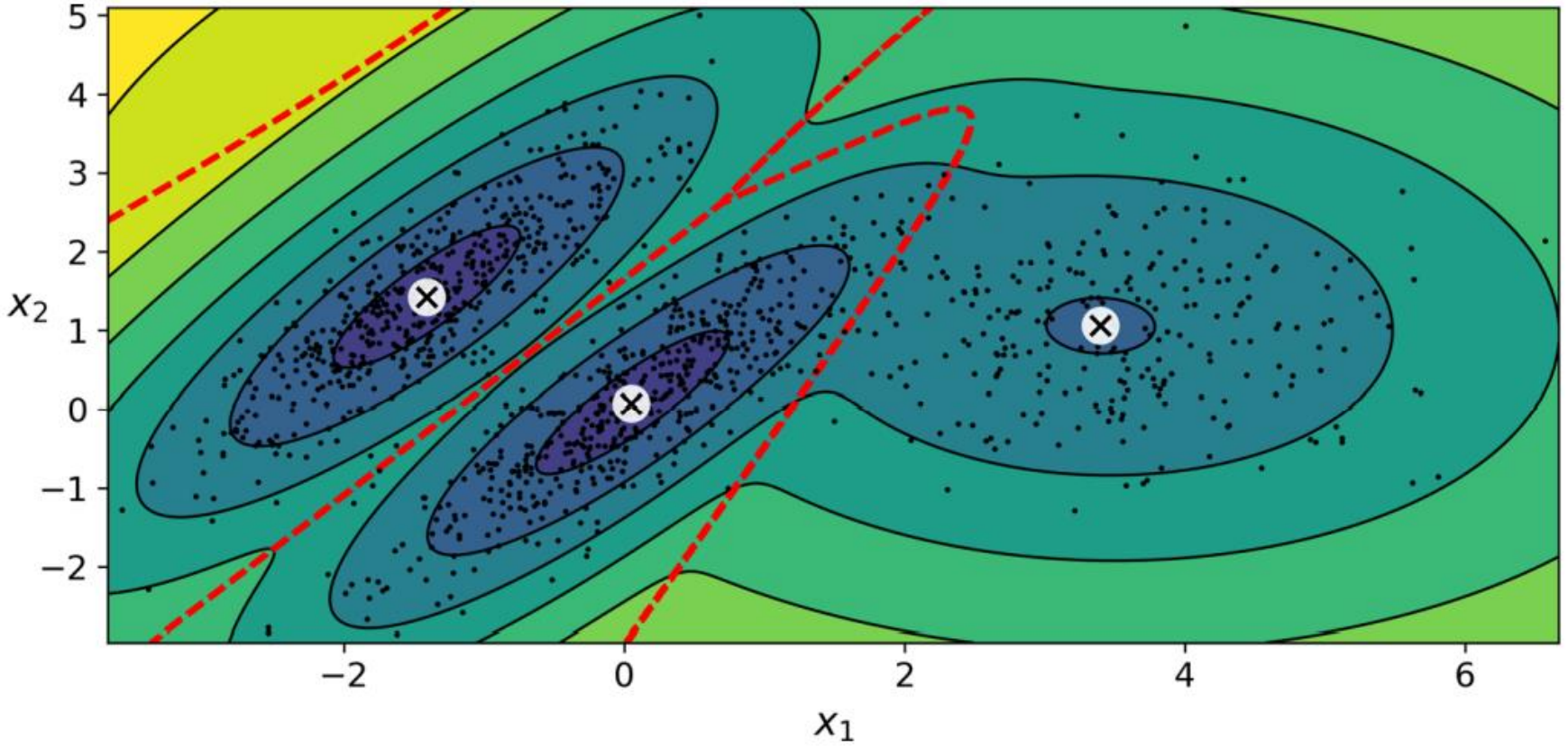


Figure 9-17. Cluster means, decision boundaries, and density contours of a trained Gaussian mixture model

Gaussian Mixtures

Nice! The algorithm clearly found an excellent solution. Of course, we made its task easy by generating the data using a set of 2D Gaussian distributions (unfortunately, real-life data is not always so Gaussian and low-dimensional). We also gave the algorithm the correct number of clusters. When there are many dimensions, or many clusters, or few instances, EM can struggle to converge to the optimal solution. You might need to reduce the difficulty of the task by limiting the number of parameters that the algorithm has to learn. One way to do this is to limit the range of shapes and orientations that the clusters can have. This can be achieved by imposing constraints on the covariance matrices. To do this, set the **covariance_type** hyperparameter to one of the following values:

Gaussian Mixtures

"spherical"

All clusters must be spherical, but they can have different diameters (i.e., different variances).

"diag"

Clusters can take on any ellipsoidal shape of any size, but the ellipsoid's axes must be parallel to the coordinate axes (i.e., the covariance matrices must be diagonal).

"tied"

All clusters must have the same ellipsoidal shape, size, and orientation (i.e., all clusters share the same covariance matrix).

Gaussian Mixtures

By default, **covariance_type** is equal to "full", which means that each cluster can take on any shape, size, and orientation (it has its own unconstrained covariance matrix). Figure 9-18 plots the solutions found by the EM algorithm when **covariance_type** is set to "tied" or "spherical."

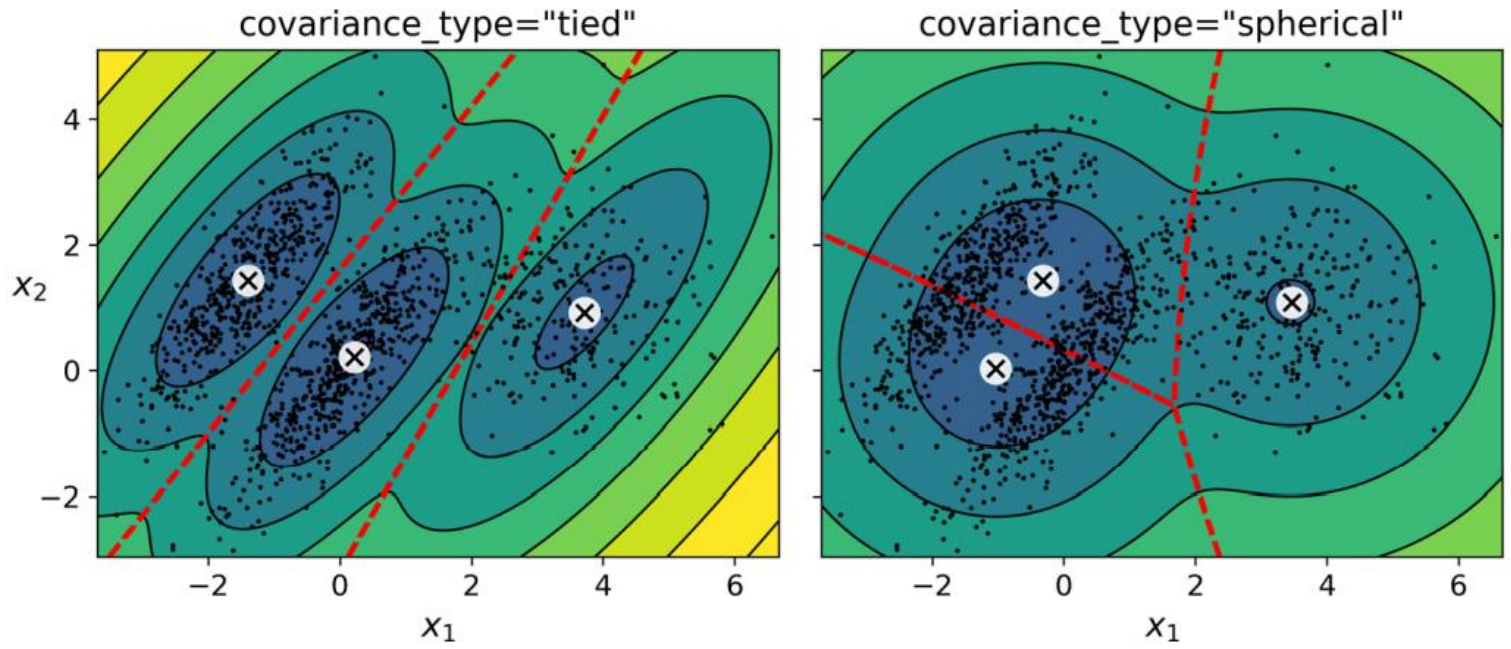


Figure 9-18. Gaussian mixtures for tied clusters (left) and spherical clusters (right)

Anomaly Detection Using Gaussian Mixtures

Anomaly detection (also called outlier detection) is the task of detecting instances that deviate strongly from the norm. These instances are called anomalies, or outliers, while the normal instances are called inliers. Anomaly detection is useful in a wide variety of applications, such as fraud detection, detecting defective products in manufacturing, or removing outliers from a dataset before training another model (which can significantly improve the performance of the resulting model).

Anomaly Detection Using Gaussian Mixtures

Using a Gaussian mixture model for anomaly detection is quite simple: any instance located in a low-density region can be considered an anomaly. You must define what density threshold you want to use. For example, in a manufacturing company that tries to detect defective products, the ratio of defective products is usually well known. Say it is equal to 4%. You then set the density threshold to be the value that results in having 4% of the instances located in areas below that threshold density. If you notice that you get too many false positives (i.e., perfectly good products that are flagged as defective), you can lower the threshold. Conversely, if you have too many false negatives (i.e., defective products that the system does not flag as defective), you can increase the threshold. This is the usual precision/recall trade-off (see Chapter 3).

Anomaly Detection Using Gaussian Mixtures

Here is how you would identify the outliers using the fourth percentile lowest density as the threshold (i.e., approximately 4% of the instances will be flagged as anomalies):

```
densities = gm.score_samples(X)
density_threshold = np.percentile(densities, 4)
anomalies = X[densities < density_threshold]
```

Figure 9-19 represents these anomalies as stars.

Anomaly Detection Using Gaussian Mixtures

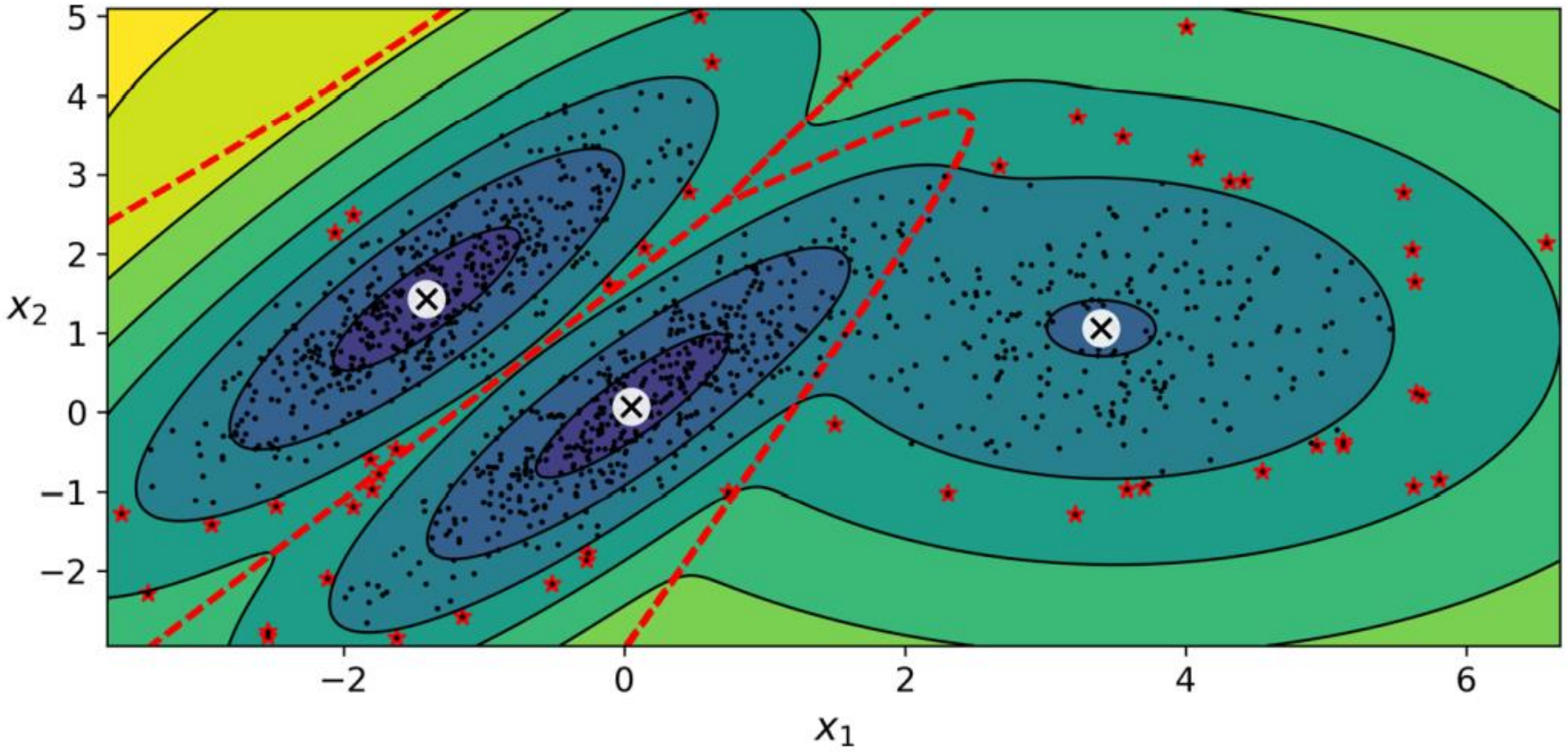


Figure 9-19. Anomaly detection using a Gaussian mixture model

Novelty Detection Using Gaussian Mixtures

A closely related task is **novelty detection**: it differs from anomaly detection in that the algorithm is assumed to be trained on a “clean” dataset, uncontaminated by outliers, whereas anomaly detection does not make this assumption. Indeed, outlier detection is often used to clean up a dataset.

TIP

Gaussian mixture models try to fit all the data, including the outliers, so if you have too many of them, this will bias the model’s view of “normality,” and some outliers may wrongly be considered as normal. If this happens, you can try to fit the model once, use it to detect and remove the most extreme outliers, then fit the model again on the cleaned-up dataset. Another approach is to use **robust covariance estimation methods** (see the **EllipticEnvelope** class).

Selecting the Number of Clusters

Just like K-Means, the $GaussianMixture$ algorithm requires you to specify the number of clusters. So, how can you find it?

With K-Means, you could use the inertia or the silhouette score to select the appropriate number of clusters. But with Gaussian mixtures, it is not possible to use these metrics because they are not reliable when the clusters are not spherical or have different sizes. Instead, you can try to find the model that **minimizes** a **theoretical information criterion**, such as the Bayesian information criterion (BIC) or the Akaike information criterion (AIC), defined in Equation 9-1.

Equation 9-1. Bayesian information criterion (BIC) and Akaike information criterion (AIC)

$$BIC = \log(m)\,p - 2\log\left(\hat{L}\right)$$

$$AIC = 2p - 2\log\left(\hat{L}\right)$$

Selecting the Number of Clusters

In these equations:

- m is the number of instances, as always.
- p is the number of parameters learned by the model.
- $\hat{L}$ is the maximized value of the likelihood function of the model.

Both the BIC and the AIC penalize models that have more parameters to learn (e.g., more clusters) and reward models that fit the data well. They often end up selecting the same model. When they differ, the model selected by the BIC tends to be simpler (fewer parameters) than the one selected by the AIC, but tends to not fit the data quite as well (this is especially true for larger datasets).

LIKELIHOOD FUNCTION

To compute the BIC and AIC, call the **bic()** and **aic()** methods:

```
>>> gm.bic(X)
8189.74345832983
>>> gm.aic(X)
8102.518178214792
```

LIKELIHOOD FUNCTION

Figure 9-21 shows the BIC for different numbers of clusters k. As you can see, both the BIC and the AIC are lowest when k=3, so it is most likely the best choice. Note that we could also search for the best value for the **covariance_type** hyperparameter. For example, if it is "spherical" rather than "full", then the model has significantly fewer parameters to learn, but it does not fit the data as well.

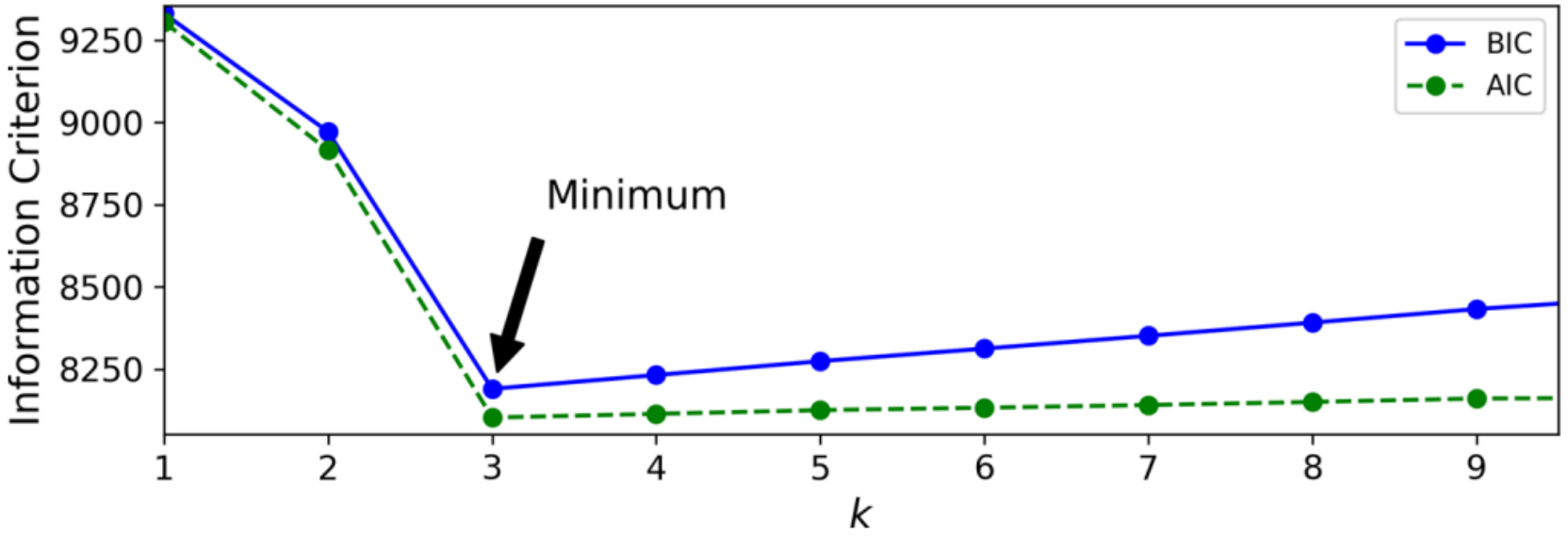


Figure 9-21. AIC and BIC for different numbers of clusters k

Bayesian Gaussian Mixture Models

Rather than manually searching for the optimal number of clusters, you can use the **BayesianGaussianMixture** class, which is capable of giving weights equal (or close) to zero to unnecessary clusters. Set the number of clusters **n_components** to a value that you have good reason to believe is greater than the optimal number of clusters (this assumes some minimal knowledge about the problem at hand), and the algorithm will eliminate the unnecessary clusters automatically. For example, let's set the number of clusters to 10 and see what happens:

```
>>> from sklearn.mixture import BayesianGaussianMixture
>>> bgm = BayesianGaussianMixture(n_components=10, n_init=10)
>>> bgm.fit(X)
>>> np.round(bgm.weights_, 2)
array([0.4 , 0.21, 0.4 , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ])
```

Perfect: the algorithm automatically detected that only three clusters are needed, and the resulting clusters are almost identical to the ones in Figure 9-17.

Limitation of Bayesian Gaussian Mixture Models

Gaussian mixture models work great on clusters with ellipsoidal shapes, but if you try to fit a dataset with different shapes, you may have bad surprises. For example, let's see what happens if we use a Bayesian Gaussian mixture model to cluster the moons dataset (see Figure 9-24).

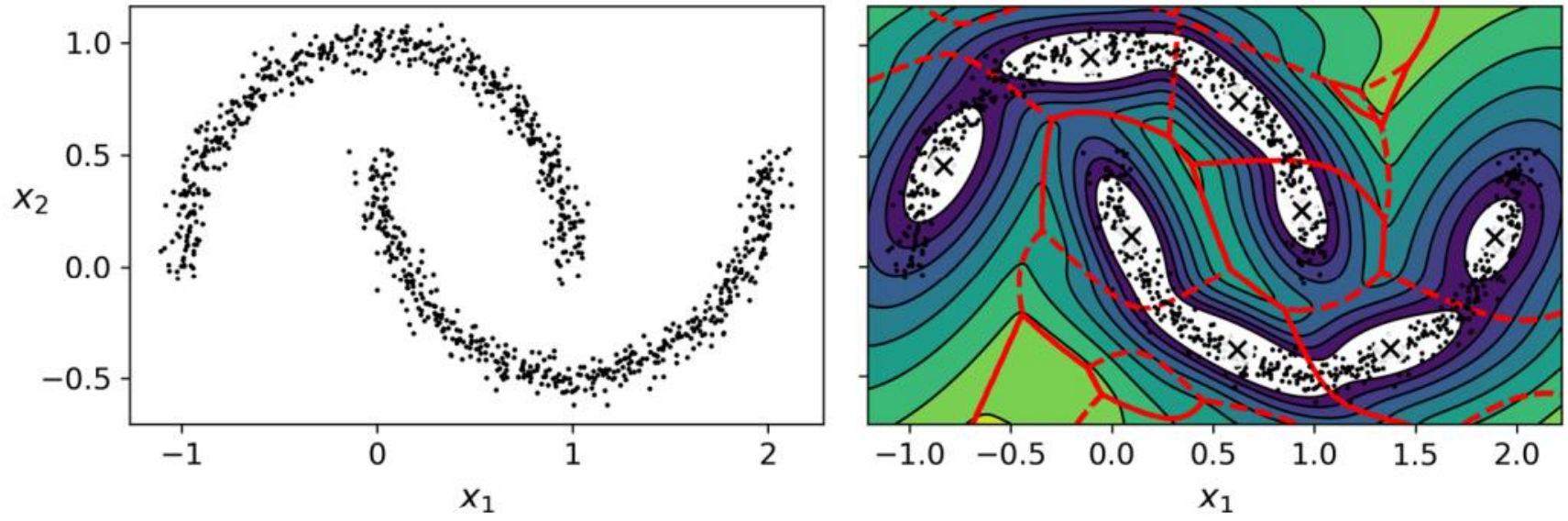


Figure 9-24. Fitting a Gaussian mixture to nonellipsoidal clusters

Limitation of Bayesian Gaussian Mixture Models

Oops! The algorithm desperately searched for ellipsoids, so it found eight different clusters instead of two. The density estimation is not too bad, so this model could perhaps be used for anomaly detection, but it failed to identify the two moons.

References

- *Gèlron, A. (2019). Hands-on machine learning with Scikit-Learn, Keras and TensorFlow: concepts, tools, and techniques to build intelligent systems (2nd ed.). O'Reilly.*