zations). If you are curious, a model's inertia is accessible via the `inertia_` instance variable:

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

The `score()` method returns the negative inertia. Why negative? Well, it is because a predictor's `score()` method must always respect the "*great is better*" rule.

```
>>> kmeans.score(X)
-211.59853725816856
```

An important improvement to the K-Means algorithm, called *K-Means+\+*, was proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii:[3] they introduced a smarter initialization step that tends to select centroids that are distant from one another, and this 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 since it makes it possible to drastically reduce the number of times the algorithm needs to be run to find the optimal solution. Here is the K-Means++ initialization algorithm:

- Take one centroid $\mathbf{c}^{(1)}$, chosen uniformly at random from the dataset.
- Take a new centroid $\mathbf{c}^{(i)}$, choosing an instance $\mathbf{x}^{(i)}$ with probability: $D\left(\mathbf{x}^{(i)}\right)^2 \Sigma_{j=1}^{m} D\left(\mathbf{x}^{(j)}\right)^2$ 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 further away from already chosen centroids are much more likely be selected as centroids.
- Repeat the previous step until all k centroids have been chosen.

The `KMeans` class actually 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.[4] It considerably accelerates the algorithm by avoiding many unnecessary distance calculations: this is achieved by exploiting the triangle inequal-

3 "k-means\++: The advantages of careful seeding," David Arthur and Sergei Vassilvitskii (2006).

4 "Using the Triangle Inequality to Accelerate k-Means," Charles Elkan (2003).

ity (i.e., the straight line is always the shortest[5]) and by keeping track of lower and upper bounds for distances between instances and centroids. This is the algorithm used by default by the `KMeans` class (but you can force it to use the original algorithm by setting the `algorithm` hyperparameter to `"full"`, although you probably will never need to).

Yet another important variant of the K-Means algorithm was proposed in a 2010 paper by David Sculley.[6] 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 3 or 4 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)
```

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 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 K-Means and regular K-Means models trained on the previous dataset using various numbers of clusters k. 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. However, 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.

5 The triangle inequality is $AC \leq AB + BC$ where A, B and C are three points, and AB, AC and BC are the distances between these points.

6 "Web-Scale K-Means Clustering," David Sculley (2010).

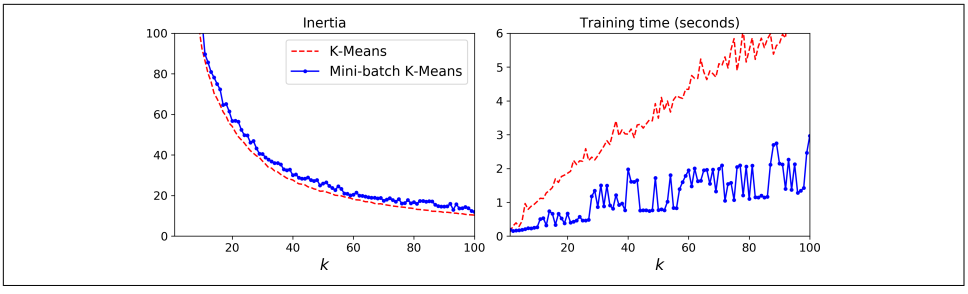

Figure 9-6. Mini-batch K-Means vs K-Means: worse inertia as k increases (left) but much faster (right)

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 is 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. For example, as you can see in Figure 9-7, setting k to 3 or 8 results in fairly bad models:

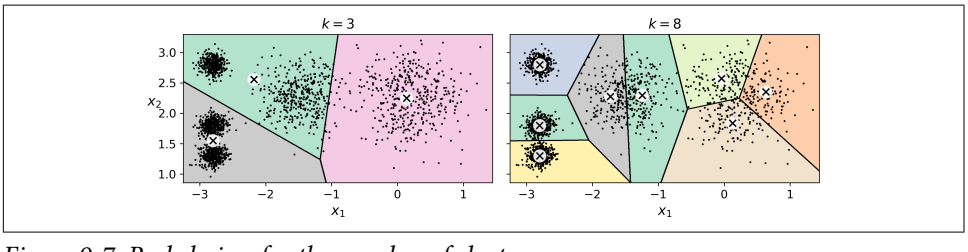

Figure 9-7. Bad choices for the number of clusters

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 since 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):

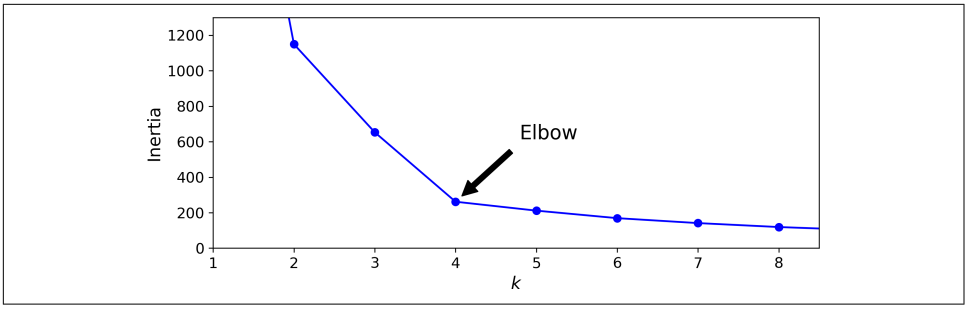

Figure 9-8. Selecting the number of clusters k using the "elbow rule"

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, it 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.

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 $(b - a) / \max(a, b)$ where a is the mean distance to the other instances in the same cluster (it is the mean intra-cluster distance), and b is the mean nearest-cluster distance, that is 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. 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):

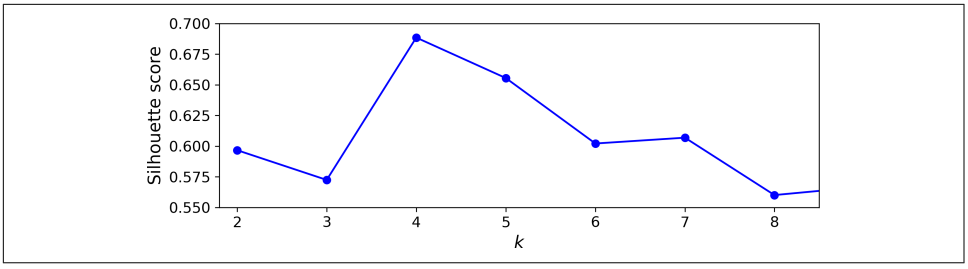

Figure 9-9. Selecting the number of clusters k using the silhouette score

As you can see, this visualization is much richer than the previous one: in particular, 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.

An even more informative visualization is obtained when you plot every instance's silhouette coefficient, sorted by the cluster they are assigned to and by the value of the coefficient. This is called a *silhouette diagram* (see Figure 9-10):

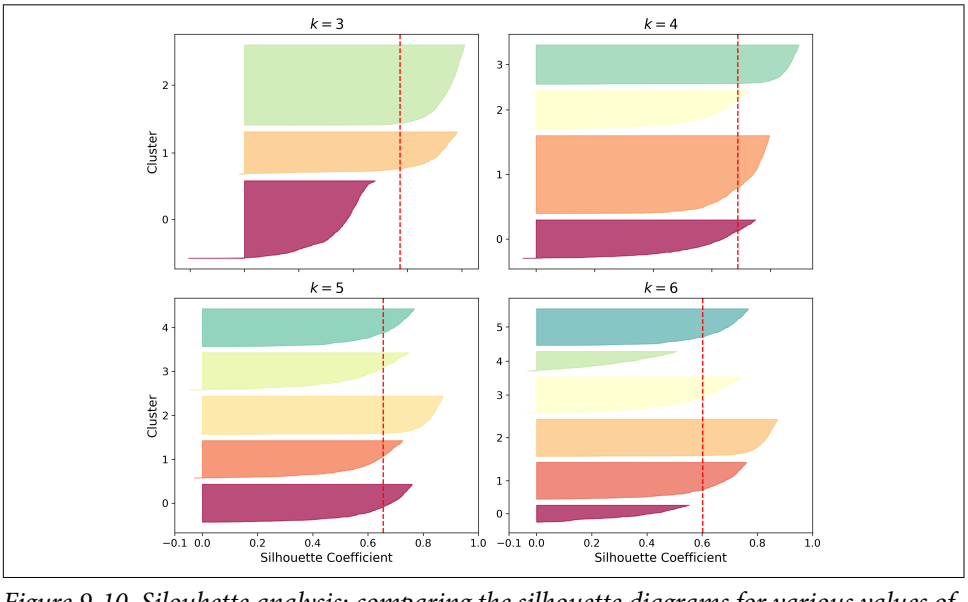

Figure 9-10. Silouhette analysis: comparing the silhouette diagrams for various values of k

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 clus-

ters. 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, while 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.

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 sub-optimal 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:

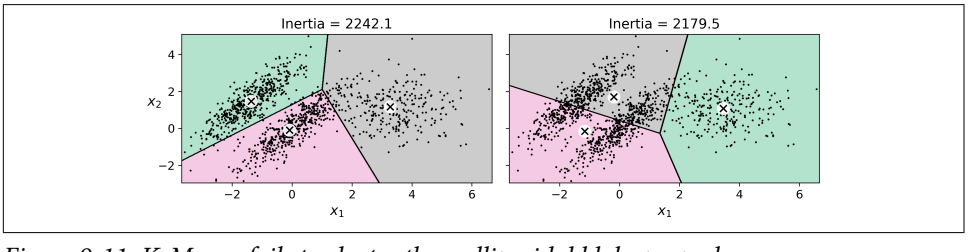

Figure 9-11. K-Means fails to cluster these ellipsoidal blobs properly

As you can see, neither of these solutions are 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. For example, on these types of elliptical clusters, Gaussian mixture models work great.

It is important to scale the input features before you run K-Means, or else 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.

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 just 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. The state of the art in semantic or instance segmentation today is achieved using complex architectures based on convolutional neural networks (see Chapter 14). 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.

First, let's load the image (see the upper left image in Figure 9-12) using Matplotlib's `imread()` function:

```
>>> from matplotlib.image import imread  # you could also use `imageio.imread()`
>>> image = imread(os.path.join("images","clustering","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). 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 less channels, such as grayscale images (one channel), or 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. 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!

```
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)
```

This outputs the image shown in the upper right of Figure 9-12. You can experiment with various numbers of clusters, as shown in the figure. When you use less than 8 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 due to the fact that the ladybug is quite 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: as mentioned earlier, K-Means prefers clusters of similar sizes.

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

That was not too hard, was it? Now let's look at another application of clustering: preprocessing.

Using Clustering for Preprocessing

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

```
from sklearn.datasets import load_digits

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

Now, let's 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, let's fit a Logistic Regression model:

```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression(random_state=42)
log_reg.fit(X_train, y_train)
```

Let's evaluate its accuracy on the test set:

```
>>> log_reg.score(X_test, y_test)
0.9666666666666667
```

Okay, that's our baseline: 96.7% 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.

Although it is tempting to define the number of clusters to 10, since there are 10 different digits, it is unlikely to perform well, because there are several different ways to write each digit.

```
from sklearn.pipeline import Pipeline

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

Now let's evaluate this classification pipeline:

```
>>> pipeline.score(X_test, y_test)
0.9822222222222222
```

How about that? We almost divided the error rate by a factor of 2!

But we chose the number of clusters k completely 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. Let's use `GridSearchCV` to find the optimal number of clusters:

```
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 best value for k, and the performance of the resulting pipeline:

```
>>> grid_clf.best_params_
{'kmeans__n_clusters': 90}
>>> grid_clf.score(X_test, y_test)
0.9844444444444445
```

With k=90 clusters, we get a small accuracy boost, reaching 98.4% accuracy on the test set. Cool!

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)
0.8266666666666667
```

The accuracy is just 82.7%: 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:

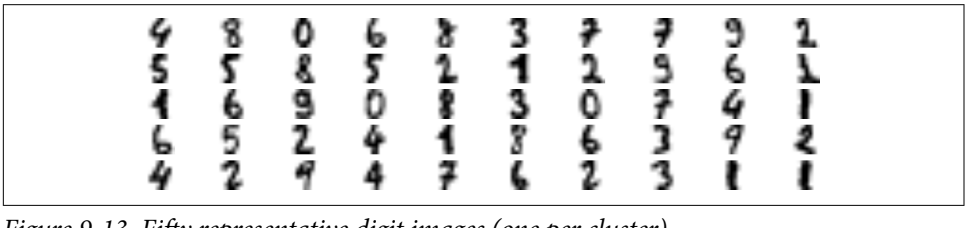

Figure 9-13. Fifty representative digit images (one per cluster)

Now 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 completely random instances, each of them is a representative image of its cluster. Let's see if the performance is any better:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_representative_digits, y_representative_digits)
>>> log_reg.score(X_test, y_test)
0.9244444444444444
```

Wow! We jumped from 82.7% accuracy to 92.4%, although we are still only training the model on 50 instances. Since it is often costly and painful to label instances, espe-