WEEK5_HW_Minju_Jo

May 14, 2020

1 Setup

In [1]:
```
# Python 3.5 is required
import sys
assert sys.version_info >= (3, 5)

# Scikit-Learn 0.20 is required
import sklearn
assert sklearn.__version__ >= "0.20"

# Common imports
import numpy as np
import os

# to make this notebook's output stable across runs
np.random.seed(42)

# To plot pretty figures
%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
mpl.rc('axes', labelsize=14)
mpl.rc('xtick', labelsize=12)
mpl.rc('ytick', labelsize=12)

# Where to save the figures
PROJECT_ROOT_DIR = "."
CHAPTER_ID = "unsupervised_learning"
IMAGES_PATH = os.path.join(PROJECT_ROOT_DIR, "images", CHAPTER_ID)
os.makedirs(IMAGES_PATH, exist_ok=True)

def save_fig(fig_id, tight_layout=True, fig_extension="png", resolution=300):
    path = os.path.join(IMAGES_PATH, fig_id + "." + fig_extension)
    print("Saving figure", fig_id)
    if tight_layout:
        plt.tight_layout()
    plt.savefig(path, format=fig_extension, dpi=resolution)
```

```
        # Ignore useless warnings (see SciPy issue #5998)
        import warnings
        warnings.filterwarnings(action="ignore", message="^internal gelsd")
```

2 Clustering

2.1 Introduction – Classification *vs* Clustering

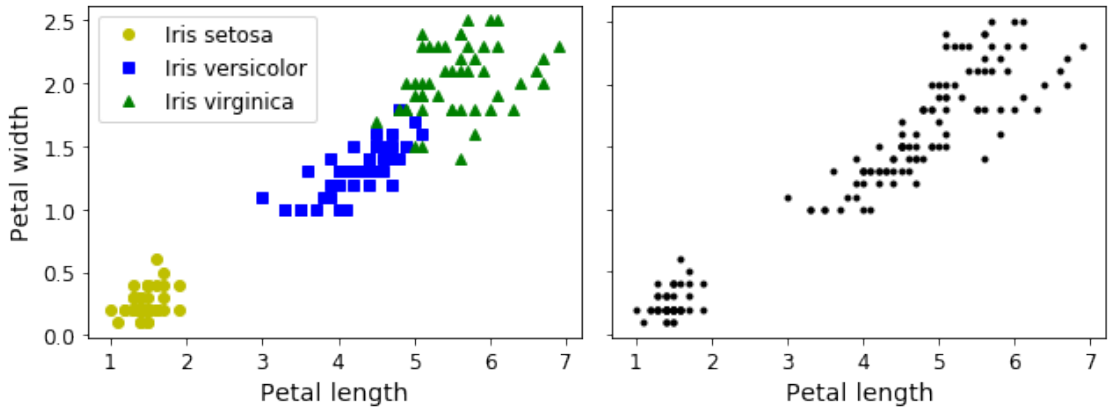
```
In [2]: from sklearn.datasets import load_iris
```

```
In [3]: data = load_iris()
        X = data.data
        y = data.target
        data.target_names
```

```
Out[3]: array(['setosa', 'versicolor', 'virginica'], dtype='<U10')
```

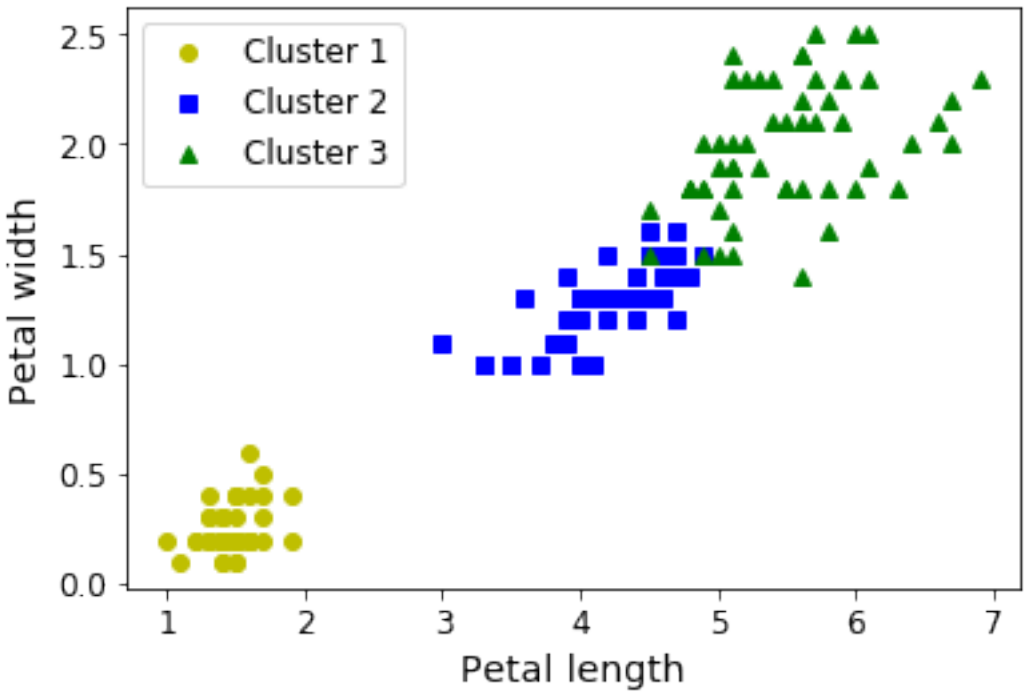
```
In [4]: plt.figure(figsize=(9, 3.5))

        plt.subplot(121)
        plt.plot(X[y==0, 2], X[y==0, 3], "yo", label="Iris setosa")
        plt.plot(X[y==1, 2], X[y==1, 3], "bs", label="Iris versicolor")
        plt.plot(X[y==2, 2], X[y==2, 3], "g^", label="Iris virginica")
        plt.xlabel("Petal length", fontsize=14)
        plt.ylabel("Petal width", fontsize=14)
        plt.legend(fontsize=12)

        plt.subplot(122)
        plt.scatter(X[:, 2], X[:, 3], c="k", marker=".")
        plt.xlabel("Petal length", fontsize=14)
        plt.tick_params(labelleft=False)

        save_fig("classification_vs_clustering_plot")
        plt.show()
```

```
Saving figure classification_vs_clustering_plot
```



A Gaussian mixture model (explained below) can actually separate these clusters pretty well (using all 4 features: petal length & width, and sepal length & width).

```
In [5]: from sklearn.mixture import GaussianMixture

In [6]: y_pred = GaussianMixture(n_components=3, random_state=42).fit(X).predict(X)
        mapping = np.array([2, 0, 1])
        y_pred = np.array([mapping[cluster_id] for cluster_id in y_pred])

In [7]: plt.plot(X[y_pred==0, 2], X[y_pred==0, 3], "yo", label="Cluster 1")
        plt.plot(X[y_pred==1, 2], X[y_pred==1, 3], "bs", label="Cluster 2")
        plt.plot(X[y_pred==2, 2], X[y_pred==2, 3], "g^", label="Cluster 3")
        plt.xlabel("Petal length", fontsize=14)
        plt.ylabel("Petal width", fontsize=14)
        plt.legend(loc="upper left", fontsize=12)
        plt.show()
```




```
In [8]: np.sum(y_pred==y)

Out[8]: 145

In [9]: np.sum(y_pred==y) / len(y_pred)

Out[9]: 0.9666666666666667
```

2.2 K-Means

Let's start by generating some blobs:

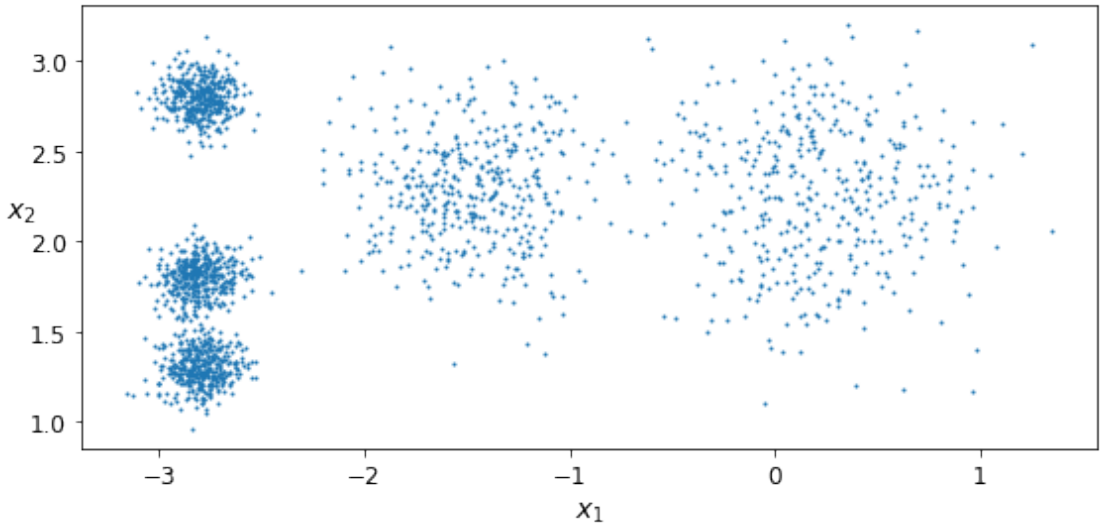
```
In [10]: from sklearn.datasets import make_blobs

In [11]: blob_centers = np.array(
             [[ 0.2,  2.3],
              [-1.5 ,  2.3],
              [-2.8,  1.8],
              [-2.8,  2.8],
              [-2.8,  1.3]])
         blob_std = np.array([0.4, 0.3, 0.1, 0.1, 0.1])

In [12]: X, y = make_blobs(n_samples=2000, centers=blob_centers,
                           cluster_std=blob_std, random_state=7)
```

Now let's plot them:

```
In [13]: def plot_clusters(X, y=None):
             plt.scatter(X[:, 0], X[:, 1], c=y, s=1)
             plt.xlabel("$x_1$", fontsize=14)
             plt.ylabel("$x_2$", fontsize=14, rotation=0)
```

```
In [14]: plt.figure(figsize=(8, 4))
         plot_clusters(X)
         save_fig("blobs_plot")
         plt.show()
```

```
Saving figure blobs_plot
```



2.2.1 Fit and Predict

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:

```
In [15]: from sklearn.cluster import KMeans
```

```
In [16]: k = 5
         kmeans = KMeans(n_clusters=k, random_state=42)
         y_pred = kmeans.fit_predict(X)
```

Each instance was assigned to one of the 5 clusters:

```
In [17]: y_pred
```

```
Out[17]: array([4, 0, 1, ..., 2, 1, 0])
```

```
In [18]: y_pred is kmeans.labels_
```

```
Out[18]: True
```

And the following 5 *centroids* (i.e., cluster centers) were estimated:

```
In [19]: kmeans.cluster_centers_

Out[19]: array([[-2.80389616,  1.80117999],
                [ 0.20876306,  2.25551336],
                [-2.79290307,  2.79641063],
                [-1.46679593,  2.28585348],
                [-2.80037642,  1.30082566]])
```

Note that the `KMeans` instance preserves the labels of the instances it was trained on. Somewhat confusingly, in this context, the *label* of an instance is the index of the cluster that instance gets assigned to:

```
In [20]: kmeans.labels_

Out[20]: array([4, 0, 1, ..., 2, 1, 0])
```

Of course, we can predict the labels of new instances:

```
In [21]: X_new = np.array([[0, 2], [3, 2], [-3, 3], [-3, 2.5]])
         kmeans.predict(X_new)

Out[21]: array([1, 1, 2, 2])
```

2.2.2 Decision Boundaries

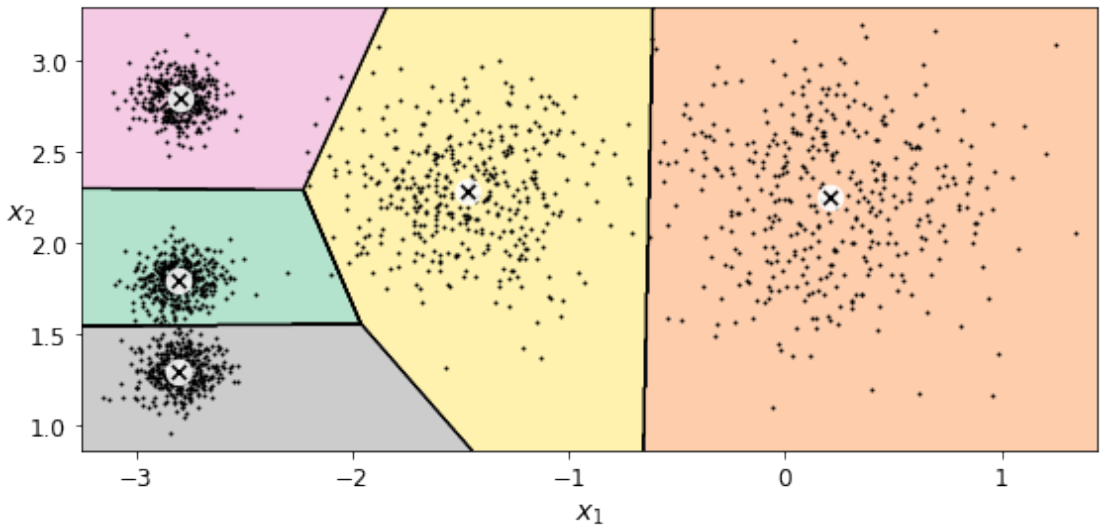
Let's plot the model's decision boundaries. This gives us a *Voronoi diagram*:

```
In [22]: def plot_data(X):
             plt.plot(X[:, 0], X[:, 1], 'k.', markersize=2)

         def plot_centroids(centroids, weights=None, circle_color='w', cross_color='k'):
             if weights is not None:
                 centroids = centroids[weights > weights.max() / 10]
             plt.scatter(centroids[:, 0], centroids[:, 1],
                         marker='o', s=30, linewidths=8,
                         color=circle_color, zorder=10, alpha=0.9)
             plt.scatter(centroids[:, 0], centroids[:, 1],
                         marker='x', s=50, linewidths=50,
                         color=cross_color, zorder=11, alpha=1)

         def plot_decision_boundaries(clusterer, X, resolution=1000, show_centroids=True,
                                      show_xlabels=True, show_ylabels=True):
             mins = X.min(axis=0) - 0.1
             maxs = X.max(axis=0) + 0.1
             xx, yy = np.meshgrid(np.linspace(mins[0], maxs[0], resolution),
                                  np.linspace(mins[1], maxs[1], resolution))
```

```
    Z = clusterer.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)

    plt.contourf(Z, extent=(mins[0], maxs[0], mins[1], maxs[1]),
                 cmap="Pastel2")
    plt.contour(Z, extent=(mins[0], maxs[0], mins[1], maxs[1]),
                linewidths=1, colors='k')
    plot_data(X)
    if show_centroids:
        plot_centroids(clusterer.cluster_centers_)

    if show_xlabels:
        plt.xlabel("$x_1$", fontsize=14)
    else:
        plt.tick_params(labelbottom=False)
    if show_ylabels:
        plt.ylabel("$x_2$", fontsize=14, rotation=0)
    else:
        plt.tick_params(labelleft=False)
```

```
In [23]: plt.figure(figsize=(8, 4))
         plot_decision_boundaries(kmeans, X)
         save_fig("voronoi_plot")
         plt.show()
```

```
Saving figure voronoi_plot
```



Not bad! Some of the instances near the edges were probably assigned to the wrong cluster, but overall it looks pretty good.

2.2.3 Hard Clustering *vs* Soft Clustering

Rather than arbitrarily choosing the closest cluster for each instance, which is called *hard clustering*, it might be better measure the distance of each instance to all 5 centroids. This is what the `transform()` method does:

```
In [24]: kmeans.transform(X_new)

Out[24]: 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]])
```

You can verify that this is indeed the Euclidian distance between each instance and each centroid:

```
In [25]: np.linalg.norm(np.tile(X_new, (1, k)).reshape(-1, k, 2) - kmeans.cluster_centers_, ax

Out[25]: 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]])
```

2.2.4 K-Means Algorithm

The K-Means algorithm is one of the fastest clustering algorithms, but also one of the simplest: * First initialize k centroids randomly: k distinct instances are chosen randomly from the dataset and the centroids are placed at their locations. * Repeat until convergence (i.e., until the centroids stop moving): * Assign each instance to the closest centroid. * Update the centroids to be the mean of the instances that are assigned to them.

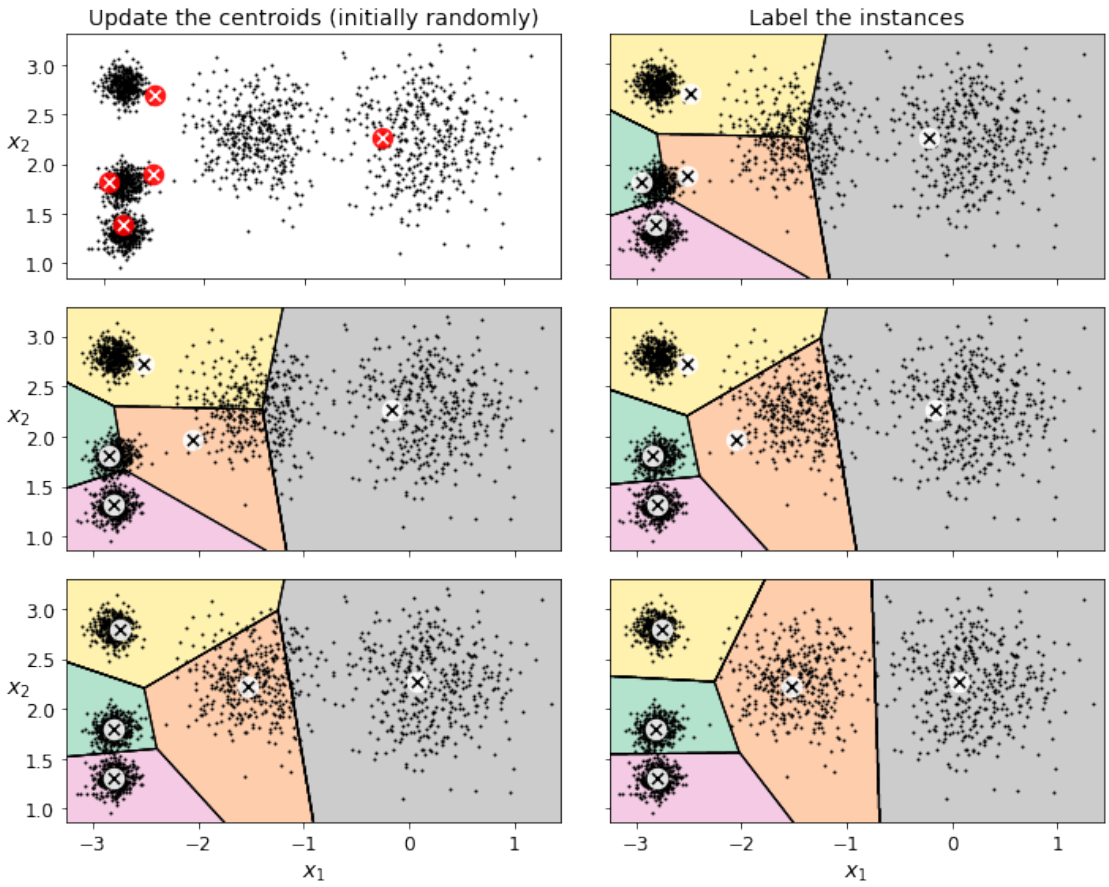
The `KMeans` class applies an optimized algorithm by default. To get the original K-Means algorithm (for educational purposes only), you must set `init="random"`, `n_init=1`and `algorithm="full"`. These hyperparameters will be explained below.

Let's run the K-Means algorithm for 1, 2 and 3 iterations, to see how the centroids move around:

```
In [26]: kmeans_iter1 = KMeans(n_clusters=5, init="random", n_init=1,
                                algorithm="full", max_iter=1, random_state=1)
         kmeans_iter2 = KMeans(n_clusters=5, init="random", n_init=1,
                                algorithm="full", max_iter=2, random_state=1)
         kmeans_iter3 = KMeans(n_clusters=5, init="random", n_init=1,
                                algorithm="full", max_iter=3, random_state=1)
         kmeans_iter1.fit(X)
         kmeans_iter2.fit(X)
         kmeans_iter3.fit(X)

Out[26]: KMeans(algorithm='full', copy_x=True, init='random', max_iter=3, n_clusters=5,
             n_init=1, n_jobs=None, precompute_distances='auto', random_state=1,
             tol=0.0001, verbose=0)
```

And let's plot this:

```
In [27]: plt.figure(figsize=(10, 8))

         plt.subplot(321)
         plot_data(X)
         plot_centroids(kmeans_iter1.cluster_centers_, circle_color='r', cross_color='w')
         plt.ylabel("$x_2$", fontsize=14, rotation=0)
         plt.tick_params(labelbottom=False)
         plt.title("Update the centroids (initially randomly)", fontsize=14)

         plt.subplot(322)
         plot_decision_boundaries(kmeans_iter1, X, show_xlabels=False, show_ylabels=False)
         plt.title("Label the instances", fontsize=14)

         plt.subplot(323)
         plot_decision_boundaries(kmeans_iter1, X, show_centroids=False, show_xlabels=False)
         plot_centroids(kmeans_iter2.cluster_centers_)

         plt.subplot(324)
         plot_decision_boundaries(kmeans_iter2, X, show_xlabels=False, show_ylabels=False)

         plt.subplot(325)
         plot_decision_boundaries(kmeans_iter2, X, show_centroids=False)
         plot_centroids(kmeans_iter3.cluster_centers_)

         plt.subplot(326)
         plot_decision_boundaries(kmeans_iter3, X, show_ylabels=False)

         save_fig("kmeans_algorithm_plot")
         plt.show()

Saving figure kmeans_algorithm_plot
```



2.2.5 K-Means Variability

In the original K-Means algorithm, the centroids are just initialized randomly, and the algorithm simply runs a single iteration to gradually improve the centroids, as we saw above.

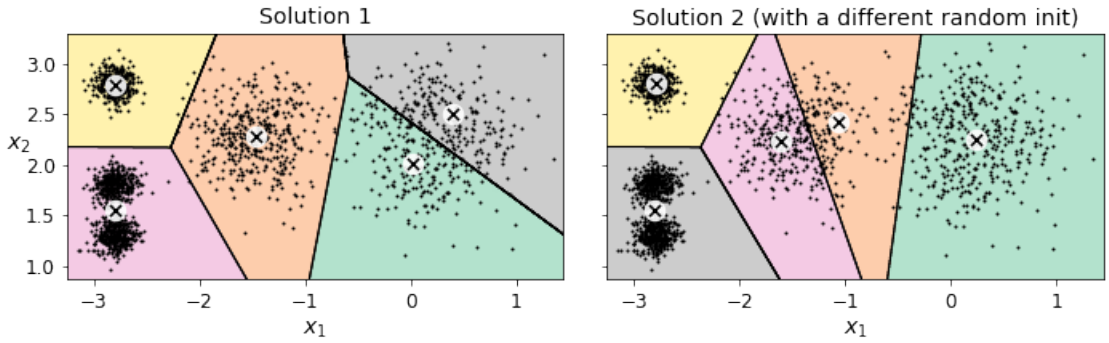
However, one major problem with this approach is that if you run K-Means multiple times (or with different random seeds), it can converge to very different solutions, as you can see below:

```
In [28]: def plot_clusterer_comparison(clusterer1, clusterer2, X, title1=None, title2=None):
             clusterer1.fit(X)
             clusterer2.fit(X)

             plt.figure(figsize=(10, 3.2))

             plt.subplot(121)
             plot_decision_boundaries(clusterer1, X)
             if title1:
                 plt.title(title1, fontsize=14)

             plt.subplot(122)
```

```
            plot_decision_boundaries(clusterer2, X, show_ylabels=False)
            if title2:
                plt.title(title2, fontsize=14)
```

```
In [29]: kmeans_rnd_init1 = KMeans(n_clusters=5, init="random", n_init=1,
                                   algorithm="full", random_state=11)
         kmeans_rnd_init2 = KMeans(n_clusters=5, init="random", n_init=1,
                                   algorithm="full", random_state=19)

         plot_clusterer_comparison(kmeans_rnd_init1, kmeans_rnd_init2, X,
                                   "Solution 1", "Solution 2 (with a different random init)")

         save_fig("kmeans_variability_plot")
         plt.show()
```

```
Saving figure kmeans_variability_plot
```



2.2.6 Inertia

To select the best model, we will need a way to evaluate a K-Mean model's performance. Unfortunately, clustering is an unsupervised task, so we do not have the targets. But at least we can measure the distance between each instance and its centroid. This is the idea behind the *inertia* metric:

```
In [30]: kmeans.inertia_
```

```
Out[30]: 211.5985372581684
```

As you can easily verify, inertia is the sum of the squared distances between each training instance and its closest centroid:

```
In [31]: X_dist = kmeans.transform(X)
         np.sum(X_dist[np.arange(len(X_dist)), kmeans.labels_]**2)
```

```
Out[31]: 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.

```
In [32]: kmeans.score(X)

Out[32]: -211.59853725816856
```

2.2.7 Multiple Initializations

So one approach to solve the variability issue is to simply run the K-Means algorithm multiple times with different random initializations, and select the solution that minimizes the inertia. For example, here are the inertias of the two "bad" models shown in the previous figure:

```
In [33]: kmeans_rnd_init1.inertia_

Out[33]: 223.29108572819035

In [34]: kmeans_rnd_init2.inertia_

Out[34]: 237.46249169442845
```

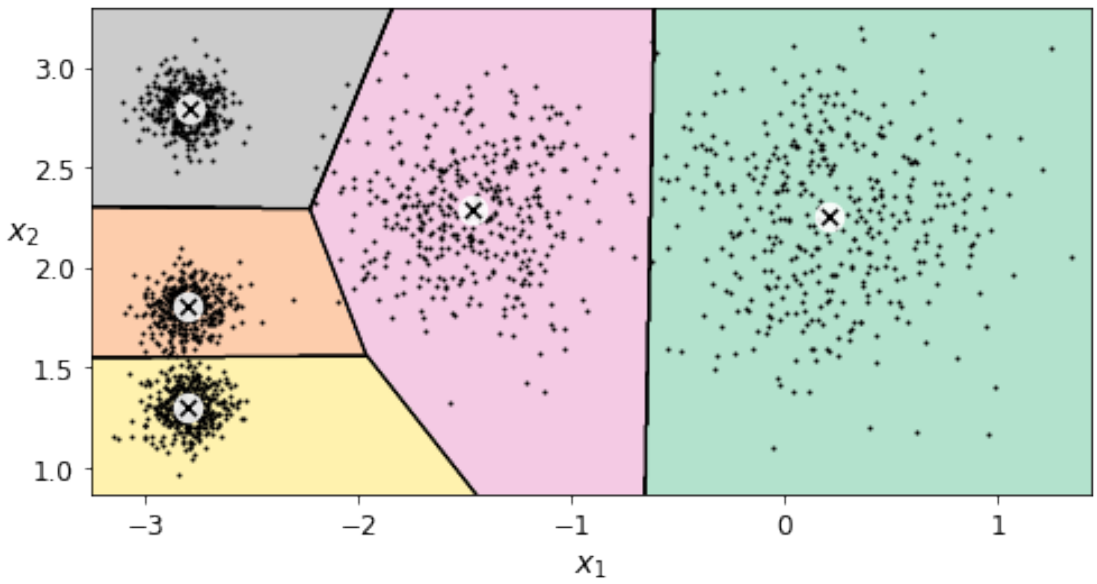
As you can see, they have a higher inertia than the first "good" model we trained, which means they are probably worse.

When you set the `n_init` hyperparameter, Scikit-Learn runs the original algorithm `n_init` times, and selects the solution that minimizes the inertia. By default, Scikit-Learn sets `n_init=10`.

```
In [35]: kmeans_rnd_10_inits = KMeans(n_clusters=5, init="random", n_init=10,
                                      algorithm="full", random_state=11)
         kmeans_rnd_10_inits.fit(X)

Out[35]: KMeans(algorithm='full', copy_x=True, init='random', max_iter=300,
             n_clusters=5, n_init=10, n_jobs=None, precompute_distances='auto',
             random_state=11, tol=0.0001, verbose=0)
```

As you can see, we end up with the initial model, which is certainly the optimal K-Means solution (at least in terms of inertia, and assuming $k = 5$).

```
In [36]: plt.figure(figsize=(8, 4))
         plot_decision_boundaries(kmeans_rnd_10_inits, X)
         plt.show()
```



2.2.8 K-Means++

Instead of initializing the centroids entirely randomly, it is preferable to initialize them using the following algorithm, proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii: * Take one centroid c_1, chosen uniformly at random from the dataset. * Take a new center c_i, choosing an instance $\mathbf{x}_i$ with probability: $D(\mathbf{x}_i)^2 \,/\, \sum_{j=1}^{m} D(\mathbf{x}_j)^2$ 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 that are 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 rest of the K-Means++ algorithm is just regular K-Means. With this initialization, the K-Means algorithm is much less likely to converge to a suboptimal solution, so it is possible to reduce `n_init` considerably. Most of the time, this largely compensates for the additional complexity of the initialization process.

To set the initialization to K-Means++, simply set `init="k-means++"` (this is actually the default):

```
In [37]: KMeans()
```

```
Out[37]: KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
             n_clusters=8, n_init=10, n_jobs=None, precompute_distances='auto',
             random_state=None, tol=0.0001, verbose=0)
```

```
In [38]: good_init = np.array([[-3, 3], [-3, 2], [-3, 1], [-1, 2], [0, 2]])
         kmeans = KMeans(n_clusters=5, init=good_init, n_init=1, random_state=42)
         kmeans.fit(X)
         kmeans.inertia_
```

```
Out[38]: 211.5985372581684
```

2.2.9 Accelerated K-Means

The K-Means algorithm can be significantly accelerated by avoiding many unnecessary distance calculations: this is achieved by exploiting the triangle inequality (given three points A, B and C, the distance AC AB + BC) and by keeping track of lower and upper bounds for distances between instances and centroids (see this 2003 paper by Charles Elkan for more details).

To use Elkan's variant of K-Means, just set `algorithm="elkan"`. Note that it does not support sparse data, so by default, Scikit-Learn uses `"elkan"` for dense data, and `"full"` (the regular K-Means algorithm) for sparse data.

```
In [39]: %timeit -n 50 KMeans(algorithm="elkan").fit(X)

274 ms ś 39.7 ms per loop (mean ś std. dev. of 7 runs, 50 loops each)


In [40]: %timeit -n 50 KMeans(algorithm="full").fit(X)

288 ms ś 46.3 ms per loop (mean ś std. dev. of 7 runs, 50 loops each)
```

2.2.10 Mini-Batch K-Means

Scikit-Learn also implements a variant of the K-Means algorithm that supports mini-batches (see this paper):

```
In [41]: from sklearn.cluster import MiniBatchKMeans

In [42]: minibatch_kmeans = MiniBatchKMeans(n_clusters=5, random_state=42)
         minibatch_kmeans.fit(X)

Out[42]: MiniBatchKMeans(batch_size=100, compute_labels=True, init='k-means++',
                 init_size=None, max_iter=100, max_no_improvement=10, n_clusters=5,
                 n_init=3, random_state=42, reassignment_ratio=0.01, tol=0.0,
                 verbose=0)

In [43]: minibatch_kmeans.inertia_

Out[43]: 211.93186531476775
```

If the dataset does not fit in memory, the simplest option is to use the `memmap` class, just like we did for incremental PCA in the previous chapter. First let's load MNIST:

```
In [44]: import urllib
         from sklearn.datasets import fetch_openml

         mnist = fetch_openml('mnist_784', version=1)
         mnist.target = mnist.target.astype(np.int64)
```

```
In [45]: from sklearn.model_selection import train_test_split

         X_train, X_test, y_train, y_test = train_test_split(
             mnist["data"], mnist["target"], random_state=42)
```

Next, let's write it to a memmap:

```
In [46]: filename = "my_mnist.data"
         X_mm = np.memmap(filename, dtype='float32', mode='write', shape=X_train.shape)
         X_mm[:] = X_train

In [47]: minibatch_kmeans = MiniBatchKMeans(n_clusters=10, batch_size=10, random_state=42)
         minibatch_kmeans.fit(X_mm)

Out[47]: MiniBatchKMeans(batch_size=10, compute_labels=True, init='k-means++',
                 init_size=None, max_iter=100, max_no_improvement=10, n_clusters=10,
                 n_init=3, random_state=42, reassignment_ratio=0.01, tol=0.0,
                 verbose=0)
```

If your data is so large that you cannot use memmap, things get more complicated. Let's start by writing a function to load the next batch (in real life, you would load the data from disk):

```
In [48]: def load_next_batch(batch_size):
             return X[np.random.choice(len(X), batch_size, replace=False)]
```

Now we can train the model by feeding it one batch at a time. We also need to implement multiple initializations and keep the model with the lowest inertia:

```
In [49]: np.random.seed(42)

In [50]: k = 5
         n_init = 10
         n_iterations = 100
         batch_size = 100
         init_size = 500  # more data for K-Means++ initialization
         evaluate_on_last_n_iters = 10

         best_kmeans = None

         for init in range(n_init):
             minibatch_kmeans = MiniBatchKMeans(n_clusters=k, init_size=init_size)
             X_init = load_next_batch(init_size)
             minibatch_kmeans.partial_fit(X_init)

             minibatch_kmeans.sum_inertia_ = 0
             for iteration in range(n_iterations):
                 X_batch = load_next_batch(batch_size)
                 minibatch_kmeans.partial_fit(X_batch)
                 if iteration >= n_iterations - evaluate_on_last_n_iters:
```

```
                    minibatch_kmeans.sum_inertia_ += minibatch_kmeans.inertia_

            if (best_kmeans is None or
                minibatch_kmeans.sum_inertia_ < best_kmeans.sum_inertia_):
                best_kmeans = minibatch_kmeans
```

```
In [51]: best_kmeans.score(X)
```

```
Out[51]: -211.70999744411483
```

Mini-batch K-Means is much faster than regular K-Means:

```
In [52]: %timeit KMeans(n_clusters=5).fit(X)
```

```
113 ms ś 7.18 ms per loop (mean ś std. dev. of 7 runs, 10 loops each)
```

```
In [53]: %timeit MiniBatchKMeans(n_clusters=5).fit(X)
```

```
52.8 ms ś 5.2 ms per loop (mean ś std. dev. of 7 runs, 10 loops each)
```

That's *much* faster! However, its performance is often lower (higher inertia), and it keeps degrading as k increases. Let's plot the inertia ratio and the training time ratio between Mini-batch K-Means and regular K-Means:

```
In [54]: from timeit import timeit
```

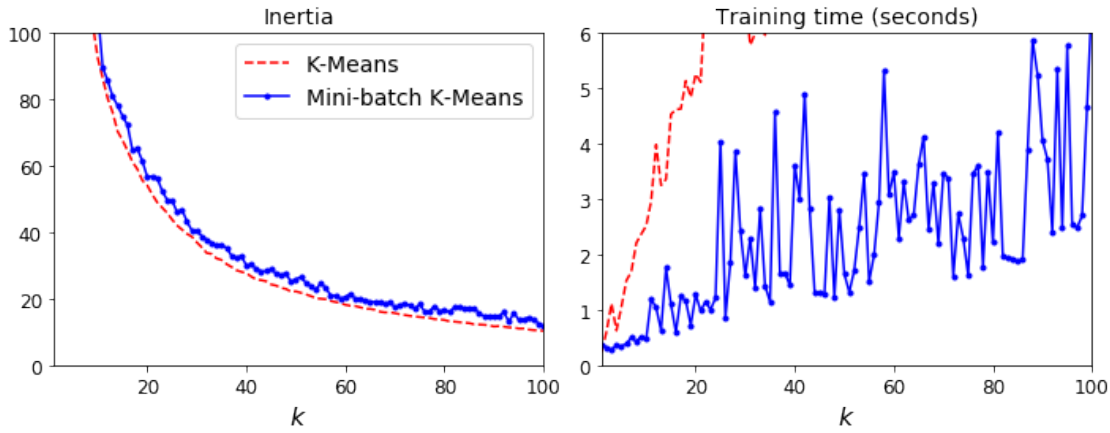
```
In [55]: times = np.empty((100, 2))
         inertias = np.empty((100, 2))
         for k in range(1, 101):
             kmeans_ = KMeans(n_clusters=k, random_state=42)
             minibatch_kmeans = MiniBatchKMeans(n_clusters=k, random_state=42)
             print("\r{}/{}".format(k, 100), end="")
             times[k-1, 0] = timeit("kmeans_.fit(X)", number=10, globals=globals())
             times[k-1, 1]  = timeit("minibatch_kmeans.fit(X)", number=10, globals=globals())
             inertias[k-1, 0] = kmeans_.inertia_
             inertias[k-1, 1] = minibatch_kmeans.inertia_
```

```
100/100
```

```
In [56]: plt.figure(figsize=(10,4))

         plt.subplot(121)
         plt.plot(range(1, 101), inertias[:, 0], "r--", label="K-Means")
         plt.plot(range(1, 101), inertias[:, 1], "b.-", label="Mini-batch K-Means")
         plt.xlabel("$k$", fontsize=16)
         plt.title("Inertia", fontsize=14)
         plt.legend(fontsize=14)
         plt.axis([1, 100, 0, 100])
```

```
plt.subplot(122)
plt.plot(range(1, 101), times[:, 0], "r--", label="K-Means")
plt.plot(range(1, 101), times[:, 1], "b.-", label="Mini-batch K-Means")
plt.xlabel("$k$", fontsize=16)
plt.title("Training time (seconds)", fontsize=14)
plt.axis([1, 100, 0, 6])

save_fig("minibatch_kmeans_vs_kmeans")
plt.show()
```

```
Saving figure minibatch_kmeans_vs_kmeans
```

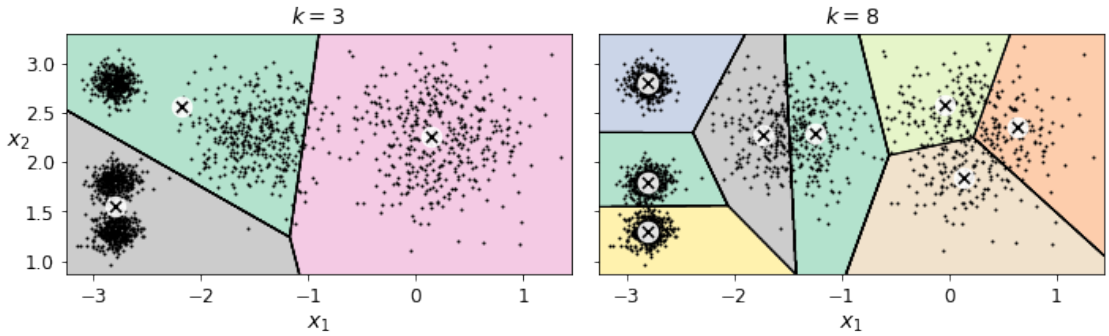


2.2.11 Finding the optimal number of clusters

What if the number of clusters was set to a lower or greater value than 5?

```
In [57]: kmeans_k3 = KMeans(n_clusters=3, random_state=42)
         kmeans_k8 = KMeans(n_clusters=8, random_state=42)

         plot_clusterer_comparison(kmeans_k3, kmeans_k8, X, "$k=3$", "$k=8$")
         save_fig("bad_n_clusters_plot")
         plt.show()
```

```
Saving figure bad_n_clusters_plot
```

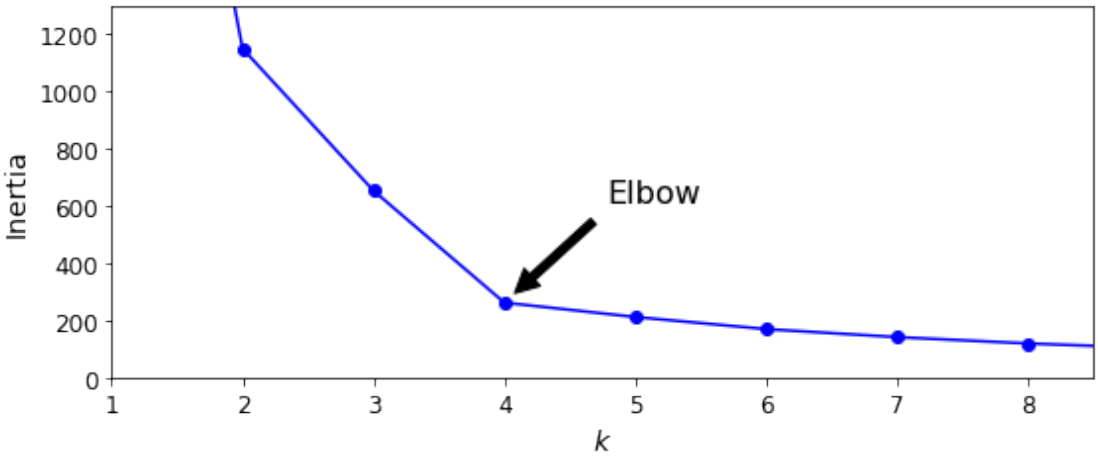


Ouch, these two models don't look great. What about their inertias?

```
In [58]: kmeans_k3.inertia_

Out[58]: 653.2167190021553

In [59]: kmeans_k8.inertia_

Out[59]: 119.11983416102879
```

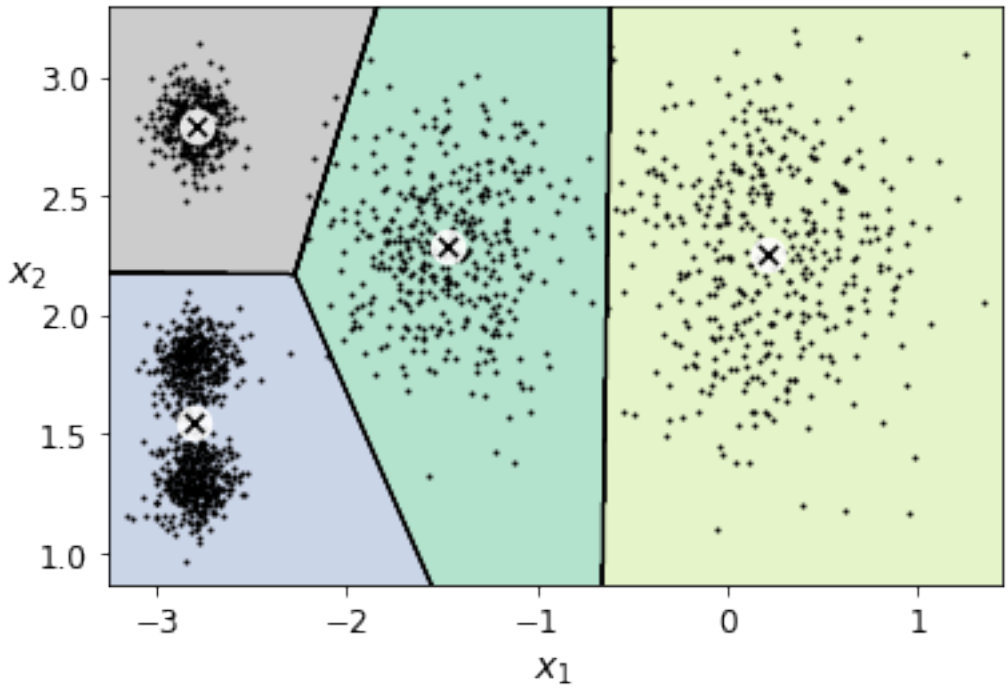
No, we cannot simply take the value of k that minimizes the inertia, since it keeps getting lower as we increase k. Indeed, the more clusters there are, the closer each instance will be to its closest centroid, and therefore the lower the inertia will be. However, we can plot the inertia as a function of k and analyze the resulting curve:

```
In [60]: kmeans_per_k = [KMeans(n_clusters=k, random_state=42).fit(X)
                         for k in range(1, 10)]
         inertias = [model.inertia_ for model in kmeans_per_k]

In [61]: plt.figure(figsize=(8, 3.5))
         plt.plot(range(1, 10), inertias, "bo-")
         plt.xlabel("$k$", fontsize=14)
         plt.ylabel("Inertia", fontsize=14)
         plt.annotate('Elbow',
                      xy=(4, inertias[3]),
                      xytext=(0.55, 0.55),
                      textcoords='figure fraction',
                      fontsize=16,
                      arrowprops=dict(facecolor='black', shrink=0.1)
                     )
         plt.axis([1, 8.5, 0, 1300])
         save_fig("inertia_vs_k_plot")
         plt.show()

Saving figure inertia_vs_k_plot
```



As you can see, there is an elbow at $k = 4$, which means that less clusters than that would be bad, and more clusters would not help much and might cut clusters in half. So $k = 4$ is a pretty good choice. Of course in this example it is not perfect since it means that the two blobs in the lower left will be considered as just a single cluster, but it's a pretty good clustering nonetheless.

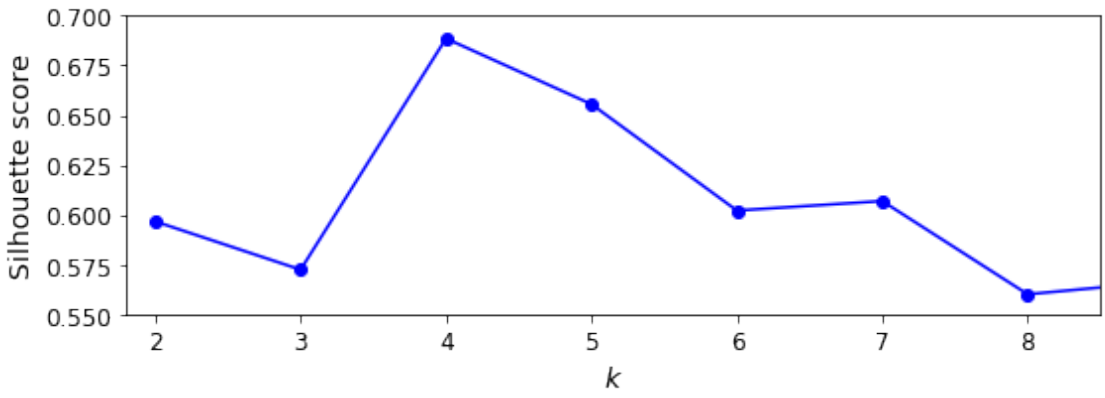
```
In [62]: plot_decision_boundaries(kmeans_per_k[4-1], X)
         plt.show()
```



Another approach is to look at 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.

Let's plot the silhouette score as a function of k:

```
In [63]: from sklearn.metrics import silhouette_score

In [64]: silhouette_score(X, kmeans.labels_)

Out[64]: 0.655517642572828

In [65]: silhouette_scores = [silhouette_score(X, model.labels_)
                              for model in kmeans_per_k[1:]]

In [66]: plt.figure(figsize=(8, 3))
         plt.plot(range(2, 10), silhouette_scores, "bo-")
         plt.xlabel("$k$", fontsize=14)
         plt.ylabel("Silhouette score", fontsize=14)
         plt.axis([1.8, 8.5, 0.55, 0.7])
         save_fig("silhouette_score_vs_k_plot")
         plt.show()

Saving figure silhouette_score_vs_k_plot
```

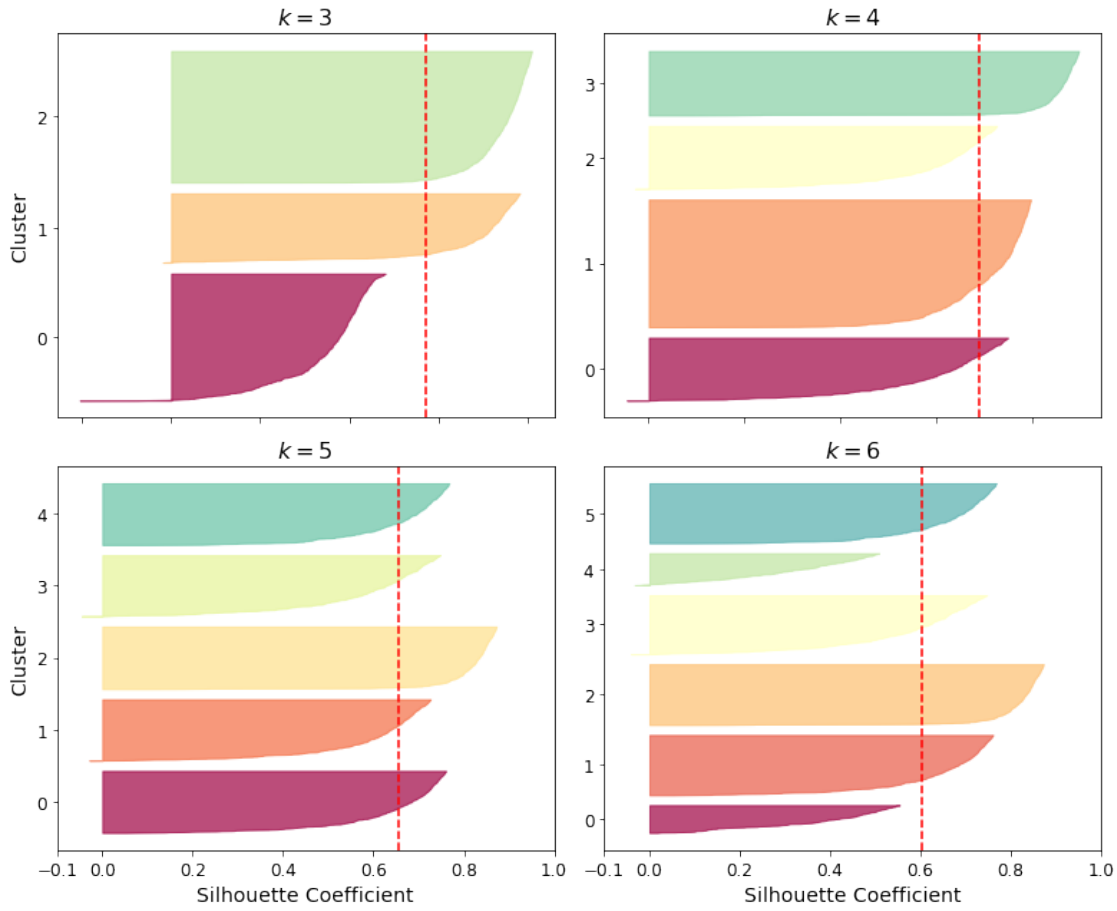


As you can see, this visualization is much richer than the previous one: in particular, although it confirms that $k = 4$ is a very good choice, but it also underlines the fact that $k = 5$ is quite good as well.

An even more informative visualization is given 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*:

In [67]:
```
from sklearn.metrics import silhouette_samples
from matplotlib.ticker import FixedLocator, FixedFormatter

plt.figure(figsize=(11, 9))

for k in (3, 4, 5, 6):
    plt.subplot(2, 2, k - 2)

    y_pred = kmeans_per_k[k - 1].labels_
    silhouette_coefficients = silhouette_samples(X, y_pred)

    padding = len(X) // 30
    pos = padding
    ticks = []
    for i in range(k):
        coeffs = silhouette_coefficients[y_pred == i]
        coeffs.sort()

        color = mpl.cm.Spectral(i / k)
        plt.fill_betweenx(np.arange(pos, pos + len(coeffs)), 0, coeffs,
                          facecolor=color, edgecolor=color, alpha=0.7)
        ticks.append(pos + len(coeffs) // 2)
        pos += len(coeffs) + padding

    plt.gca().yaxis.set_major_locator(FixedLocator(ticks))
    plt.gca().yaxis.set_major_formatter(FixedFormatter(range(k)))
    if k in (3, 5):
        plt.ylabel("Cluster")

    if k in (5, 6):
        plt.gca().set_xticks([-0.1, 0, 0.2, 0.4, 0.6, 0.8, 1])
        plt.xlabel("Silhouette Coefficient")
    else:
        plt.tick_params(labelbottom=False)

    plt.axvline(x=silhouette_scores[k - 2], color="red", linestyle="--")
    plt.title("$k={}$".format(k), fontsize=16)

save_fig("silhouette_analysis_plot")
plt.show()
```

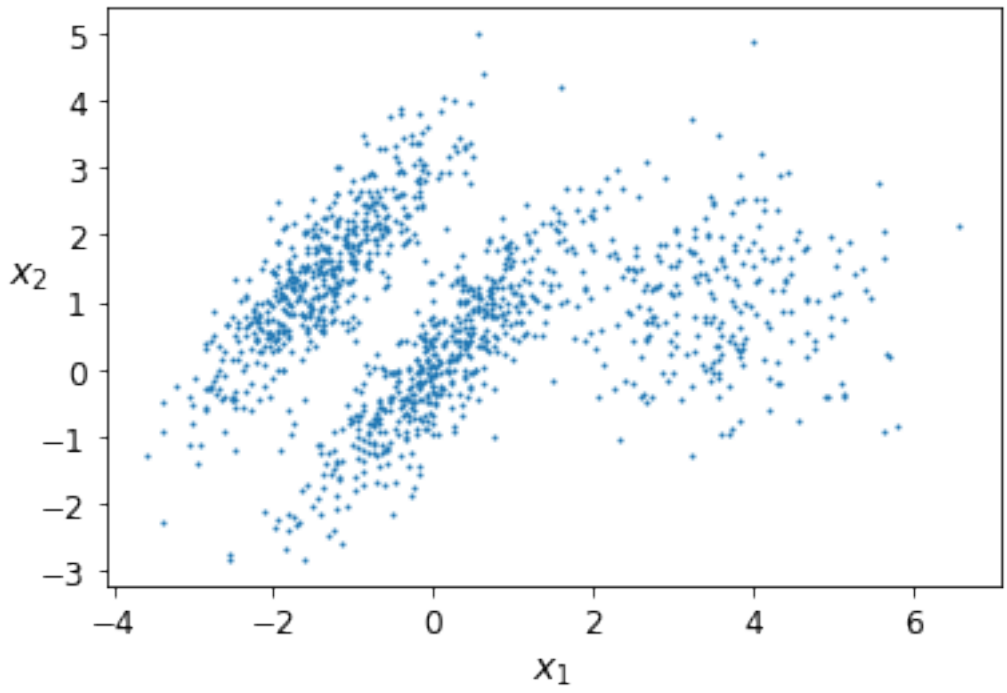
```
Saving figure silhouette_analysis_plot
```



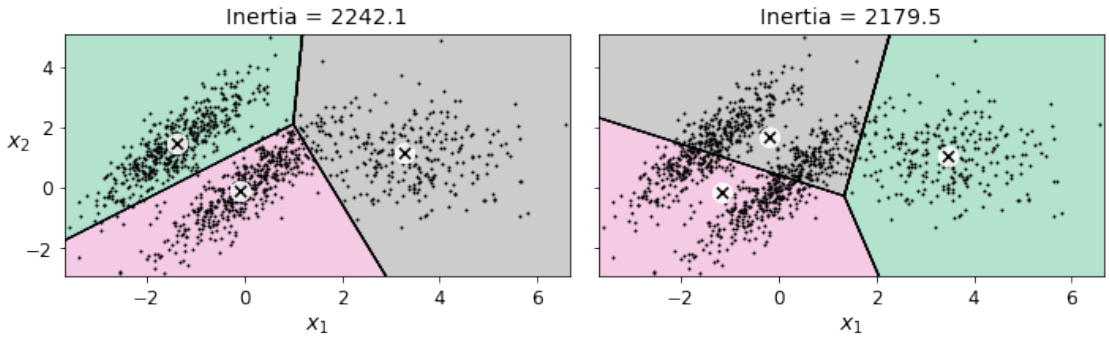
2.2.12 Limits of K-Means

```
In [68]: X1, y1 = make_blobs(n_samples=1000, centers=((4, -4), (0, 0)), random_state=42)
         X1 = X1.dot(np.array([[0.374, 0.95], [0.732, 0.598]]))
         X2, y2 = make_blobs(n_samples=250, centers=1, random_state=42)
         X2 = X2 + [6, -8]
         X = np.r_[X1, X2]
         y = np.r_[y1, y2]
```

```
In [69]: plot_clusters(X)
```




```
In [70]: kmeans_good = KMeans(n_clusters=3, init=np.array([[-1.5, 2.5], [0.5, 0], [4, 0]]), n_
         kmeans_bad = KMeans(n_clusters=3, random_state=42)
         kmeans_good.fit(X)
         kmeans_bad.fit(X)

Out[70]: KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
             n_clusters=3, n_init=10, n_jobs=None, precompute_distances='auto',
             random_state=42, tol=0.0001, verbose=0)

In [71]: plt.figure(figsize=(10, 3.2))

         plt.subplot(121)
         plot_decision_boundaries(kmeans_good, X)
         plt.title("Inertia = {:.1f}".format(kmeans_good.inertia_), fontsize=14)

         plt.subplot(122)
         plot_decision_boundaries(kmeans_bad, X, show_ylabels=False)
         plt.title("Inertia = {:.1f}".format(kmeans_bad.inertia_), fontsize=14)

         save_fig("bad_kmeans_plot")
         plt.show()

Saving figure bad_kmeans_plot
```



2.2.13 Using clustering for image segmentation

```
In [72]: # Download the ladybug image
         images_path = os.path.join(PROJECT_ROOT_DIR, "images", "unsupervised_learning")
         os.makedirs(images_path, exist_ok=True)
         DOWNLOAD_ROOT = "https://raw.githubusercontent.com/ageron/handson-ml2/master/"
         filename = "ladybug.png"
         print("Downloading", filename)
         url = DOWNLOAD_ROOT + "images/unsupervised_learning/" + filename
         urllib.request.urlretrieve(url, os.path.join(images_path, filename))
```

```
Downloading ladybug.png
```

```
Out[72]: ('.\\images\\unsupervised_learning\\ladybug.png',
          <http.client.HTTPMessage at 0x1a0daa526d8>)
```

```
In [73]: from matplotlib.image import imread
         image = imread(os.path.join(images_path, filename))
         image.shape
```

```
Out[73]: (533, 800, 3)
```

```
In [74]: X = image.reshape(-1, 3)
         kmeans = KMeans(n_clusters=8, random_state=42).fit(X)
         segmented_img = kmeans.cluster_centers_[kmeans.labels_]
         segmented_img = segmented_img.reshape(image.shape)
```

```
In [75]: segmented_imgs = []
         n_colors = (10, 8, 6, 4, 2)
         for n_clusters in n_colors:
             kmeans = KMeans(n_clusters=n_clusters, random_state=42).fit(X)
             segmented_img = kmeans.cluster_centers_[kmeans.labels_]
             segmented_imgs.append(segmented_img.reshape(image.shape))
```

```
In [76]: plt.figure(figsize=(10,5))
         plt.subplots_adjust(wspace=0.05, hspace=0.1)

         plt.subplot(231)
         plt.imshow(image)
         plt.title("Original image")
         plt.axis('off')

         for idx, n_clusters in enumerate(n_colors):
             plt.subplot(232 + idx)
             plt.imshow(segmented_imgs[idx])
             plt.title("{} colors".format(n_clusters))
             plt.axis('off')

         save_fig('image_segmentation_diagram', tight_layout=False)
         plt.show()
```

```
Saving figure image_segmentation_diagram
```

2.2.14 Using Clustering for Preprocessing

Let's tackle the *digits dataset* which is a simple MNIST-like dataset containing 1,797 grayscale 8Œ8 images representing digits 0 to 9.

```
In [77]: from sklearn.datasets import load_digits
```

```
In [78]: X_digits, y_digits = load_digits(return_X_y=True)
```

Let's split it into a training set and a test set:

```
In [79]: from sklearn.model_selection import train_test_split

In [80]: X_train, X_test, y_train, y_test = train_test_split(X_digits, y_digits, random_state=
```

Now let's fit a Logistic Regression model and evaluate it on the test set:

```
In [81]: from sklearn.linear_model import LogisticRegression

In [82]: log_reg = LogisticRegression(multi_class="ovr", solver="lbfgs", max_iter=5000, random_
         log_reg.fit(X_train, y_train)

Out[82]: LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
                            intercept_scaling=1, max_iter=5000, multi_class='ovr',
                            n_jobs=None, penalty='l2', random_state=42, solver='lbfgs',
                            tol=0.0001, verbose=0, warm_start=False)

In [83]: log_reg.score(X_test, y_test)

Out[83]: 0.9688888888888889
```

Okay, that's our baseline: 96.89% 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 the 50 clusters, then apply a logistic regression model:

```
In [84]: from sklearn.pipeline import Pipeline

In [85]: pipeline = Pipeline([
             ("kmeans", KMeans(n_clusters=50, random_state=42)),
             ("log_reg", LogisticRegression(multi_class="ovr", solver="lbfgs", max_iter=5000, r
         ])
         pipeline.fit(X_train, y_train)

Out[85]: Pipeline(memory=None,
              steps=[('kmeans', KMeans(algorithm='auto', copy_x=True, init='k-means++', max_ite
                     n_clusters=50, n_init=10, n_jobs=None, precompute_distances='auto',
                     random_state=42, tol=0.0001, verbose=0)), ('log_reg', LogisticRegression(C=1.0, cl
                            intercept_scaling=1, max_iter=5000, multi_class='ovr',
                            n_jobs=None, penalty='l2', random_state=42, solver='lbfgs',
                            tol=0.0001, verbose=0, warm_start=False))])

In [86]: pipeline.score(X_test, y_test)

Out[86]: 0.9777777777777777

In [87]: 1 - (1 - 0.977777) / (1 - 0.968888)

Out[87]: 0.28570969400874346
```

How about that? We reduced the error rate by over 28%! 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.

```
In [88]: from sklearn.model_selection import GridSearchCV

In [89]: 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)

Fitting 3 folds for each of 98 candidates, totalling 294 fits
[CV] kmeans__n_clusters=2 ...


[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.


[CV] ... kmeans__n_clusters=2, total=   0.3s
[CV] kmeans__n_clusters=2 ...


[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:    0.3s remaining:    0.0s


[CV] ... kmeans__n_clusters=2, total=   0.2s
[CV] kmeans__n_clusters=2 ...
[CV] ... kmeans__n_clusters=2, total=   0.4s
[CV] kmeans__n_clusters=3 ...
[CV] ... kmeans__n_clusters=3, total=   0.4s
[CV] kmeans__n_clusters=3 ...
[CV] ... kmeans__n_clusters=3, total=   0.3s
[CV] kmeans__n_clusters=3 ...
[CV] ... kmeans__n_clusters=3, total=   0.2s
[CV] kmeans__n_clusters=4 ...
[CV] ... kmeans__n_clusters=4, total=   0.3s
[CV] kmeans__n_clusters=4 ...
[CV] ... kmeans__n_clusters=4, total=   0.3s
[CV] kmeans__n_clusters=4 ...
[CV] ... kmeans__n_clusters=4, total=   0.3s
[CV] kmeans__n_clusters=5 ...
[CV] ... kmeans__n_clusters=5, total=   0.4s
[CV] kmeans__n_clusters=5 ...
[CV] ... kmeans__n_clusters=5, total=   0.4s
[CV] kmeans__n_clusters=5 ...
[CV] ... kmeans__n_clusters=5, total=   0.4s
[CV] kmeans__n_clusters=6 ...
[CV] ... kmeans__n_clusters=6, total=   0.5s
```

```
[CV] kmeans__n_clusters=6 ...
[CV] ... kmeans__n_clusters=6, total=   0.5s
[CV] kmeans__n_clusters=6 ...
[CV] ... kmeans__n_clusters=6, total=   0.5s
[CV] kmeans__n_clusters=7 ...
[CV] ... kmeans__n_clusters=7, total=   0.5s
[CV] kmeans__n_clusters=7 ...
[CV] ... kmeans__n_clusters=7, total=   0.5s
[CV] kmeans__n_clusters=7 ...
[CV] ... kmeans__n_clusters=7, total=   0.6s
[CV] kmeans__n_clusters=8 ...
[CV] ... kmeans__n_clusters=8, total=   0.8s
[CV] kmeans__n_clusters=8 ...
[CV] ... kmeans__n_clusters=8, total=   0.9s
[CV] kmeans__n_clusters=8 ...
[CV] ... kmeans__n_clusters=8, total=   0.8s
[CV] kmeans__n_clusters=9 ...
[CV] ... kmeans__n_clusters=9, total=   0.9s
[CV] kmeans__n_clusters=9 ...
[CV] ... kmeans__n_clusters=9, total=   1.0s
[CV] kmeans__n_clusters=9 ...
[CV] ... kmeans__n_clusters=9, total=   1.0s
[CV] kmeans__n_clusters=10 ...
[CV] ... kmeans__n_clusters=10, total=   1.2s
[CV] kmeans__n_clusters=10 ...
[CV] ... kmeans__n_clusters=10, total=   1.2s
[CV] kmeans__n_clusters=10 ...
[CV] ... kmeans__n_clusters=10, total=   1.0s
[CV] kmeans__n_clusters=11 ...
[CV] ... kmeans__n_clusters=11, total=   1.4s
[CV] kmeans__n_clusters=11 ...
[CV] ... kmeans__n_clusters=11, total=   1.5s
[CV] kmeans__n_clusters=11 ...
[CV] ... kmeans__n_clusters=11, total=   1.5s
[CV] kmeans__n_clusters=12 ...
[CV] ... kmeans__n_clusters=12, total=   2.0s
[CV] kmeans__n_clusters=12 ...
[CV] ... kmeans__n_clusters=12, total=   2.1s
[CV] kmeans__n_clusters=12 ...
[CV] ... kmeans__n_clusters=12, total=   1.9s
[CV] kmeans__n_clusters=13 ...
[CV] ... kmeans__n_clusters=13, total=   2.1s
[CV] kmeans__n_clusters=13 ...
[CV] ... kmeans__n_clusters=13, total=   2.0s
[CV] kmeans__n_clusters=13 ...
[CV] ... kmeans__n_clusters=13, total=   1.7s
[CV] kmeans__n_clusters=14 ...
[CV] ... kmeans__n_clusters=14, total=   2.4s
```

```
[CV] kmeans__n_clusters=14 ...
[CV] ... kmeans__n_clusters=14, total=   2.3s
[CV] kmeans__n_clusters=14 ...
[CV] ... kmeans__n_clusters=14, total=   2.4s
[CV] kmeans__n_clusters=15 ...
[CV] ... kmeans__n_clusters=15, total=   3.2s
[CV] kmeans__n_clusters=15 ...
[CV] ... kmeans__n_clusters=15, total=   2.8s
[CV] kmeans__n_clusters=15 ...
[CV] ... kmeans__n_clusters=15, total=   2.5s
[CV] kmeans__n_clusters=16 ...
[CV] ... kmeans__n_clusters=16, total=   2.9s
[CV] kmeans__n_clusters=16 ...
[CV] ... kmeans__n_clusters=16, total=   3.1s
[CV] kmeans__n_clusters=16 ...
[CV] ... kmeans__n_clusters=16, total=   2.7s
[CV] kmeans__n_clusters=17 ...
[CV] ... kmeans__n_clusters=17, total=   3.6s
[CV] kmeans__n_clusters=17 ...
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[CV] ... kmeans__n_clusters=88, total=   6.9s
[CV] kmeans__n_clusters=88 ...
[CV] ... kmeans__n_clusters=88, total=   6.4s
[CV] kmeans__n_clusters=88 ...
[CV] ... kmeans__n_clusters=88, total=   6.0s
[CV] kmeans__n_clusters=89 ...
[CV] ... kmeans__n_clusters=89, total=   6.4s
[CV] kmeans__n_clusters=89 ...
[CV] ... kmeans__n_clusters=89, total=   7.7s
[CV] kmeans__n_clusters=89 ...
[CV] ... kmeans__n_clusters=89, total=   6.7s
[CV] kmeans__n_clusters=90 ...
[CV] ... kmeans__n_clusters=90, total=   6.6s
[CV] kmeans__n_clusters=90 ...
[CV] ... kmeans__n_clusters=90, total=   6.9s
[CV] kmeans__n_clusters=90 ...
[CV] ... kmeans__n_clusters=90, total=   5.8s
[CV] kmeans__n_clusters=91 ...
[CV] ... kmeans__n_clusters=91, total=   6.3s
[CV] kmeans__n_clusters=91 ...
[CV] ... kmeans__n_clusters=91, total=   7.0s
[CV] kmeans__n_clusters=91 ...
[CV] ... kmeans__n_clusters=91, total=   6.5s
[CV] kmeans__n_clusters=92 ...
[CV] ... kmeans__n_clusters=92, total=   7.8s
[CV] kmeans__n_clusters=92 ...
[CV] ... kmeans__n_clusters=92, total=   6.7s
[CV] kmeans__n_clusters=92 ...
[CV] ... kmeans__n_clusters=92, total=   6.4s
[CV] kmeans__n_clusters=93 ...
[CV] ... kmeans__n_clusters=93, total=   6.3s
[CV] kmeans__n_clusters=93 ...
[CV] ... kmeans__n_clusters=93, total=   6.8s
[CV] kmeans__n_clusters=93 ...
[CV] ... kmeans__n_clusters=93, total=   7.5s
[CV] kmeans__n_clusters=94 ...
[CV] ... kmeans__n_clusters=94, total=   6.2s
```

```
[CV] kmeans__n_clusters=94 ...
[CV] ... kmeans__n_clusters=94, total=   7.1s
[CV] kmeans__n_clusters=94 ...
[CV] ... kmeans__n_clusters=94, total=   6.0s
[CV] kmeans__n_clusters=95 ...
[CV] ... kmeans__n_clusters=95, total=   6.3s
[CV] kmeans__n_clusters=95 ...
[CV] ... kmeans__n_clusters=95, total=   6.3s
[CV] kmeans__n_clusters=95 ...
[CV] ... kmeans__n_clusters=95, total=   6.5s
[CV] kmeans__n_clusters=96 ...
[CV] ... kmeans__n_clusters=96, total=   7.1s
[CV] kmeans__n_clusters=96 ...
[CV] ... kmeans__n_clusters=96, total=   7.1s
[CV] kmeans__n_clusters=96 ...
[CV] ... kmeans__n_clusters=96, total=   7.1s
[CV] kmeans__n_clusters=97 ...
[CV] ... kmeans__n_clusters=97, total=   7.6s
[CV] kmeans__n_clusters=97 ...
[CV] ... kmeans__n_clusters=97, total=   6.7s
[CV] kmeans__n_clusters=97 ...
[CV] ... kmeans__n_clusters=97, total=   6.3s
[CV] kmeans__n_clusters=98 ...
[CV] ... kmeans__n_clusters=98, total=   6.8s
[CV] kmeans__n_clusters=98 ...
[CV] ... kmeans__n_clusters=98, total=   8.5s
[CV] kmeans__n_clusters=98 ...
[CV] ... kmeans__n_clusters=98, total=   7.3s
[CV] kmeans__n_clusters=99 ...
[CV] ... kmeans__n_clusters=99, total=   6.8s
[CV] kmeans__n_clusters=99 ...
[CV] ... kmeans__n_clusters=99, total=   6.4s
[CV] kmeans__n_clusters=99 ...
[CV] ... kmeans__n_clusters=99, total=   8.3s

[Parallel(n_jobs=1)]: Done 294 out of 294 | elapsed: 30.1min finished

Out[89]: GridSearchCV(cv=3, error_score='raise-deprecating',
               estimator=Pipeline(memory=None,
              steps=[('kmeans', KMeans(algorithm='auto', copy_x=True, init='k-means++', max_ite
             n_clusters=50, n_init=10, n_jobs=None, precompute_distances='auto',
             random_state=42, tol=0.0001, verbose=0)), ('log_reg', LogisticRegression(C=1.0, cl
                   tol=0.0001, verbose=0, warm_start=False))]),
               fit_params=None, iid='warn', n_jobs=None,
               param_grid={'kmeans__n_clusters': range(2, 100)},
               pre_dispatch='2*n_jobs', refit=True, return_train_score='warn',
               scoring=None, verbose=2)
```

Let's see what the best number of clusters is:

```
In [90]: grid_clf.best_params_

Out[90]: {'kmeans__n_clusters': 77}

In [91]: grid_clf.score(X_test, y_test)

Out[91]: 0.9822222222222222
```

2.2.15 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 look at the performance of a logistic regression model when we only have 50 labeled instances:

```
In [92]: n_labeled = 50

In [93]: log_reg = LogisticRegression(multi_class="ovr", solver="lbfgs", random_state=42)
         log_reg.fit(X_train[:n_labeled], y_train[:n_labeled])
         log_reg.score(X_test, y_test)

Out[93]: 0.8333333333333334
```

It's much less than earlier of course. 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:

```
In [94]: k = 50

In [95]: kmeans = KMeans(n_clusters=k, random_state=42)
         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]
```

Now let's plot these representative images and label them manually:

```
In [96]: plt.figure(figsize=(8, 2))
         for index, X_representative_digit in enumerate(X_representative_digits):
             plt.subplot(k // 10, 10, index + 1)
             plt.imshow(X_representative_digit.reshape(8, 8), cmap="binary", interpolation="bi
             plt.axis('off')

         save_fig("representative_images_diagram", tight_layout=False)
         plt.show()

Saving figure representative_images_diagram
```

```
In [97]: y_representative_digits = np.array([
             4, 8, 0, 6, 8, 3, 7, 7, 9, 2,
             5, 5, 8, 5, 2, 1, 2, 9, 6, 1,
             1, 6, 9, 0, 8, 3, 0, 7, 4, 1,
             6, 5, 2, 4, 1, 8, 6, 3, 9, 2,
             4, 2, 9, 4, 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:

```
In [98]: log_reg = LogisticRegression(multi_class="ovr", solver="lbfgs", max_iter=5000, random
         log_reg.fit(X_representative_digits, y_representative_digits)
         log_reg.score(X_test, y_test)

Out[98]: 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's often costly and painful to label instances, especially when it has to be done manually by experts, it's a good idea to make them 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?

```
In [99]: 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]

In [100]: log_reg = LogisticRegression(multi_class="ovr", solver="lbfgs", max_iter=5000, rando
          log_reg.fit(X_train, y_train_propagated)

Out[100]: LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
                    intercept_scaling=1, max_iter=5000, multi_class='ovr',
                    n_jobs=None, penalty='l2', random_state=42, solver='lbfgs',
                    tol=0.0001, verbose=0, warm_start=False)
```

```
In [101]: log_reg.score(X_test, y_test)

Out[101]: 0.9333333333333333
```

We got a tiny little accuracy boost. Better than nothing, but we should probably have propagated the labels only to the instances closest to the centroid, because by propagating to the full cluster, we have certainly included some outliers. Let's only propagate the labels to the 20th percentile closest to the centroid:

```
In [102]: 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

In [103]: partially_propagated = (X_cluster_dist != -1)
          X_train_partially_propagated = X_train[partially_propagated]
          y_train_partially_propagated = y_train_propagated[partially_propagated]

In [104]: log_reg = LogisticRegression(multi_class="ovr", solver="lbfgs", max_iter=5000, rando
          log_reg.fit(X_train_partially_propagated, y_train_partially_propagated)

Out[104]: LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
                    intercept_scaling=1, max_iter=5000, multi_class='ovr',
                    n_jobs=None, penalty='l2', random_state=42, solver='lbfgs',
                    tol=0.0001, verbose=0, warm_start=False)

In [105]: log_reg.score(X_test, y_test)

Out[105]: 0.94
```

Nice! With just 50 labeled instances (just 5 examples per class on average!), we got 94% performance, which is pretty close to the performance of logistic regression on the fully labeled *digits* dataset (which was 96.9%).

This is because the propagated labels are actually pretty good: their accuracy is very close to 99%:

```
In [106]: np.mean(y_train_partially_propagated == y_train[partially_propagated])

Out[106]: 0.9896907216494846
```

You could now do a few iterations of *active learning*: 1. Manually label the instances that the classifier is least sure about, if possible by picking them in distinct clusters. 2. Train a new model with these additional labels.

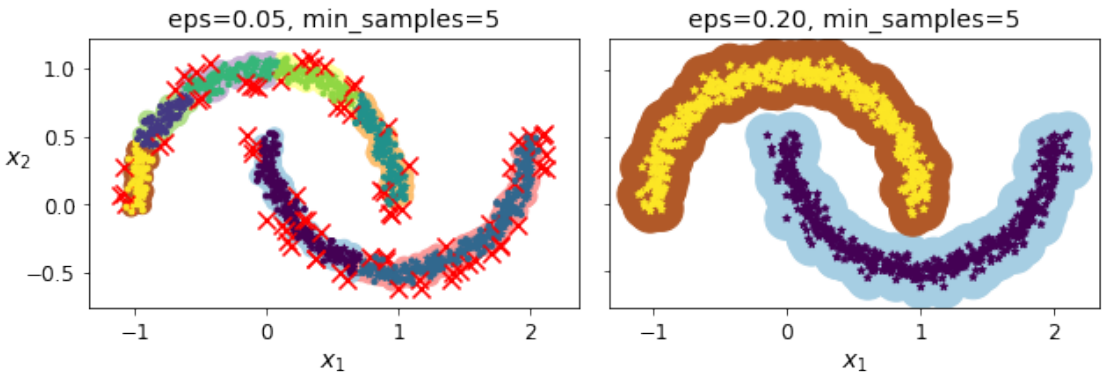
2.3 DBSCAN

```
In [107]: from sklearn.datasets import make_moons

In [108]: X, y = make_moons(n_samples=1000, noise=0.05, random_state=42)

In [109]: from sklearn.cluster import DBSCAN

In [110]: dbscan = DBSCAN(eps=0.05, min_samples=5)
          dbscan.fit(X)

Out[110]: DBSCAN(algorithm='auto', eps=0.05, leaf_size=30, metric='euclidean',
              metric_params=None, min_samples=5, n_jobs=None, p=None)

In [111]: dbscan.labels_[:10]

Out[111]: array([ 0,  2, -1, -1,  1,  0,  0,  0,  2,  5], dtype=int64)

In [112]: len(dbscan.core_sample_indices_)

Out[112]: 808

In [113]: dbscan.core_sample_indices_[:10]

Out[113]: array([ 0,  4,  5,  6,  7,  8, 10, 11, 12, 13], dtype=int64)

In [114]: dbscan.components_[:3]

Out[114]: array([[-0.02137124,  0.40618608],
                 [-0.84192557,  0.53058695],
                 [ 0.58930337, -0.32137599]])

In [115]: np.unique(dbscan.labels_)

Out[115]: array([-1,  0,  1,  2,  3,  4,  5,  6], dtype=int64)

In [116]: dbscan2 = DBSCAN(eps=0.2)
          dbscan2.fit(X)

Out[116]: DBSCAN(algorithm='auto', eps=0.2, leaf_size=30, metric='euclidean',
              metric_params=None, min_samples=5, n_jobs=None, p=None)

In [117]: def plot_dbscan(dbscan, X, size, show_xlabels=True, show_ylabels=True):
              core_mask = np.zeros_like(dbscan.labels_, dtype=bool)
              core_mask[dbscan.core_sample_indices_] = True
              anomalies_mask = dbscan.labels_ == -1
              non_core_mask = ~(core_mask | anomalies_mask)

              cores = dbscan.components_
              anomalies = X[anomalies_mask]
              non_cores = X[non_core_mask]
```

```
            plt.scatter(cores[:, 0], cores[:, 1],
                        c=dbscan.labels_[core_mask], marker='o', s=size, cmap="Paired")
            plt.scatter(cores[:, 0], cores[:, 1], marker='*', s=20, c=dbscan.labels_[core_mas
            plt.scatter(anomalies[:, 0], anomalies[:, 1],
                        c="r", marker="x", s=100)
            plt.scatter(non_cores[:, 0], non_cores[:, 1], c=dbscan.labels_[non_core_mask], ma
            if show_xlabels:
                plt.xlabel("$x_1$", fontsize=14)
            else:
                plt.tick_params(labelbottom=False)
            if show_ylabels:
                plt.ylabel("$x_2$", fontsize=14, rotation=0)
            else:
                plt.tick_params(labelleft=False)
            plt.title("eps={:.2f}, min_samples={}".format(dbscan.eps, dbscan.min_samples), fo
```

In [118]:
```
plt.figure(figsize=(9, 3.2))

plt.subplot(121)
plot_dbscan(dbscan, X, size=100)

plt.subplot(122)
plot_dbscan(dbscan2, X, size=600, show_ylabels=False)

save_fig("dbscan_plot")
plt.show()
```

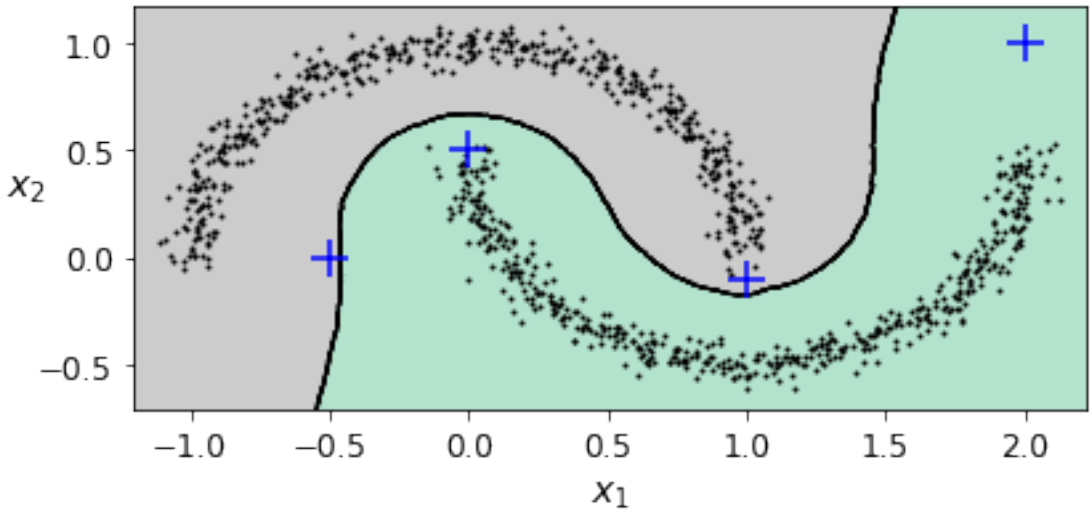
```
Saving figure dbscan_plot
```



In [119]:
```
dbscan = dbscan2
```

In [120]:
```
from sklearn.neighbors import KNeighborsClassifier
```

```
In [121]: knn = KNeighborsClassifier(n_neighbors=50)
          knn.fit(dbscan.components_, dbscan.labels_[dbscan.core_sample_indices_])

Out[121]: KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                               metric_params=None, n_jobs=None, n_neighbors=50, p=2,
                               weights='uniform')

In [122]: X_new = np.array([[-0.5, 0], [0, 0.5], [1, -0.1], [2, 1]])
          knn.predict(X_new)

Out[122]: array([1, 0, 1, 0], dtype=int64)

In [123]: knn.predict_proba(X_new)

Out[123]: array([[0.18, 0.82],
                 [1.  , 0.  ],
                 [0.12, 0.88],
                 [1.  , 0.  ]])

In [124]: plt.figure(figsize=(6, 3))
          plot_decision_boundaries(knn, X, show_centroids=False)
          plt.scatter(X_new[:, 0], X_new[:, 1], c="b", marker="+", s=200, zorder=10)
          save_fig("cluster_classification_plot")
          plt.show()

Saving figure cluster_classification_plot
```

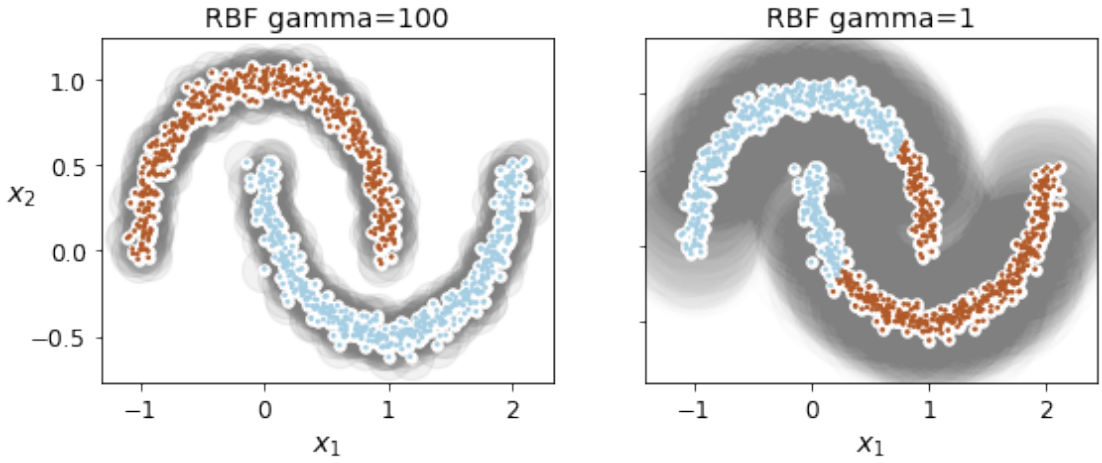



```
In [125]: y_dist, y_pred_idx = knn.kneighbors(X_new, n_neighbors=1)
          y_pred = dbscan.labels_[dbscan.core_sample_indices_][y_pred_idx]
          y_pred[y_dist > 0.2] = -1
          y_pred.ravel()

Out[125]: array([-1,  0,  1, -1], dtype=int64)
```

2.4 Other Clustering Algorithms

2.4.1 Spectral Clustering

```
In [126]: from sklearn.cluster import SpectralClustering

In [127]: sc1 = SpectralClustering(n_clusters=2, gamma=100, random_state=42)
          sc1.fit(X)

Out[127]: SpectralClustering(affinity='rbf', assign_labels='kmeans', coef0=1, degree=3,
                    eigen_solver=None, eigen_tol=0.0, gamma=100, kernel_params=None,
                    n_clusters=2, n_init=10, n_jobs=None, n_neighbors=10,
                    random_state=42)

In [128]: sc2 = SpectralClustering(n_clusters=2, gamma=1, random_state=42)
          sc2.fit(X)

Out[128]: SpectralClustering(affinity='rbf', assign_labels='kmeans', coef0=1, degree=3,
                    eigen_solver=None, eigen_tol=0.0, gamma=1, kernel_params=None,
                    n_clusters=2, n_init=10, n_jobs=None, n_neighbors=10,
                    random_state=42)

In [129]: np.percentile(sc1.affinity_matrix_, 95)

Out[129]: 0.04251990648936265

In [130]: def plot_spectral_clustering(sc, X, size, alpha, show_xlabels=True, show_ylabels=Tru
              plt.scatter(X[:, 0], X[:, 1], marker='o', s=size, c='gray', cmap="Paired", alpha=
              plt.scatter(X[:, 0], X[:, 1], marker='o', s=30, c='w')
              plt.scatter(X[:, 0], X[:, 1], marker='.', s=10, c=sc.labels_, cmap="Paired")

              if show_xlabels:
                  plt.xlabel("$x_1$", fontsize=14)
              else:
                  plt.tick_params(labelbottom=False)
              if show_ylabels:
                  plt.ylabel("$x_2$", fontsize=14, rotation=0)
              else:
                  plt.tick_params(labelleft=False)
              plt.title("RBF gamma={}".format(sc.gamma), fontsize=14)

In [131]: plt.figure(figsize=(9, 3.2))

          plt.subplot(121)
          plot_spectral_clustering(sc1, X, size=500, alpha=0.1)

          plt.subplot(122)
          plot_spectral_clustering(sc2, X, size=4000, alpha=0.01, show_ylabels=False)

          plt.show()
```



2.4.2 Agglomerative Clustering

```
In [132]: from sklearn.cluster import AgglomerativeClustering

In [133]: X = np.array([0, 2, 5, 8.5]).reshape(-1, 1)
          agg = AgglomerativeClustering(linkage="complete").fit(X)

In [134]: def learned_parameters(estimator):
              return [attrib for attrib in dir(estimator)
                      if attrib.endswith("_") and not attrib.startswith("_")]

In [135]: learned_parameters(agg)

Out[135]: ['children_', 'labels_', 'n_components_', 'n_leaves_']

In [136]: agg.children_

Out[136]: array([[0, 1],
                 [2, 3],
                 [4, 5]])
```

3 Gaussian Mixtures

```
In [137]: X1, y1 = make_blobs(n_samples=1000, centers=((4, -4), (0, 0)), random_state=42)
          X1 = X1.dot(np.array([[0.374, 0.95], [0.732, 0.598]]))
          X2, y2 = make_blobs(n_samples=250, centers=1, random_state=42)
          X2 = X2 + [6, -8]
          X = np.r_[X1, X2]
          y = np.r_[y1, y2]
```

Let's train a Gaussian mixture model on the previous dataset:

```
In [138]: from sklearn.mixture import GaussianMixture

In [139]: gm = GaussianMixture(n_components=3, n_init=10, random_state=42)
          gm.fit(X)

Out[139]: GaussianMixture(covariance_type='full', init_params='kmeans', max_iter=100,
                  means_init=None, n_components=3, n_init=10, precisions_init=None,
                  random_state=42, reg_covar=1e-06, tol=0.001, verbose=0,
                  verbose_interval=10, warm_start=False, weights_init=None)
```

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

```
In [140]: gm.weights_

Out[140]: array([0.20965228, 0.4000662 , 0.39028152])

In [141]: gm.means_

Out[141]: array([[ 3.39909717,  1.05933727],
                 [-1.40763984,  1.42710194],
                 [ 0.05135313,  0.07524095]])

In [142]: gm.covariances_

Out[142]: 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]]])
```

Did the algorithm actually converge?

```
In [143]: gm.converged_

Out[143]: True
```

Yes, good. How many iterations did it take?

```
In [144]: gm.n_iter_

Out[144]: 4
```

You can now use the model to predict which cluster each instance belongs to (hard clustering) or the probabilities that it came from each cluster. For this, just use `predict()` method or the `predict_proba()` method:

```
In [145]: gm.predict(X)
```

```
Out[145]: array([2, 2, 1, ..., 0, 0, 0], dtype=int64)

In [146]: gm.predict_proba(X)

Out[146]: 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]])
```

This is a generative model, so you can sample new instances from it (and get their labels):

```
In [147]: X_new, y_new = gm.sample(6)
          X_new

Out[147]: 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]])

In [148]: y_new

Out[148]: array([0, 1, 2, 2, 2, 2])
```

Notice that they are sampled sequentially from each cluster.

You can also estimate the log of the *probability density function* (PDF) at any location using the `score_samples()` method:

```
In [149]: gm.score_samples(X)

Out[149]: array([-2.60782346, -3.57106041, -3.33003479, ..., -3.51352783,
                 -4.39802535, -3.80743859])
```

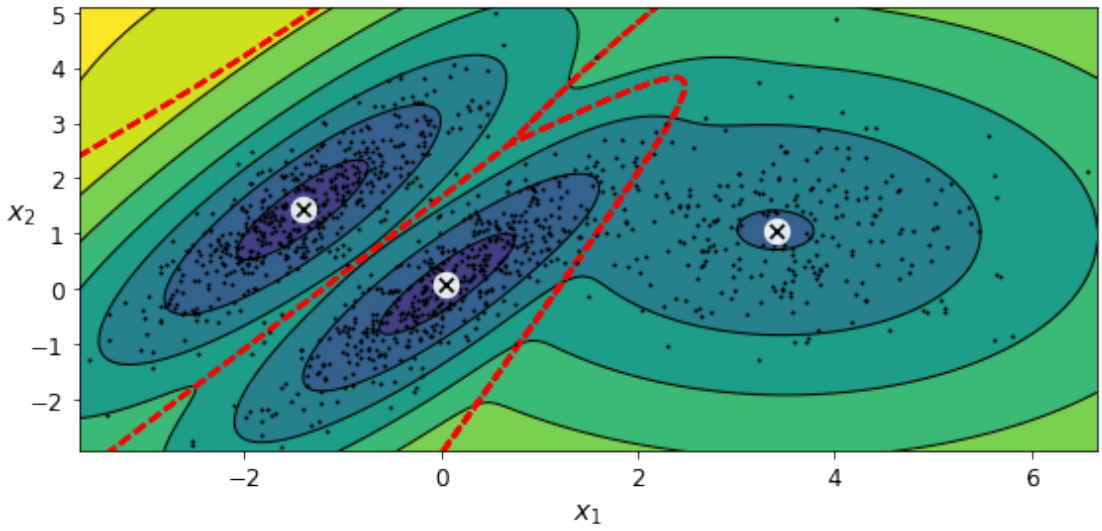
Let's check that the PDF integrates to 1 over the whole space. We just take a large square around the clusters, and chop it into a grid of tiny squares, then we compute the approximate probability that the instances will be generated in each tiny square (by multiplying the PDF at one corner of the tiny square by the area of the square), and finally summing all these probabilities). The result is very close to 1:

```
In [150]: resolution = 100
          grid = np.arange(-10, 10, 1 / resolution)
          xx, yy = np.meshgrid(grid, grid)
          X_full = np.vstack([xx.ravel(), yy.ravel()]).T

          pdf = np.exp(gm.score_samples(X_full))
          pdf_probas = pdf * (1 / resolution) ** 2
          pdf_probas.sum()
```

```
Out[150]: 0.9999999999217849
```

Now let's plot the resulting decision boundaries (dashed lines) and density contours:

```
In [151]: from matplotlib.colors import LogNorm

          def plot_gaussian_mixture(clusterer, X, resolution=1000, show_ylabels=True):
              mins = X.min(axis=0) - 0.1
              maxs = X.max(axis=0) + 0.1
              xx, yy = np.meshgrid(np.linspace(mins[0], maxs[0], resolution),
                                   np.linspace(mins[1], maxs[1], resolution))
              Z = -clusterer.score_samples(np.c_[xx.ravel(), yy.ravel()])
              Z = Z.reshape(xx.shape)

              plt.contourf(xx, yy, Z,
                           norm=LogNorm(vmin=1.0, vmax=30.0),
                           levels=np.logspace(0, 2, 12))
              plt.contour(xx, yy, Z,
                          norm=LogNorm(vmin=1.0, vmax=30.0),
                          levels=np.logspace(0, 2, 12),
                          linewidths=1, colors='k')

              Z = clusterer.predict(np.c_[xx.ravel(), yy.ravel()])
              Z = Z.reshape(xx.shape)
              plt.contour(xx, yy, Z,
                          linewidths=2, colors='r', linestyles='dashed')

              plt.plot(X[:, 0], X[:, 1], 'k.', markersize=2)
              plot_centroids(clusterer.means_, clusterer.weights_)

              plt.xlabel("$x_1$", fontsize=14)
              if show_ylabels:
                  plt.ylabel("$x_2$", fontsize=14, rotation=0)
              else:
                  plt.tick_params(labelleft=False)

In [152]: plt.figure(figsize=(8, 4))

          plot_gaussian_mixture(gm, X)

          save_fig("gaussian_mixtures_plot")
          plt.show()

Saving figure gaussian_mixtures_plot
```



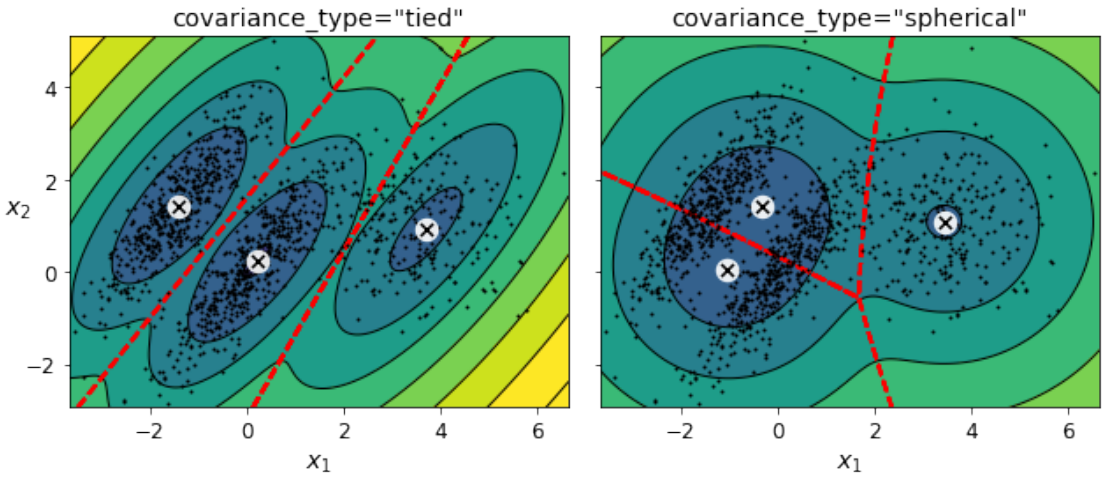
You can impose constraints on the covariance matrices that the algorithm looks for by setting the `covariance_type` hyperparameter: * `"full"` (default): no constraint, all clusters can take on any ellipsoidal shape of any size. * `"tied"`: all clusters must have the same shape, which can be any ellipsoid (i.e., they all share the same covariance matrix). * `"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 axes (i.e., the covariance matrices must be diagonal).

```
In [153]: gm_full = GaussianMixture(n_components=3, n_init=10, covariance_type="full", random_s
          gm_tied = GaussianMixture(n_components=3, n_init=10, covariance_type="tied", random_s
          gm_spherical = GaussianMixture(n_components=3, n_init=10, covariance_type="spherical"
          gm_diag = GaussianMixture(n_components=3, n_init=10, covariance_type="diag", random_s
          gm_full.fit(X)
          gm_tied.fit(X)
          gm_spherical.fit(X)
          gm_diag.fit(X)

Out[153]: GaussianMixture(covariance_type='diag', init_params='kmeans', max_iter=100,
                  means_init=None, n_components=3, n_init=10, precisions_init=None,
                  random_state=42, reg_covar=1e-06, tol=0.001, verbose=0,
                  verbose_interval=10, warm_start=False, weights_init=None)

In [154]: def compare_gaussian_mixtures(gm1, gm2, X):
              plt.figure(figsize=(9, 4))

              plt.subplot(121)
              plot_gaussian_mixture(gm1, X)
              plt.title('covariance_type="{}"'.format(gm1.covariance_type), fontsize=14)

              plt.subplot(122)
```

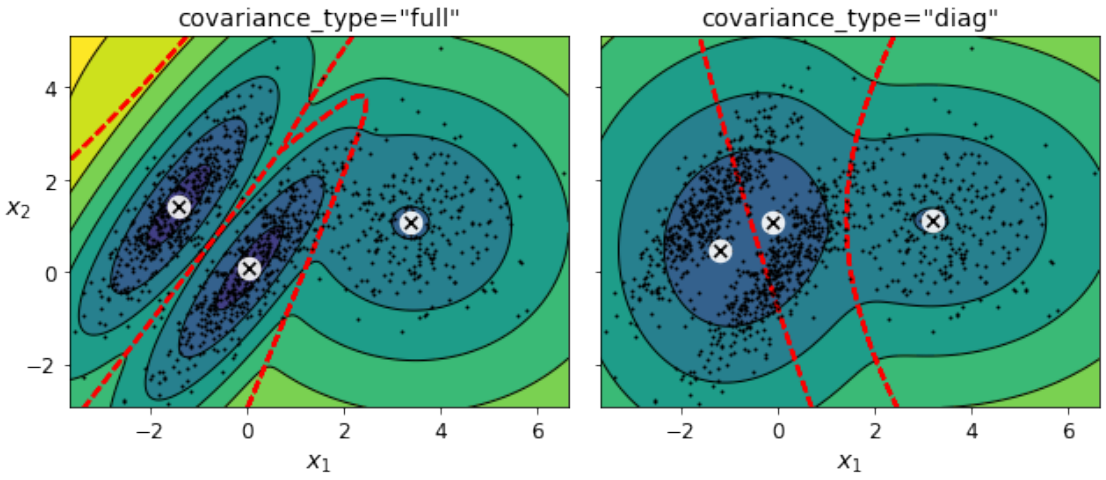
```
        plot_gaussian_mixture(gm2, X, show_ylabels=False)
        plt.title('covariance_type="{}"'.format(gm2.covariance_type), fontsize=14)
```

In [155]:
```
compare_gaussian_mixtures(gm_tied, gm_spherical, X)

save_fig("covariance_type_plot")
plt.show()
```

```
Saving figure covariance_type_plot
```



In [156]:
```
compare_gaussian_mixtures(gm_full, gm_diag, X)
plt.tight_layout()
plt.show()
```

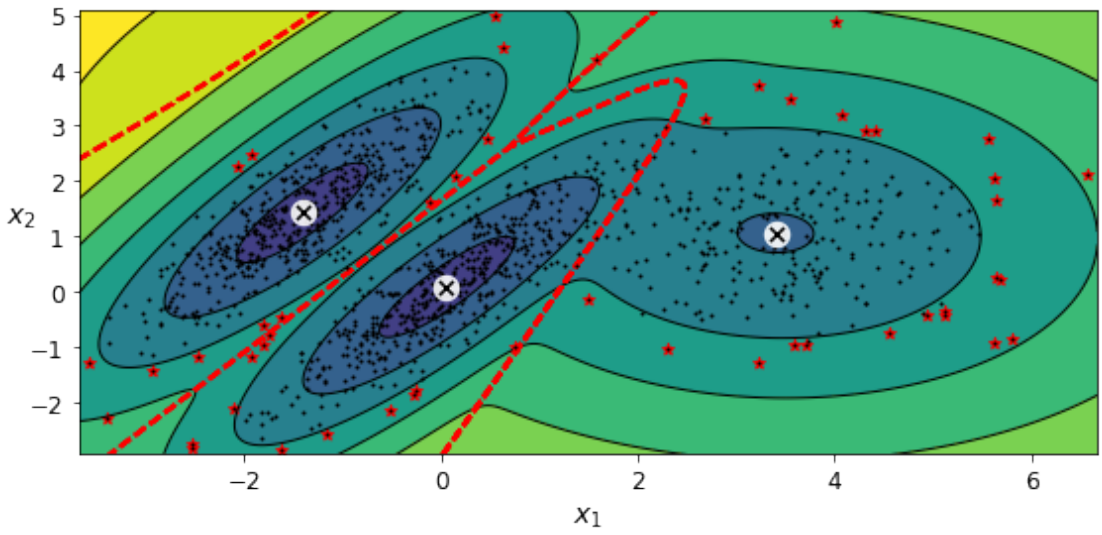


3.1 Anomaly Detection using Gaussian Mixtures

Gaussian Mixtures can be used for *anomaly detection*: instances located in low-density regions can be considered anomalies. 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%, then you can set the density threshold to be the value that results in having 4% of the instances located in areas below that threshold density:

```
In [157]: densities = gm.score_samples(X)
          density_threshold = np.percentile(densities, 4)
          anomalies = X[densities < density_threshold]

In [158]: plt.figure(figsize=(8, 4))

          plot_gaussian_mixture(gm, X)
          plt.scatter(anomalies[:, 0], anomalies[:, 1], color='r', marker='*')
          plt.ylim(top=5.1)

          save_fig("mixture_anomaly_detection_plot")
          plt.show()
```

```
Saving figure mixture_anomaly_detection_plot
```



3.2 Model selection

We cannot use the inertia or the silhouette score because they both assume that the clusters are spherical. Instead, we 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):

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

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

- m is the number of instances.
- p is the number of parameters learned by the model.
- $\hat{L}$ is the maximized value of the likelihood function of the model. This is the conditional probability of the observed data $\mathbf{X}$, given the model and its optimized parameters.

Both BIC and AIC penalize models that have more parameters to learn (e.g., more clusters), and reward models that fit the data well (i.e., models that give a high likelihood to the observed data).

```
In [159]: gm.bic(X)

Out[159]: 8189.74345832983

In [160]: gm.aic(X)

Out[160]: 8102.518178214792
```

We could compute the BIC manually like this:

```
In [161]: n_clusters = 3
          n_dims = 2
          n_params_for_weights = n_clusters - 1
          n_params_for_means = n_clusters * n_dims
          n_params_for_covariance = n_clusters * n_dims * (n_dims + 1) // 2
          n_params = n_params_for_weights + n_params_for_means + n_params_for_covariance
          max_log_likelihood = gm.score(X) * len(X) # log(L^)
          bic = np.log(len(X)) * n_params - 2 * max_log_likelihood
          aic = 2 * n_params - 2 * max_log_likelihood

In [162]: bic, aic

Out[162]: (8189.74345832983, 8102.518178214792)

In [163]: n_params

Out[163]: 17
```

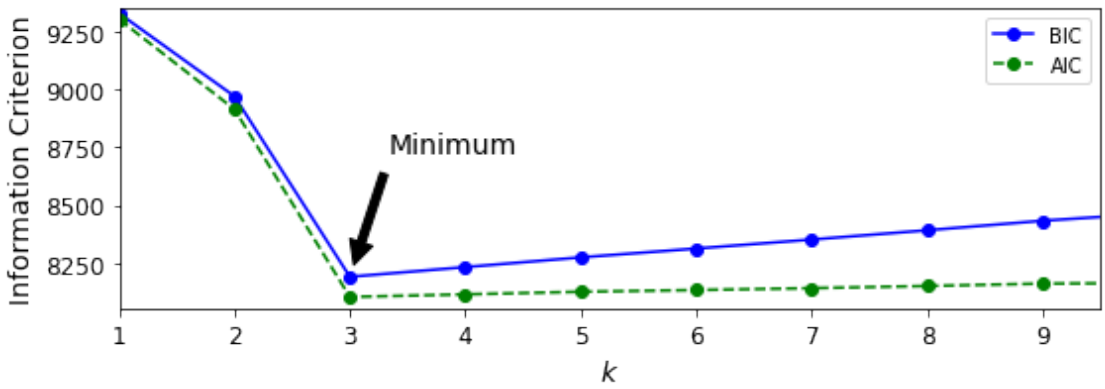
There's one weight per cluster, but the sum must be equal to 1, so we have one degree of freedom less, hence the -1. Similarly, the degrees of freedom for an $n \times n$ covariance matrix is not n^2, but $1 + 2 + \cdots + n = \frac{n(n+1)}{2}$.

Let's train Gaussian Mixture models with various values of k and measure their BIC:

```
In [164]: gms_per_k = [GaussianMixture(n_components=k, n_init=10, random_state=42).fit(X)
                       for k in range(1, 11)]

In [165]: bics = [model.bic(X) for model in gms_per_k]
          aics = [model.aic(X) for model in gms_per_k]
```

```
In [166]: plt.figure(figsize=(8, 3))
          plt.plot(range(1, 11), bics, "bo-", label="BIC")
          plt.plot(range(1, 11), aics, "go--", label="AIC")
          plt.xlabel("$k$", fontsize=14)
          plt.ylabel("Information Criterion", fontsize=14)
          plt.axis([1, 9.5, np.min(aics) - 50, np.max(aics) + 50])
          plt.annotate('Minimum',
                       xy=(3, bics[2]),
                       xytext=(0.35, 0.6),
                       textcoords='figure fraction',
                       fontsize=14,
                       arrowprops=dict(facecolor='black', shrink=0.1)
                      )
          plt.legend()
          save_fig("aic_bic_vs_k_plot")
          plt.show()
```

```
Saving figure aic_bic_vs_k_plot
```



Let's search for best combination of values for both the number of clusters and the `covariance_type` hyperparameter:

```
In [167]: min_bic = np.infty

          for k in range(1, 11):
              for covariance_type in ("full", "tied", "spherical", "diag"):
                  bic = GaussianMixture(n_components=k, n_init=10,
                                        covariance_type=covariance_type,
                                        random_state=42).fit(X).bic(X)
                  if bic < min_bic:
                      min_bic = bic
                      best_k = k
                      best_covariance_type = covariance_type
```

```
In [168]: best_k

Out[168]: 3

In [169]: best_covariance_type

Out[169]: 'full'
```

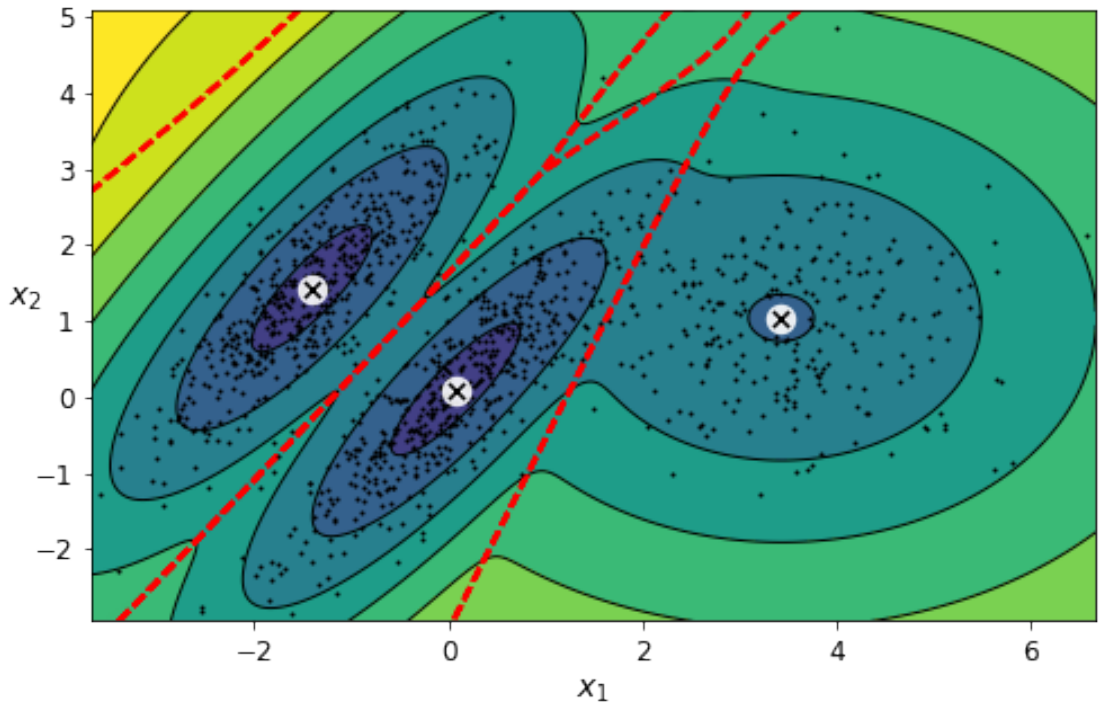
3.3 Variational Bayesian Gaussian Mixtures

Rather than manually searching for the optimal number of clusters, it is possible to use instead the `BayesianGaussianMixture` class which is capable of giving weights equal (or close) to zero to unnecessary clusters. Just set the number of components to a value that you believe is greater than the optimal number of clusters, and the algorithm will eliminate the unnecessary clusters automatically.

```
In [170]: from sklearn.mixture import BayesianGaussianMixture

In [171]: bgm = BayesianGaussianMixture(n_components=10, n_init=10, random_state=42)
          bgm.fit(X)

Out[171]: BayesianGaussianMixture(covariance_prior=None, covariance_type='full',
                      degrees_of_freedom_prior=None, init_params='kmeans',
                      max_iter=100, mean_precision_prior=None, mean_prior=None,
                      n_components=10, n_init=10, random_state=42, reg_covar=1e-06,
                      tol=0.001, verbose=0, verbose_interval=10, warm_start=False,
                      weight_concentration_prior=None,
                      weight_concentration_prior_type='dirichlet_process')
```

The algorithm automatically detected that only 3 components are needed:

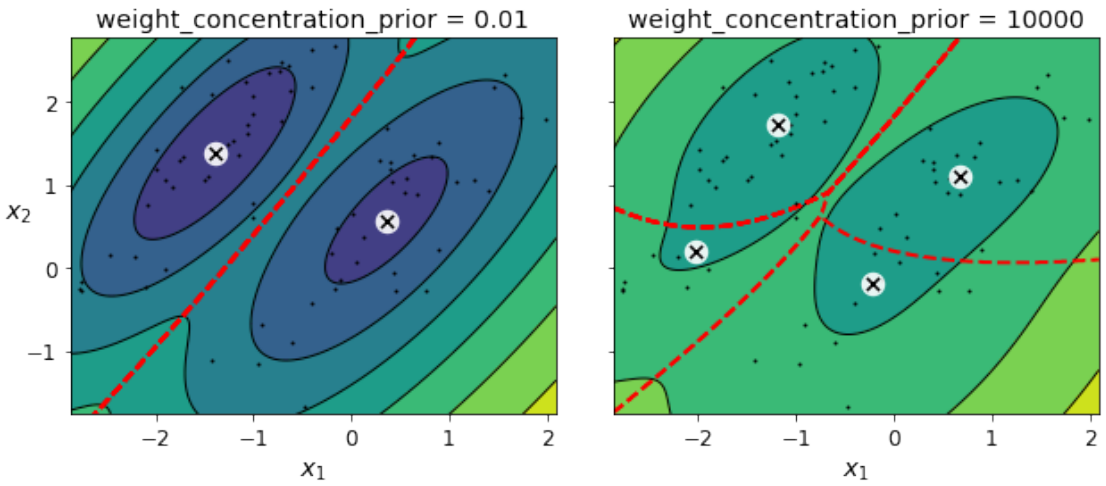
```
In [172]: np.round(bgm.weights_, 2)

Out[172]: array([0.4 , 0.21, 0.4 , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ])

In [173]: plt.figure(figsize=(8, 5))
          plot_gaussian_mixture(bgm, X)
          plt.show()
```




```
In [174]: bgm_low = BayesianGaussianMixture(n_components=10, max_iter=1000, n_init=1,
                                            weight_concentration_prior=0.01, random_state=42)
          bgm_high = BayesianGaussianMixture(n_components=10, max_iter=1000, n_init=1,
                                             weight_concentration_prior=10000, random_state=42)
          nn = 73
          bgm_low.fit(X[:nn])
          bgm_high.fit(X[:nn])

Out[174]: BayesianGaussianMixture(covariance_prior=None, covariance_type='full',
                      degrees_of_freedom_prior=None, init_params='kmeans',
                      max_iter=1000, mean_precision_prior=None, mean_prior=None,
                      n_components=10, n_init=1, random_state=42, reg_covar=1e-06,
                      tol=0.001, verbose=0, verbose_interval=10, warm_start=False,
                      weight_concentration_prior=10000,
                      weight_concentration_prior_type='dirichlet_process')

In [175]: np.round(bgm_low.weights_, 2)

Out[175]: array([0.52, 0.48, 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ])

In [176]: np.round(bgm_high.weights_, 2)

Out[176]: array([0.01, 0.18, 0.27, 0.11, 0.01, 0.01, 0.01, 0.01, 0.37, 0.01])
```

```
In [177]: plt.figure(figsize=(9, 4))

          plt.subplot(121)
          plot_gaussian_mixture(bgm_low, X[:nn])
          plt.title("weight_concentration_prior = 0.01", fontsize=14)

          plt.subplot(122)
          plot_gaussian_mixture(bgm_high, X[:nn], show_ylabels=False)
          plt.title("weight_concentration_prior = 10000", fontsize=14)

          save_fig("mixture_concentration_prior_plot")
          plt.show()
```

```
Saving figure mixture_concentration_prior_plot
```

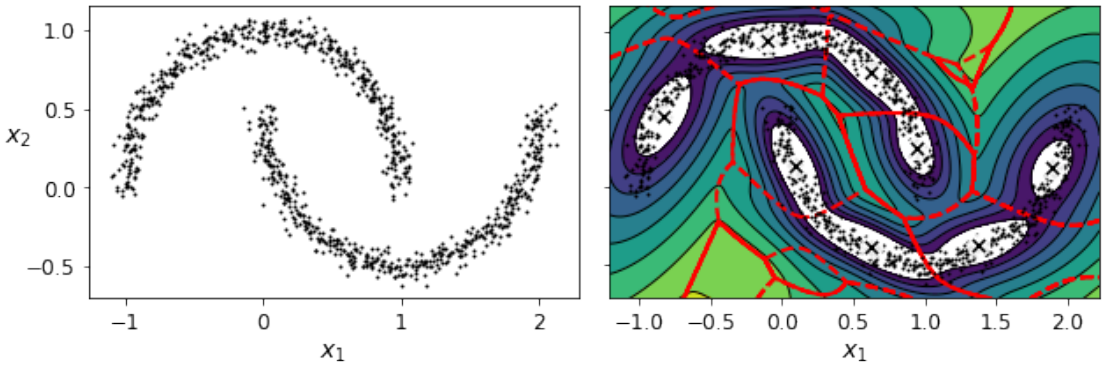


Note: the fact that you see only 3 regions in the right plot although there are 4 centroids is not a bug. The weight of the top-right cluster is much larger than the weight of the lower-right cluster, so the probability that any given point in this region belongs to the top right cluster is greater than the probability that it belongs to the lower-right cluster.

```
In [178]: X_moons, y_moons = make_moons(n_samples=1000, noise=0.05, random_state=42)

In [179]: bgm = BayesianGaussianMixture(n_components=10, n_init=10, random_state=42)
          bgm.fit(X_moons)

Out[179]: BayesianGaussianMixture(covariance_prior=None, covariance_type='full',
                    degrees_of_freedom_prior=None, init_params='kmeans',
                    max_iter=100, mean_precision_prior=None, mean_prior=None,
                    n_components=10, n_init=10, random_state=42, reg_covar=1e-06,
                    tol=0.001, verbose=0, verbose_interval=10, warm_start=False,
                    weight_concentration_prior=None,
                    weight_concentration_prior_type='dirichlet_process')
```

```
In [180]: plt.figure(figsize=(9, 3.2))

          plt.subplot(121)
          plot_data(X_moons)
          plt.xlabel("$x_1$", fontsize=14)
          plt.ylabel("$x_2$", fontsize=14, rotation=0)

          plt.subplot(122)
          plot_gaussian_mixture(bgm, X_moons, show_ylabels=False)

          save_fig("moons_vs_bgm_plot")
          plt.show()
```

```
Saving figure moons_vs_bgm_plot
```



Oops, not great... instead of detecting 2 moon-shaped clusters, the algorithm detected 8 ellipsoidal clusters. However, the density plot does not look too bad, so it might be usable for anomaly detection.

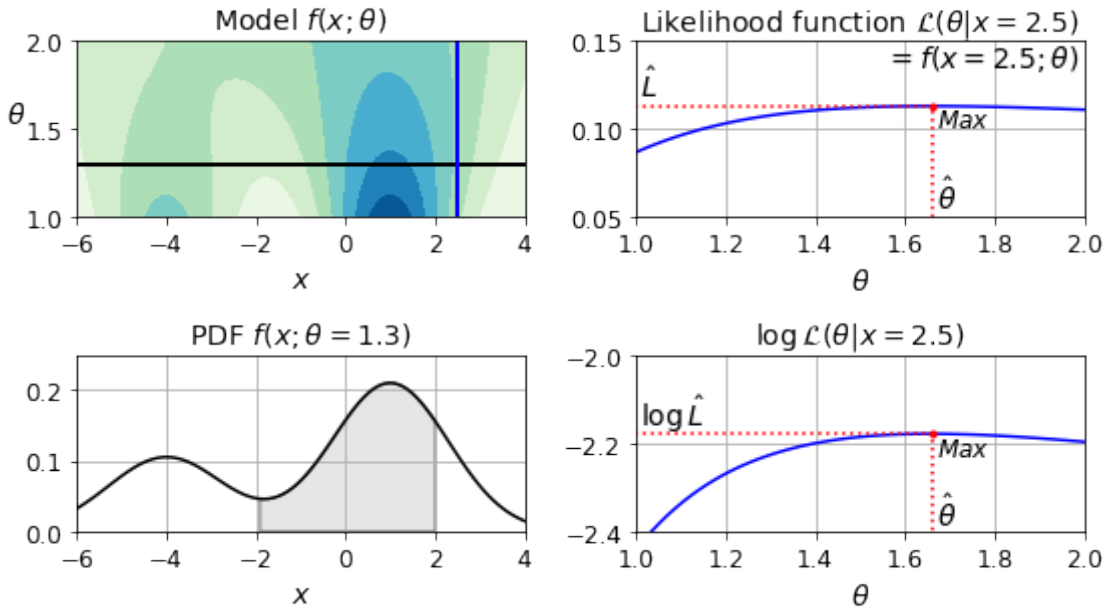
3.4 Likelihood Function

```
In [181]: from scipy.stats import norm

In [182]: xx = np.linspace(-6, 4, 101)
          ss = np.linspace(1, 2, 101)
          XX, SS = np.meshgrid(xx, ss)
          ZZ = 2 * norm.pdf(XX - 1.0, 0, SS) + norm.pdf(XX + 4.0, 0, SS)
          ZZ = ZZ / ZZ.sum(axis=1)[:,np.newaxis] / (xx[1] - xx[0])

In [183]: from matplotlib.patches import Polygon

          plt.figure(figsize=(8, 4.5))

          x_idx = 85
```

```
s_idx = 30

plt.subplot(221)
plt.contourf(XX, SS, ZZ, cmap="GnBu")
plt.plot([-6, 4], [ss[s_idx], ss[s_idx]], "k-", linewidth=2)
plt.plot([xx[x_idx], xx[x_idx]], [1, 2], "b-", linewidth=2)
plt.xlabel(r"$x$")
plt.ylabel(r"$\theta$", fontsize=14, rotation=0)
plt.title(r"Model $f(x; \theta)$", fontsize=14)

plt.subplot(222)
plt.plot(ss, ZZ[:, x_idx], "b-")
max_idx = np.argmax(ZZ[:, x_idx])
max_val = np.max(ZZ[:, x_idx])
plt.plot(ss[max_idx], max_val, "r.")
plt.plot([ss[max_idx], ss[max_idx]], [0, max_val], "r:")
plt.plot([0, ss[max_idx]], [max_val, max_val], "r:")
plt.text(1.01, max_val + 0.005, r"$\hat{L}$", fontsize=14)
plt.text(ss[max_idx]+ 0.01, 0.055, r"$\hat{\theta}$", fontsize=14)
plt.text(ss[max_idx]+ 0.01, max_val - 0.012, r"$Max$", fontsize=12)
plt.axis([1, 2, 0.05, 0.15])
plt.xlabel(r"$\theta$", fontsize=14)
plt.grid(True)
plt.text(1.99, 0.135, r"$=f(x=2.5; \theta)$", fontsize=14, ha="right")
plt.title(r"Likelihood function $\mathcal{L}(\theta|x=2.5)$", fontsize=14)

plt.subplot(223)
plt.plot(xx, ZZ[s_idx], "k-")
plt.axis([-6, 4, 0, 0.25])
plt.xlabel(r"$x$", fontsize=14)
plt.grid(True)
plt.title(r"PDF $f(x; \theta=1.3)$", fontsize=14)
verts = [(xx[41], 0)] + list(zip(xx[41:81], ZZ[s_idx, 41:81])) + [(xx[80], 0)]
poly = Polygon(verts, facecolor='0.9', edgecolor='0.5')
plt.gca().add_patch(poly)

plt.subplot(224)
plt.plot(ss, np.log(ZZ[:, x_idx]), "b-")
max_idx = np.argmax(np.log(ZZ[:, x_idx]))
max_val = np.max(np.log(ZZ[:, x_idx]))
plt.plot(ss[max_idx], max_val, "r.")
plt.plot([ss[max_idx], ss[max_idx]], [-5, max_val], "r:")
plt.plot([0, ss[max_idx]], [max_val, max_val], "r:")
plt.axis([1, 2, -2.4, -2])
plt.xlabel(r"$\theta$", fontsize=14)
plt.text(ss[max_idx]+ 0.01, max_val - 0.05, r"$Max$", fontsize=12)
plt.text(ss[max_idx]+ 0.01, -2.39, r"$\hat{\theta}$", fontsize=14)
plt.text(1.01, max_val + 0.02, r"$\log \, \hat{L}$", fontsize=14)
```

```
plt.grid(True)
plt.title(r"$\log \, \mathcal{L}(\theta|x=2.5)$", fontsize=14)

save_fig("likelihood_function_plot")
plt.show()
```

```
Saving figure likelihood_function_plot
```



In [ ]:

4 Exercise solutions

4.1 1. to 9.

See Appendix A.

4.2 10. Cluster the Olivetti Faces Dataset

Exercise: The classic Olivetti faces dataset contains 400 grayscale 64 Œ 64–pixel images of faces. Each image is flattened to a 1D vector of size 4,096. 40 different people were photographed (10 times each), and the usual task is to train a model that can predict which person is represented in each picture. Load the dataset using the `sklearn.datasets.fetch_olivetti_faces()` function.

In [184]:
```
from sklearn.datasets import fetch_olivetti_faces

olivetti = fetch_olivetti_faces()
```

```
downloading Olivetti faces from https://ndownloader.figshare.com/files/5976027 to C:\Users\MIN.
```

```
In [185]: print(olivetti.DESCR)
```

```
.. _olivetti_faces_dataset:

The Olivetti faces dataset
--------------------------

`This dataset contains a set of face images`_ taken between April 1992 and
April 1994 at AT&T Laboratories Cambridge. The
:func:`sklearn.datasets.fetch_olivetti_faces` function is the data
fetching / caching function that downloads the data
archive from AT&T.

.. _This dataset contains a set of face images: http://www.cl.cam.ac.uk/research/dtg/attarchive

As described on the original website:

    There are ten different images of each of 40 distinct subjects. For some
    subjects, the images were taken at different times, varying the lighting,
    facial expressions (open / closed eyes, smiling / not smiling) and facial
    details (glasses / no glasses). All the images were taken against a dark
    homogeneous background with the subjects in an upright, frontal position
    (with tolerance for some side movement).

**Data Set Characteristics:**

    =================   ====================
    Classes                              40
    Samples total                       400
    Dimensionality                     4096
    Features            real, between 0 and 1
    =================   ====================

The image is quantized to 256 grey levels and stored as unsigned 8-bit
integers; the loader will convert these to floating point values on the
interval [0, 1], which are easier to work with for many algorithms.

The "target" for this database is an integer from 0 to 39 indicating the
identity of the person pictured; however, with only 10 examples per class, this
relatively small dataset is more interesting from an unsupervised or
semi-supervised perspective.

The original dataset consisted of 92 x 112, while the version available here
consists of 64x64 images.
```

```
When using these images, please give credit to AT&T Laboratories Cambridge.
```

```
In [186]: olivetti.target
```

```
Out[186]: array([ 0,  0,  0,  0,  0,  0,  0,  0,  0,  0,  1,  1,  1,  1,  1,  1,  1,
                  1,  1,  1,  2,  2,  2,  2,  2,  2,  2,  2,  2,  2,  3,  3,  3,  3,
                  3,  3,  3,  3,  3,  3,  4,  4,  4,  4,  4,  4,  4,  4,  4,  4,  5,
                  5,  5,  5,  5,  5,  5,  5,  5,  5,  6,  6,  6,  6,  6,  6,  6,  6,
                  6,  6,  7,  7,  7,  7,  7,  7,  7,  7,  7,  7,  8,  8,  8,  8,  8,
                  8,  8,  8,  8,  8,  9,  9,  9,  9,  9,  9,  9,  9,  9,  9, 10, 10,
                 10, 10, 10, 10, 10, 10, 10, 10, 11, 11, 11, 11, 11, 11, 11, 11, 11,
                 11, 12, 12, 12, 12, 12, 12, 12, 12, 12, 12, 13, 13, 13, 13, 13, 13,
                 13, 13, 13, 13, 14, 14, 14, 14, 14, 14, 14, 14, 14, 14, 15, 15, 15,
                 15, 15, 15, 15, 15, 15, 15, 16, 16, 16, 16, 16, 16, 16, 16, 16, 16,
                 17, 17, 17, 17, 17, 17, 17, 17, 17, 17, 18, 18, 18, 18, 18, 18, 18,
                 18, 18, 18, 19, 19, 19, 19, 19, 19, 19, 19, 19, 19, 20, 20, 20, 20,
                 20, 20, 20, 20, 20, 20, 21, 21, 21, 21, 21, 21, 21, 21, 21, 21, 22,
                 22, 22, 22, 22, 22, 22, 22, 22, 22, 23, 23, 23, 23, 23, 23, 23, 23,
                 23, 23, 24, 24, 24, 24, 24, 24, 24, 24, 24, 24, 25, 25, 25, 25, 25,
                 25, 25, 25, 25, 25, 26, 26, 26, 26, 26, 26, 26, 26, 26, 26, 27, 27,
                 27, 27, 27, 27, 27, 27, 28, 28, 28, 28, 28, 28, 28, 28, 28, 28, 28,
                 28, 29, 29, 29, 29, 29, 29, 29, 29, 29, 29, 30, 30, 30, 30, 30, 30,
                 30, 30, 30, 30, 31, 31, 31, 31, 31, 31, 31, 31, 31, 31, 32, 32, 32,
                 32, 32, 32, 32, 32, 33, 33, 33, 33, 33, 33, 33, 33, 33, 33, 33, 33,
                 34, 34, 34, 34, 34, 34, 34, 34, 34, 34, 35, 35, 35, 35, 35, 35, 35,
                 35, 35, 35, 36, 36, 36, 36, 36, 36, 36, 36, 36, 36, 37, 37, 37, 37,
                 37, 37, 37, 37, 37, 37, 38, 38, 38, 38, 38, 38, 38, 38, 38, 38, 39,
                 39, 39, 39, 39, 39, 39, 39, 39])
```

Exercise: Then split it into a training set, a validation set, and a test set (note that the dataset is already scaled between 0 and 1). Since the dataset is quite small, you probably want to use stratified sampling to ensure that there are the same number of images per person in each set.

```
In [187]: from sklearn.model_selection import StratifiedShuffleSplit

          strat_split = StratifiedShuffleSplit(n_splits=1, test_size=40, random_state=42)
          train_valid_idx, test_idx = next(strat_split.split(olivetti.data, olivetti.target))
          X_train_valid = olivetti.data[train_valid_idx]
          y_train_valid = olivetti.target[train_valid_idx]
          X_test = olivetti.data[test_idx]
          y_test = olivetti.target[test_idx]

          strat_split = StratifiedShuffleSplit(n_splits=1, test_size=80, random_state=43)
          train_idx, valid_idx = next(strat_split.split(X_train_valid, y_train_valid))
          X_train = X_train_valid[train_idx]
          y_train = y_train_valid[train_idx]
```

```
X_valid = X_train_valid[valid_idx]
y_valid = y_train_valid[valid_idx]
```

```
In [188]: print(X_train.shape, y_train.shape)
          print(X_valid.shape, y_valid.shape)
          print(X_test.shape, y_test.shape)
```

```
(280, 4096) (280,)
(80, 4096) (80,)
(40, 4096) (40,)
```

To speed things up, we'll reduce the data's dimensionality using PCA:

```
In [189]: from sklearn.decomposition import PCA

          pca = PCA(0.99)
          X_train_pca = pca.fit_transform(X_train)
          X_valid_pca = pca.transform(X_valid)
          X_test_pca = pca.transform(X_test)

          pca.n_components_
```

```
Out[189]: 199
```

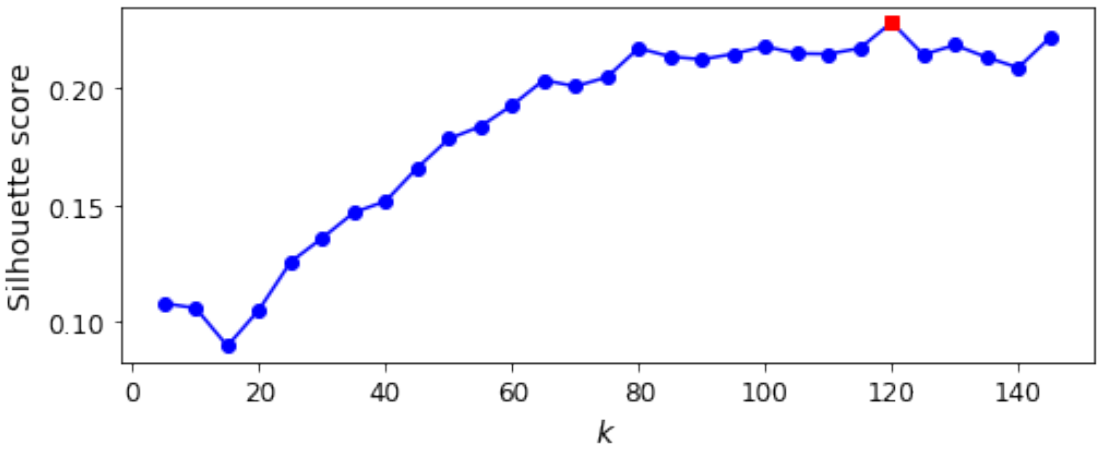
Exercise: Next, cluster the images using K-Means, and ensure that you have a good number of clusters (using one of the techniques discussed in this chapter).

```
In [190]: from sklearn.cluster import KMeans

          k_range = range(5, 150, 5)
          kmeans_per_k = []
          for k in k_range:
              print("k={}".format(k))
              kmeans = KMeans(n_clusters=k, random_state=42).fit(X_train_pca)
              kmeans_per_k.append(kmeans)
```

```
k=5
k=10
k=15
k=20
k=25
k=30
k=35
k=40
k=45
k=50
k=55
k=60
```

```
k=65
k=70
k=75
k=80
k=85
k=90
k=95
k=100
k=105
k=110
k=115
k=120
k=125
k=130
k=135
k=140
k=145
```

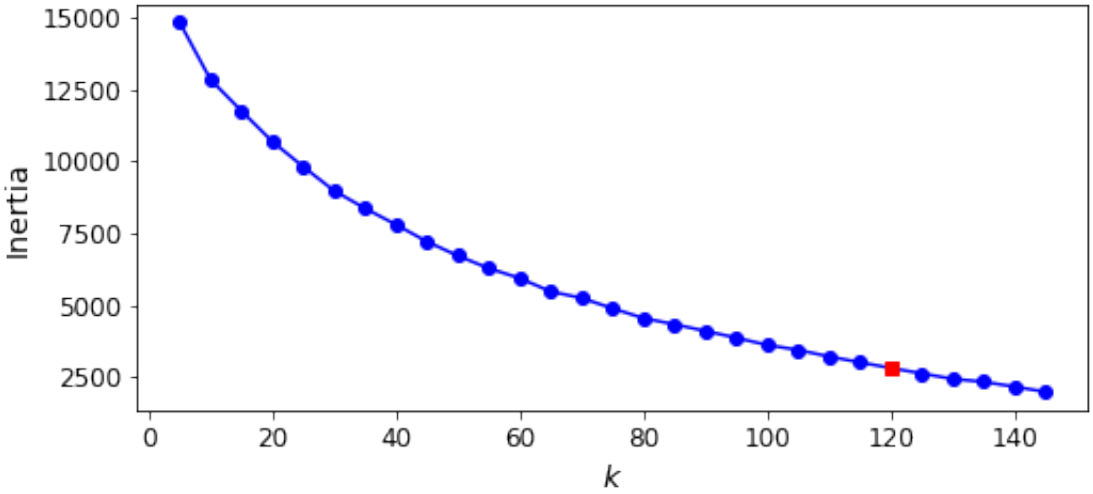
In [191]:
```
from sklearn.metrics import silhouette_score

silhouette_scores = [silhouette_score(X_train_pca, model.labels_)
                     for model in kmeans_per_k]
best_index = np.argmax(silhouette_scores)
best_k = k_range[best_index]
best_score = silhouette_scores[best_index]

plt.figure(figsize=(8, 3))
plt.plot(k_range, silhouette_scores, "bo-")
plt.xlabel("$k$", fontsize=14)
plt.ylabel("Silhouette score", fontsize=14)
plt.plot(best_k, best_score, "rs")
plt.show()
```



```
In [192]: best_k

Out[192]: 120
```

It looks like the best number of clusters is quite high, at 120. You might have expected it to be 40, since there are 40 different people on the pictures. However, the same person may look quite different on different pictures (e.g., with or without glasses, or simply shifted left or right).

```
In [193]: inertias = [model.inertia_ for model in kmeans_per_k]
          best_inertia = inertias[best_index]

          plt.figure(figsize=(8, 3.5))
          plt.plot(k_range, inertias, "bo-")
          plt.xlabel("$k$", fontsize=14)
          plt.ylabel("Inertia", fontsize=14)
          plt.plot(best_k, best_inertia, "rs")
          plt.show()
```



The optimal number of clusters is not clear on this inertia diagram, as there is no obvious elbow, so let's stick with k=120.

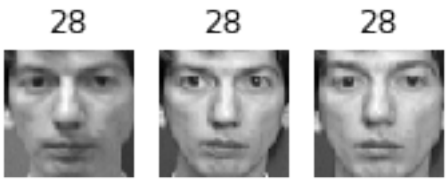
```
In [194]: best_model = kmeans_per_k[best_index]
```

Exercise: Visualize the clusters: do you see similar faces in each cluster?

```
In [195]: def plot_faces(faces, labels, n_cols=5):
              n_rows = (len(faces) - 1) // n_cols + 1
              plt.figure(figsize=(n_cols, n_rows * 1.1))
```

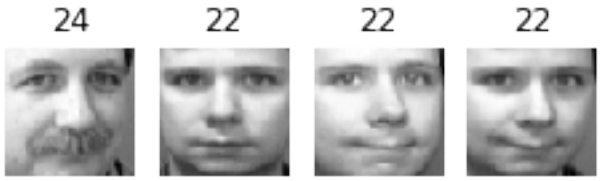
```
            for index, (face, label) in enumerate(zip(faces, labels)):
                plt.subplot(n_rows, n_cols, index + 1)
                plt.imshow(face.reshape(64, 64), cmap="gray")
                plt.axis("off")
                plt.title(label)
            plt.show()

        for cluster_id in np.unique(best_model.labels_):
            print("Cluster", cluster_id)
            in_cluster = best_model.labels_==cluster_id
            faces = X_train[in_cluster].reshape(-1, 64, 64)
            labels = y_train[in_cluster]
            plot_faces(faces, labels)
```

```
Cluster 0
```

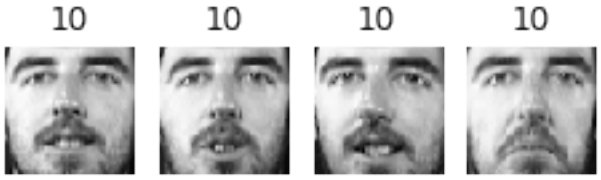



```
Cluster 1
```


```
Cluster 2
```



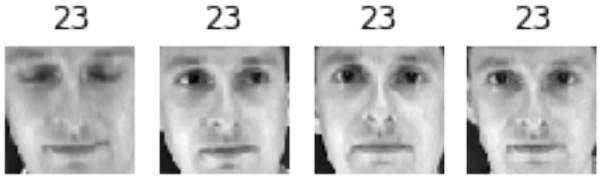
Cluster 3



Cluster 4

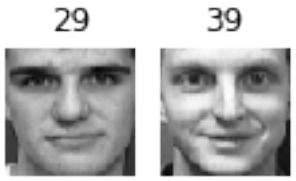
Cluster 5

Cluster 6



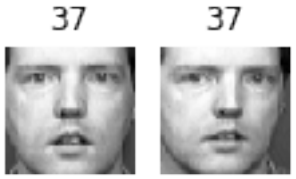
Cluster 7

Cluster 8



Cluster 9

Cluster 10



Cluster 11

Cluster 12

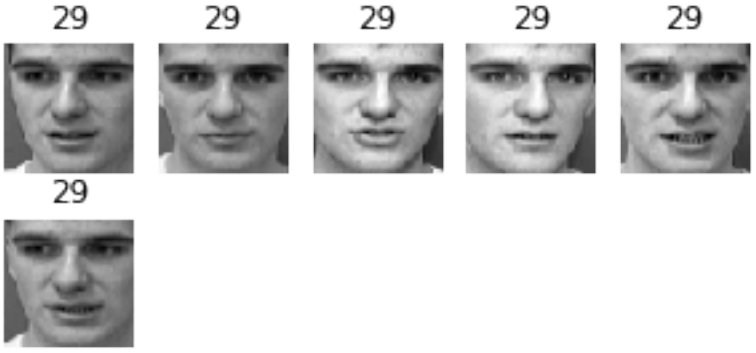
Cluster 13

Cluster 14

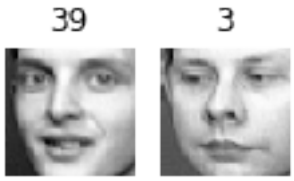
Cluster 15

Cluster 16

Cluster 17



Cluster 18

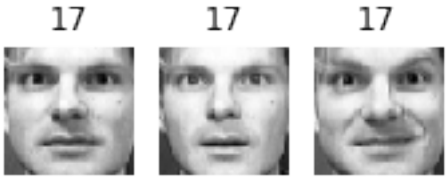


Cluster 19

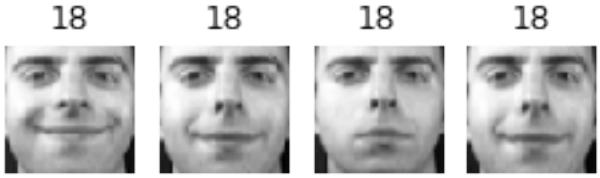
Cluster 20

Cluster 21

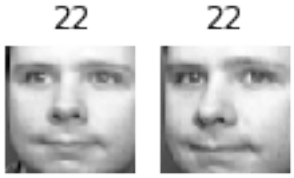
Cluster 22



Cluster 23



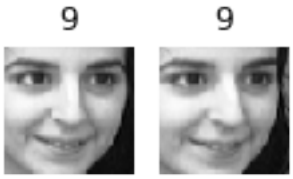
Cluster 24



Cluster 25

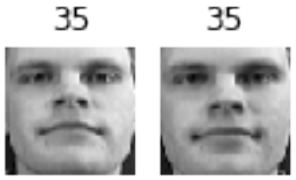
Cluster 26

Cluster 27



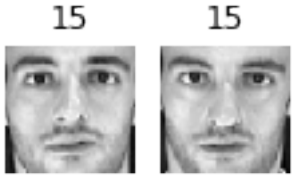
Cluster 28

Cluster 29



Cluster 30

Cluster 31



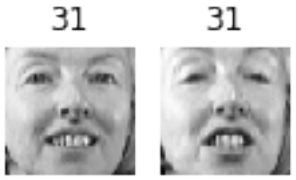
Cluster 32

Cluster 33

Cluster 34

Cluster 35

Cluster 36



Cluster 37

Cluster 38

Cluster 39

Cluster 40

Cluster 41

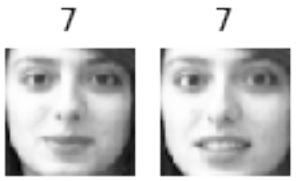
Cluster 42

Cluster 43

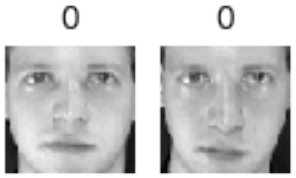
Cluster 44

Cluster 45

Cluster 46



Cluster 47



Cluster 48

Cluster 49

Cluster 50

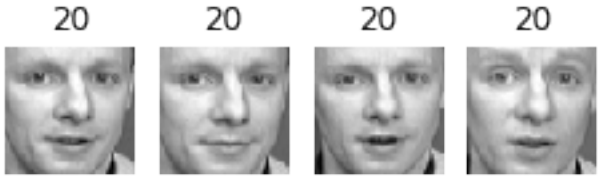
Cluster 51

Cluster 52

Cluster 53

Cluster 54

Cluster 55



Cluster 56

Cluster 57

Cluster 58

Cluster 59

Cluster 60

27

Cluster 61

9

Cluster 62

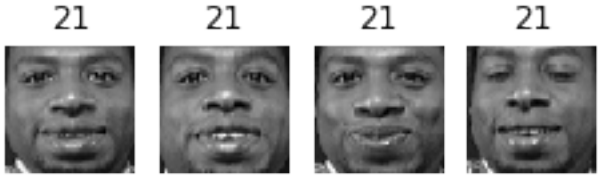
8 8

Cluster 63

27

Cluster 64

Cluster 65



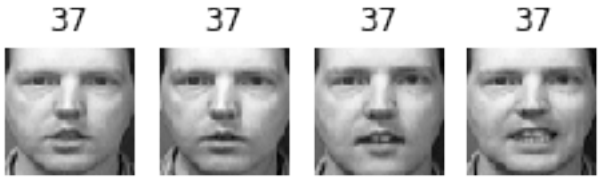
Cluster 66

Cluster 67

Cluster 68

Cluster 69

Cluster 70



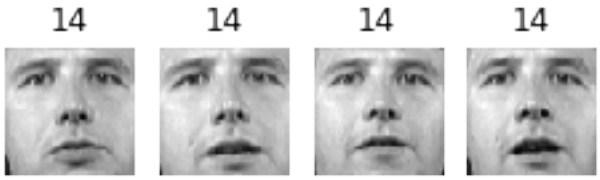
Cluster 71

Cluster 72

Cluster 73

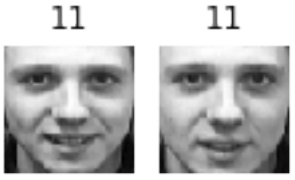
Cluster 74

Cluster 75



Cluster 76

Cluster 77



Cluster 78

Cluster 79

Cluster 80

Cluster 81

Cluster 82

Cluster 83

Cluster 84

Cluster 85

Cluster 86

Cluster 87

Cluster 88

Cluster 89

Cluster 90

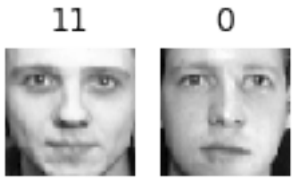
Cluster 91

Cluster 92

Cluster 93

Cluster 94

Cluster 95



Cluster 96

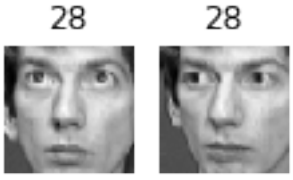
Cluster 97

Cluster 98

Cluster 99

Cluster 100

Cluster 101



Cluster 102

Cluster 103

Cluster 104

Cluster 105

Cluster 106

Cluster 107

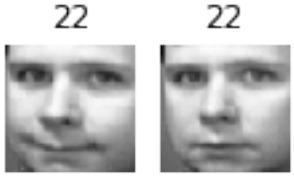
Cluster 108

Cluster 109

Cluster 110

Cluster 111

Cluster 112

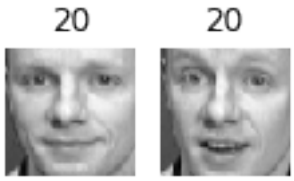


Cluster 113

Cluster 114

Cluster 115

Cluster 116



Cluster 117

Cluster 118

Cluster 119

About 2 out of 3 clusters are useful: that is, they contain at least 2 pictures, all of the same person. However, the rest of the clusters have either one or more intruders, or they have just a single picture.

Clustering images this way may be too imprecise to be directly useful when training a model (as we will see below), but it can be tremendously useful when labeling images in a new dataset: it will usually make labelling much faster.

4.3 11. Using Clustering as Preprocessing for Classification

Exercise: Continuing with the Olivetti faces dataset, train a classifier to predict which person is represented in each picture, and evaluate it on the validation set.

```
In [196]: from sklearn.ensemble import RandomForestClassifier

          clf = RandomForestClassifier(n_estimators=150, random_state=42)
          clf.fit(X_train_pca, y_train)
          clf.score(X_valid_pca, y_valid)
```

```
Out[196]: 0.9
```

Exercise: Next, use K-Means as a dimensionality reduction tool, and train a classifier on the reduced set.

```
In [197]: X_train_reduced = best_model.transform(X_train_pca)
          X_valid_reduced = best_model.transform(X_valid_pca)
          X_test_reduced = best_model.transform(X_test_pca)

          clf = RandomForestClassifier(n_estimators=150, random_state=42)
          clf.fit(X_train_reduced, y_train)

          clf.score(X_valid_reduced, y_valid)
```

```
Out[197]: 0.7
```

Yikes! That's not better at all! Let's see if tuning the number of clusters helps.

Exercise: Search for the number of clusters that allows the classifier to get the best performance: what performance can you reach?

We could use a `GridSearchCV` like we did earlier in this notebook, but since we already have a validation set, we don't need K-fold cross-validation, and we're only exploring a single hyperparameter, so it's simpler to just run a loop manually:

```
In [198]: from sklearn.pipeline import Pipeline

          for n_clusters in k_range:
              pipeline = Pipeline([
                  ("kmeans", KMeans(n_clusters=n_clusters, random_state=n_clusters)),
                  ("forest_clf", RandomForestClassifier(n_estimators=150, random_state=42))
```

```
        ])
        pipeline.fit(X_train_pca, y_train)
        print(n_clusters, pipeline.score(X_valid_pca, y_valid))
```

```
5 0.3625
10 0.55
15 0.6125
20 0.6625
25 0.6625
30 0.7
35 0.6875
40 0.7125
45 0.7
50 0.7375
55 0.7375
60 0.75
65 0.725
70 0.7375
75 0.7875
80 0.7125
85 0.725
90 0.775
95 0.7625
100 0.65
105 0.7125
110 0.725
115 0.7625
120 0.75
125 0.725
130 0.775
135 0.7375
140 0.7375
145 0.725
```

Oh well, even by tuning the number of clusters, we never get beyond 80% accuracy. Looks like the distances to the cluster centroids are not as informative as the original images.

Exercise: What if you append the features from the reduced set to the original features (again, searching for the best number of clusters)?

```
In [199]: X_train_extended = np.c_[X_train_pca, X_train_reduced]
          X_valid_extended = np.c_[X_valid_pca, X_valid_reduced]
          X_test_extended = np.c_[X_test_pca, X_test_reduced]

In [200]: clf = RandomForestClassifier(n_estimators=150, random_state=42)
          clf.fit(X_train_extended, y_train)
          clf.score(X_valid_extended, y_valid)

Out[200]: 0.8125
```

That's a bit better, but still worse than without the cluster features. The clusters are not useful to directly train a classifier in this case (but they can still help when labelling new training instances).

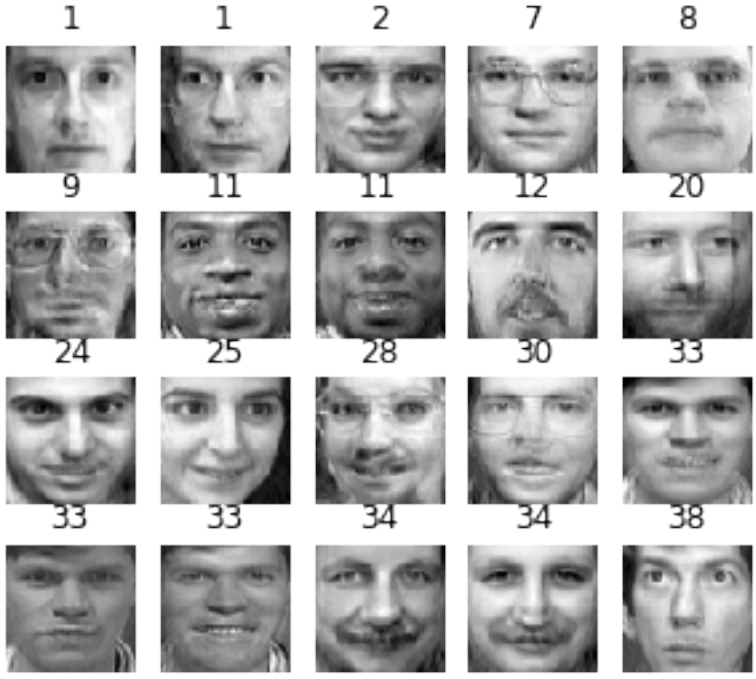
4.4 12. A Gaussian Mixture Model for the Olivetti Faces Dataset

Exercise: Train a Gaussian mixture model on the Olivetti faces dataset. To speed up the algorithm, you should probably reduce the dataset's dimensionality (e.g., use PCA, preserving 99% of the variance).

```
In [201]: from sklearn.mixture import GaussianMixture

          gm = GaussianMixture(n_components=40, random_state=42)
          y_pred = gm.fit_predict(X_train_pca)
```

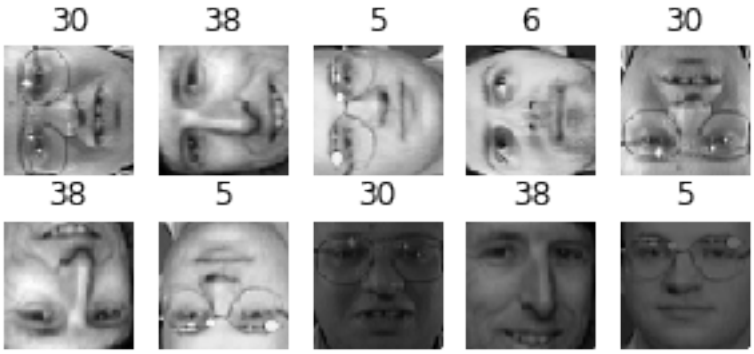
Exercise: Use the model to generate some new faces (using the `sample()` method), and visualize them (if you used PCA, you will need to use its `inverse_transform()` method).

```
In [202]: n_gen_faces = 20
          gen_faces_reduced, y_gen_faces = gm.sample(n_samples=n_gen_faces)
          gen_faces = pca.inverse_transform(gen_faces_reduced)

In [203]: plot_faces(gen_faces, y_gen_faces)
```



Exercise: Try to modify some images (e.g., rotate, flip, darken) and see if the model can detect the anomalies (i.e., compare the output of the `score_samples()` method for normal images and for anomalies).

```
In [204]: n_rotated = 4
          rotated = np.transpose(X_train[:n_rotated].reshape(-1, 64, 64), axes=[0, 2, 1])
          rotated = rotated.reshape(-1, 64*64)
          y_rotated = y_train[:n_rotated]

          n_flipped = 3
          flipped = X_train[:n_flipped].reshape(-1, 64, 64)[:, ::-1]
          flipped = flipped.reshape(-1, 64*64)
          y_flipped = y_train[:n_flipped]

          n_darkened = 3
          darkened = X_train[:n_darkened].copy()
          darkened[:, 1:-1] *= 0.3
          darkened = darkened.reshape(-1, 64*64)
          y_darkened = y_train[:n_darkened]

          X_bad_faces = np.r_[rotated, flipped, darkened]
          y_bad = np.concatenate([y_rotated, y_flipped, y_darkened])

          plot_faces(X_bad_faces, y_bad)
```




```
In [205]: X_bad_faces_pca = pca.transform(X_bad_faces)

In [206]: gm.score_samples(X_bad_faces_pca)

Out[206]: array([-2.43643037e+07, -1.89785096e+07, -3.78112303e+07, -4.98187816e+07,
                 -3.20479116e+07, -1.37530878e+07, -2.92374167e+07, -1.05488962e+08,
                 -1.19575241e+08, -6.74255912e+07])
```

The bad faces are all considered highly unlikely by the Gaussian Mixture model. Compare this to the scores of some training instances:

```
In [207]: gm.score_samples(X_train_pca[:10])
```

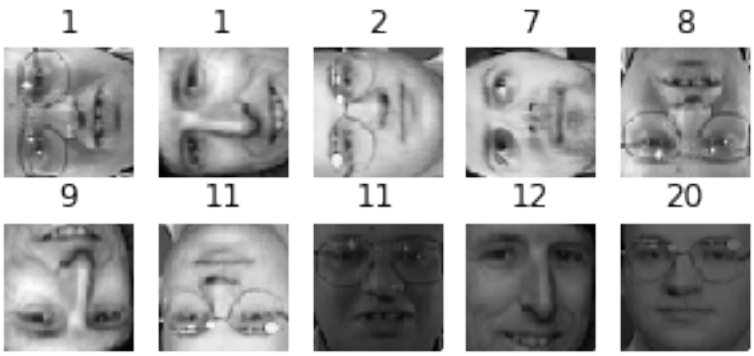
```
Out[207]: array([1163.02020782, 1134.03637955, 1156.32132916, 1170.67602877,
                 1141.45404923, 1154.35205244, 1091.32894658, 1111.41149605,
                 1096.43049398, 1132.98982653])
```

4.5 13. Using Dimensionality Reduction Techniques for Anomaly Detection

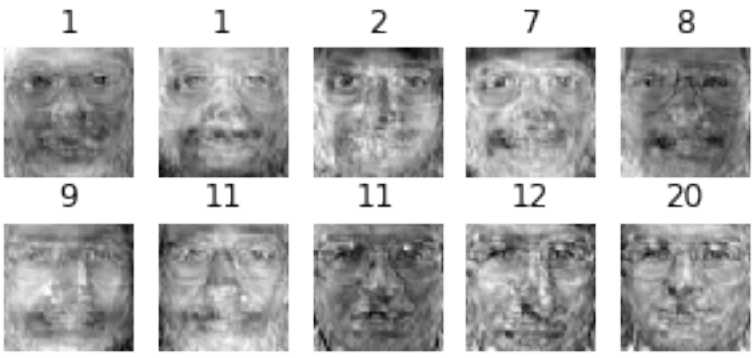
Exercise: Some dimensionality reduction techniques can also be used for anomaly detection. For example, take the Olivetti faces dataset and reduce it with PCA, preserving 99% of the variance. Then compute the reconstruction error for each image. Next, take some of the modified images you built in the previous exercise, and look at their reconstruction error: notice how much larger the reconstruction error is. If you plot a reconstructed image, you will see why: it tries to reconstruct a normal face.

We already reduced the dataset using PCA earlier:

```
In [208]: X_train_pca

Out[208]: array([[ 3.78081155e+00, -1.85478246e+00, -5.14402437e+00, ...,
                   -1.35636762e-01, -2.14078009e-01,  6.11925423e-02],
                 [ 1.01488543e+01, -1.52754021e+00, -7.66989529e-01, ...,
                    1.23924956e-01, -1.35271937e-01, -2.32602730e-02],
                 [-1.00152893e+01,  2.87728882e+00, -9.19888139e-01, ...,
                    7.26130083e-02, -2.96292058e-03,  1.24880552e-01],
                 ...,
                 [ 2.47586727e+00,  2.95597124e+00,  1.29985118e+00, ...,
                   -2.09054109e-02,  3.48596871e-02, -1.54340118e-01],
                 [-3.22031713e+00,  5.34897852e+00,  1.39426589e+00, ...,
                    5.75408675e-02, -2.28313506e-01,  1.55569553e-01],
                 [-9.22876954e-01, -3.64702487e+00,  2.26088190e+00, ...,
                    1.36844069e-01, -6.91413283e-02,  6.27049729e-02]], dtype=float32)

In [209]: def reconstruction_errors(pca, X):
              X_pca = pca.transform(X)
              X_reconstructed = pca.inverse_transform(X_pca)
              mse = np.square(X_reconstructed - X).mean(axis=-1)
              return mse

In [210]: reconstruction_errors(pca, X_train).mean()

Out[210]: 0.0001920535

In [211]: reconstruction_errors(pca, X_bad_faces).mean()

Out[211]: 0.0047073546

In [212]: plot_faces(X_bad_faces, y_gen_faces)
```



In [213]:
```
X_bad_faces_reconstructed = pca.inverse_transform(X_bad_faces_pca)
plot_faces(X_bad_faces_reconstructed, y_gen_faces)
```



In [ ]: