# Unsupervised Learning

## Introduction

This "walk-through" lab will give some examples of the unsupervised learning methods covered in lectures. First we look into applying dimensionality reduction using PCA. Next we apply $k$-means clustering, as well as the EM algorithm discussed in lectures. We finish with some toy examples of some other clustering algorithms we did not cover but which you may find useful.

### Acknowledgement

*This notebook contains several excerpts from the Python Data Science Handbook (http://shop.oreilly.com/product/0636920034919.do) by Jake VanderPlas; the original content is available on GitHub (https://github.com/jakevdp/PythonDataScienceHandbook).*

## Overview

The objective is to expose some of the methods and to show some visualizations, since this is a key aspect of dimensionality reduction and clustering. We will use the `Seaborn` visualization package which builds on and extends the capabilities of the standard `Matplotlib` package. *You will need to install these if you want to run this notebook locally.*

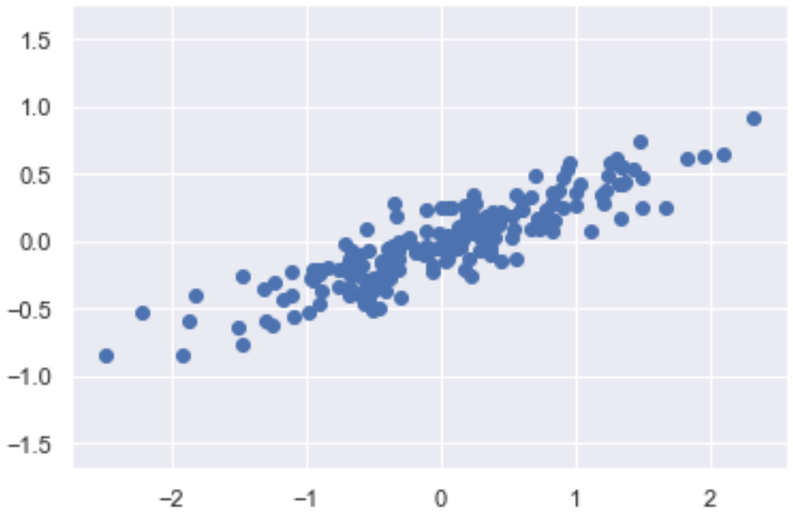
In [40]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()

import pandas as pd
# pandas.__version__
```

## Principal Component Analysis (PCA)

Principal component analysis is an unsupervised method for dimensionality reduction that is designed to search for a set of linear combinations of the original features. If this set of new features is smaller than the set of original features, it forms a *sub-space* onto which the data can be projected, reducing the number of dimensions. PCA is easiest to visualize by looking at a two-dimensional dataset. Consider the following 200 points:

In [41]:
```
rng = np.random.RandomState(1)
A=rng.rand(2, 2)
B=rng.randn(2, 200)
X = np.dot(A,B).T
plt.scatter(X[:, 0], X[:, 1])
plt.axis('equal')
```

Out[41]:
```
(-2.7391278364515688,
 2.5801310701596343,
 -0.9477947579593763,
 1.0195904306706842)
```



Clearly there is a nearly linear relationship here between the two axes. We could apply linear regression to model the dependency of the y values on the x values, but the problem setting here is slightly different: rather than attempting to *predict* the y values from the x values, the unsupervised learning problem attempts to learn about the *relationship* between the x and y values. To do this, PCA zero-centres the data matrix, generates the covariance matrix, then applies a Singular Value Decomposition (SVD), as outlined in the lecture notes. However, here we simply call Scikit-Learn's `PCA` estimator to do this. PCA will return a list of the orthogonal *principal axes* (eigenvectors) in the data, ordered in terms of decreasing variance (decreasing eigenvalues).

In [42]:
```
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
pca.fit(X)
```

Out[42]:
```
PCA(copy=True, iterated_power='auto', n_components=2, random_state
=None,
  svd_solver='auto', tol=0.0, whiten=False)
```

The fit learns some quantities from the data, most importantly the "components" and "explained variance":

In [43]:
```
print(pca.components_)
```

```
[[-0.94446029 -0.32862557]
 [-0.32862557  0.94446029]]
```

In [44]:
```
print(pca.explained_variance_)
```

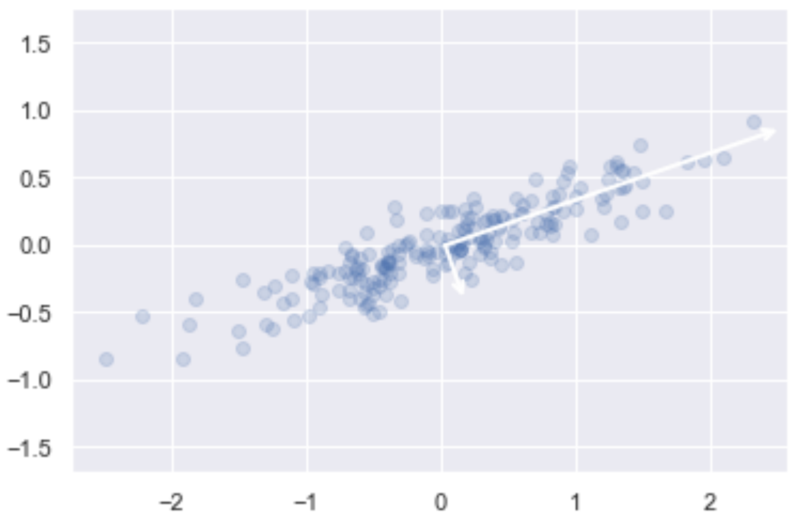
```
[0.7625315 0.0184779]
```

To see what these numbers mean, let's visualize them as vectors over the input data, using the "components" to define the direction of the vector, and the "explained variance" to define the squared-length of the vector:

In [45]:
```
def draw_vector(v0, v1, ax=None):
    ax = ax or plt.gca()
    arrowprops=dict(arrowstyle='->',
                    linewidth=2,
                    shrinkA=0, shrinkB=0)
    ax.annotate('', v1, v0, arrowprops=arrowprops)

# plot data
plt.scatter(X[:, 0], X[:, 1], alpha=0.2)
for length, vector in zip(pca.explained_variance_, pca.components_):
    print(length,vector)
    v = vector * 3 * np.sqrt(length)
    draw_vector(pca.mean_, pca.mean_ - v)
plt.axis('equal')
```

```
0.7625315008826115 [-0.94446029 -0.32862557]
0.018477895513562572 [-0.32862557  0.94446029]
```

Out[45]:
```
(-2.7391278364515688,
 2.5801310701596343,
 -0.9477947579593763,
 1.0195904306706842)
```



These vectors represent the *principal axes* of the data, and the length of the vector is an indication of how "important" that axis is in describing the distribution of the data—more precisely, it is a measure of the variance of the data when projected onto that axis. The projection of each data point onto the principal axes are the "principal components" of the data.

This transformation from data axes to principal axes is an *affine transformation*, which basically means it is composed of a translation, rotation, and uniform scaling, which is implemented by the SVD algorithm.

While this algorithm to find principal components may seem like just a mathematical curiosity, it turns out to have very far-reaching applications in the world of machine learning and data exploration.

## PCA as dimensionality reduction

Using PCA for dimensionality reduction involves *zeroing out* one or more of the smallest principal components, resulting in a lower-dimensional projection of the data that preserves the maximal data variance. (You can think of this as setting the eigenvalues below some threshold in the diagonal matrix to zero).

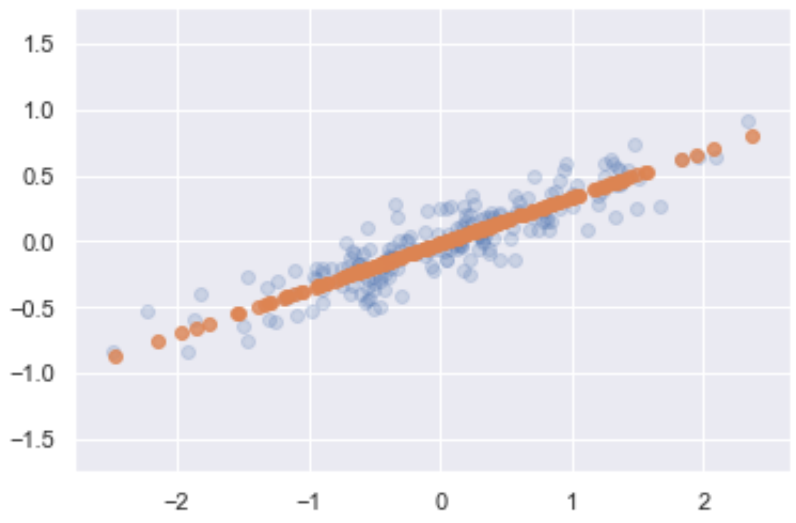
Here is an example of using PCA as a dimensionality reduction transform:

In [46]:
```
pca = PCA(n_components=1)
pca.fit(X)
X_pca = pca.transform(X)
print("original shape:   ", X.shape)
print("transformed shape:", X_pca.shape)
```

```
original shape:    (200, 2)
transformed shape: (200, 1)
```

The transformed data has been reduced to a single dimension. To understand the effect of this dimensionality reduction, we can perform the inverse transform of this reduced data and plot it along with the original data:

In [47]:
```
X_new = pca.inverse_transform(X_pca)
plt.scatter(X[:, 0], X[:, 1], alpha=0.2)
plt.scatter(X_new[:, 0], X_new[:, 1], alpha=0.8)
plt.axis('equal');
```



The light points are the original data, while the dark points are the projected version. This makes clear what a PCA dimensionality reduction means: ***the information along the least important principal axis or axes is removed, leaving only the component(s) of the data with the highest variance***. The fraction of variance that is cut out (proportional to the spread of points about the line formed in this figure) is roughly a measure of how much "information" is discarded in this reduction of dimensionality.

This reduced-dimension dataset is in some senses "good enough" to encode the most important relationships between the points: despite reducing the dimension of the data by 50%, the overall relationship between the data points are mostly preserved.

## PCA for visualization: Hand-written digits

The usefulness of the dimensionality reduction may not be entirely apparent in only two dimensions, but becomes much more clear when looking at high-dimensional data. To see this, let's take a quick look at the application of PCA to the built-in digits dataset.

We start by loading the data:

In [48]:
```
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
```

Out[48]:
```
(1797, 64)
```

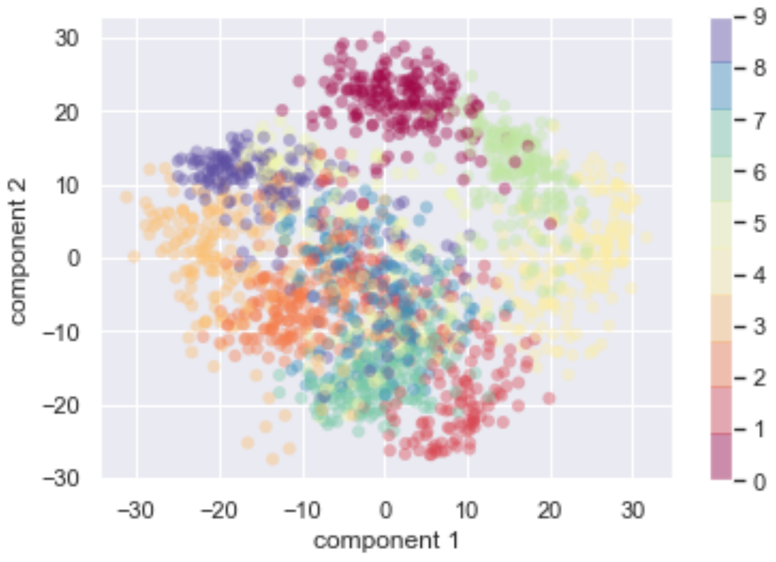
Recall that the data consists of 8×8 pixel images, meaning that they are 64-dimensional. To gain some intuition into the relationships between these points, we can use PCA to project them to a more manageable number of dimensions, say two:

In [49]:
```
pca = PCA(n_components=2)  # project from 64 to 2 dimensions
projected = pca.fit_transform(digits.data)
print(digits.data.shape)
print(projected.shape)
```

```
(1797, 64)
(1797, 2)
```

We can now plot the first two principal components of each point to learn about the data:

In [50]:
```
import matplotlib.cm

plt.scatter(projected[:, 0], projected[:, 1],
            c=digits.target, edgecolor='none', alpha=0.4,
            # cmap=plt.cm.get_cmap('spectral', 10))
            cmap=plt.cm.get_cmap('Spectral', 10))
plt.xlabel('component 1')
plt.ylabel('component 2')
plt.colorbar();
```



Recall what these components mean: the full data is a 64-dimensional point cloud, and these points are the projection of each data point along the directions with the largest variance. Essentially, we have found the optimal stretch and rotation in 64-dimensional space that allows us to see the layout of the digits in two dimensions, and have done this in an unsupervised manner—that is, without reference to the labels. The set of examples for each digit has been colour-coded using the key on the right. This is the sense in which PCA can provide a low-dimensional representation of the data: it discovers a set of functions (linear combinations of the original features) that are more efficient at encoding the data than the native pixel features of the input data.

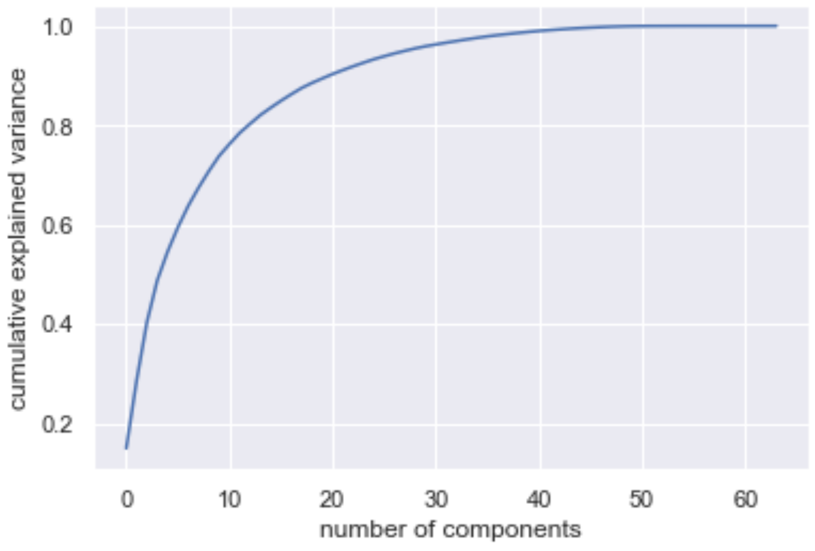
## Choosing the number of components

A vital part of using PCA in practice is the ability to estimate how many components are needed to describe the data. This can be determined by looking at the cumulative *explained variance ratio*.

On the cumulative *explained variance ratio* plot, we want to find the turning point where its cumulative *explained variance ratio* reach one threshold.

In [51]:
```
pca = PCA().fit(digits.data)
plt.plot(np.cumsum(pca.explained_variance_ratio_))
plt.xlabel('number of components')
plt.ylabel('cumulative explained variance')
```

Out[51]:
```
Text(0, 0.5, 'cumulative explained variance')
```



This curve quantifies how much of the total, 64-dimensional variance is contained within the first $N$ components. For example, we see that with the digits the first 10 components contain approximately 75% of the variance, while you need around 50 components to describe close to 100% of the variance.

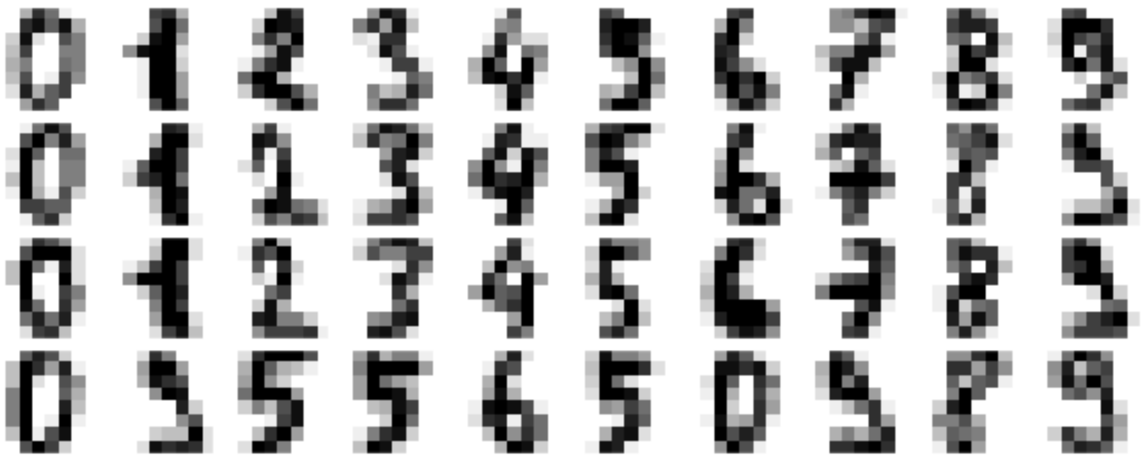
Here we see that our two-dimensional projection loses a lot of information (as measured by the explained variance) and that we'd need about 20 components to retain 90% of the variance. Looking at this plot for a high-dimensional dataset can help you understand the level of redundancy present in multiple observations.

## PCA as Noise Filtering

PCA can also be used as a filtering approach for noisy data. The idea is this: any components with variance much larger than the effect of the noise should be relatively unaffected by the noise. So if you reconstruct the data using just the largest subset of principal components, you should be preferentially keeping the signal and throwing out the noise.

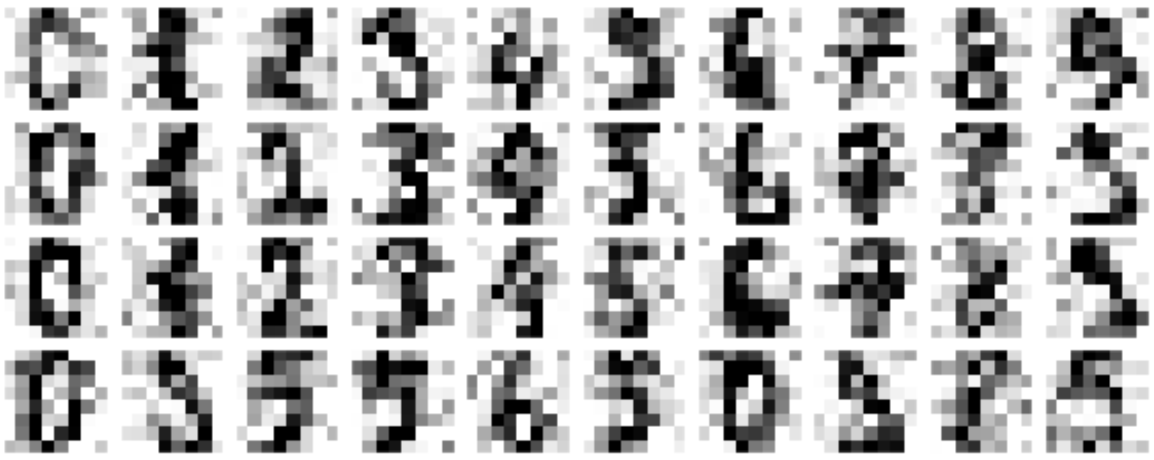
Let's see how this looks with the digits data. First we will plot several of the input noise-free data:

In [52]:
```
def plot_digits(data):
    fig, axes = plt.subplots(4, 10, figsize=(10, 4),
                             subplot_kw={'xticks':[], 'yticks':[]},
                             gridspec_kw=dict(hspace=0.1, wspace=0.
    for i, ax in enumerate(axes.flat):
        ax.imshow(data[i].reshape(8, 8),
                  cmap='binary', interpolation='nearest',
                  clim=(0, 16))
plot_digits(digits.data)
```



Now lets add some random noise to create a noisy dataset, and re-plot it:

In [53]:
```
np.random.seed(42)
noisy = np.random.normal(digits.data, 4)
plot_digits(noisy)
```



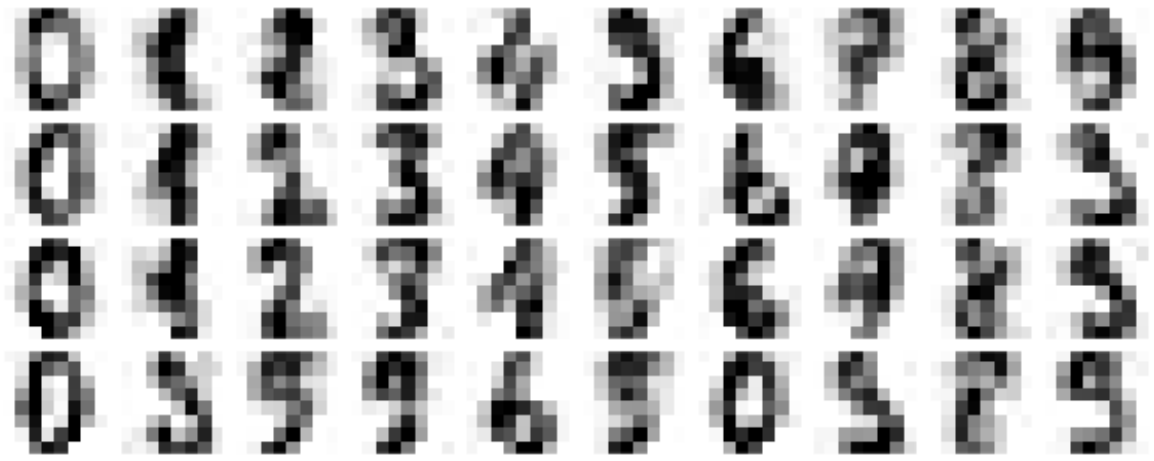
It's clear by eye that the images are noisy, and contain spurious pixels. Let's train a PCA on the noisy data, requesting that the projection preserve 50% of the variance:

In [54]:
```
pca = PCA(0.50).fit(noisy)
pca.n_components_
```

Out[54]:
```
12
```

Here 50% of the variance amounts to 12 principal components. Now we compute these components, and then use the inverse of the transform to reconstruct the filtered digits:

In [55]:
```
components = pca.transform(noisy)
filtered = pca.inverse_transform(components)
plot_digits(filtered)
```



This signal preserving/noise filtering property makes PCA a very useful feature selection routine—for example, rather than training a classifier on very high-dimensional data, you might instead train the classifier on the lower-dimensional representation, which will automatically serve to filter out random noise in the inputs.

## Example: Eigenfaces

This example applies a PCA projection to facial image data using the Labeled Faces in the Wild dataset made available through Scikit-Learn:

In [56]:
```
from sklearn.datasets import fetch_lfw_people
faces = fetch_lfw_people(min_faces_per_person=60)
print(faces.target_names)
print(faces.images.shape)
```

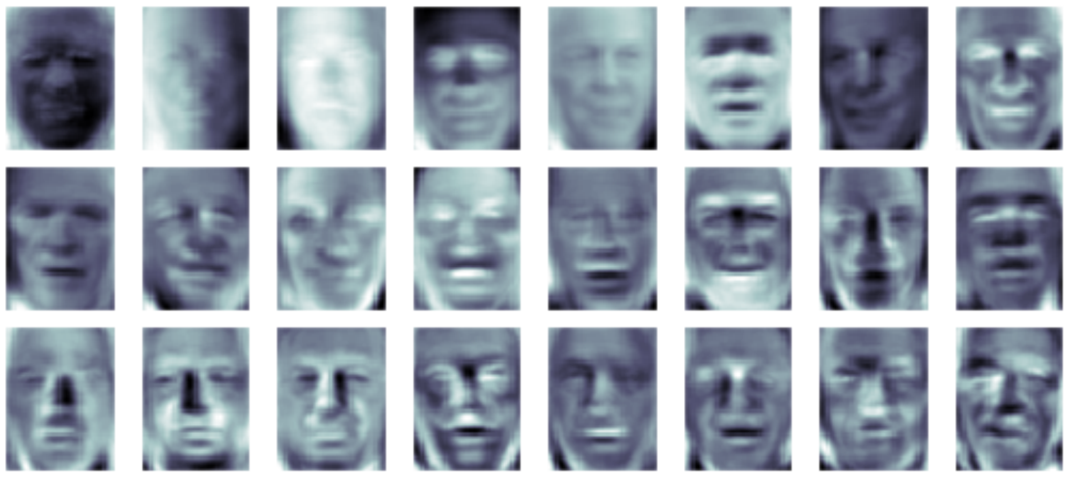
```
['Ariel Sharon' 'Colin Powell' 'Donald Rumsfeld' 'George W Bush'
 'Gerhard Schroeder' 'Hugo Chavez' 'Junichiro Koizumi' 'Tony Blair
']
(1348, 62, 47)
```

Let's take a look at the principal axes that span this dataset. Because this is a large dataset, we will use a `Randomized` version of PCA which contains a randomized method to approximate the first $N$ principal components much more quickly than the standard `PCA` estimator, and thus is very useful for high-dimensional data (here, a dimensionality of nearly 3,000). We will take a look at the first 150 components:

In [57]:
```
# from sklearn.decomposition import RandomizedPCA
# pca = RandomizedPCA(150)
# pca.fit(faces.data)
pca = PCA(n_components=150,svd_solver='randomized').fit(faces.data)
```

In this case, it can be interesting to visualize the images associated with the first several principal components (these components are technically known as "eigenvectors," so these types of images are often called "eigenfaces"). As you can see in this figure, they are as creepy as they sound:

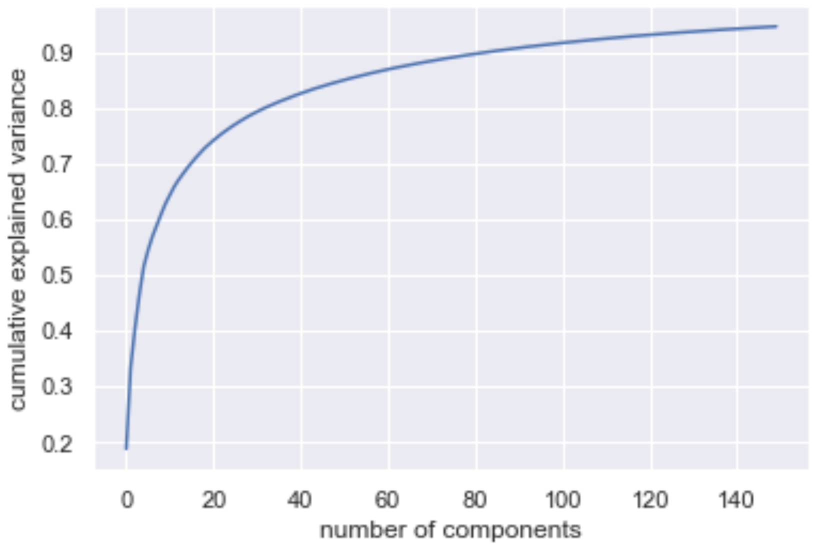
In [58]:
```
fig, axes = plt.subplots(3, 8, figsize=(9, 4),
                         subplot_kw={'xticks':[], 'yticks':[]},
                         gridspec_kw=dict(hspace=0.1, wspace=0.1))
for i, ax in enumerate(axes.flat):
    ax.imshow(pca.components_[i].reshape(62, 47), cmap='bone')
```



The results are very interesting, and give us insight into how the images vary: for example, the first few eigenfaces (from the top left) seem to be associated with the angle of lighting on the face, and later principal vectors seem to be picking out certain features, such as eyes, noses, and lips. Let's take a look at the cumulative variance of these components to see how much of the data information the projection is preserving:

In [59]:
```
plt.plot(np.cumsum(pca.explained_variance_ratio_))
plt.xlabel('number of components')
plt.ylabel('cumulative explained variance');
plt.figure()
```

Out[59]:
```
<Figure size 432x288 with 0 Axes>
```

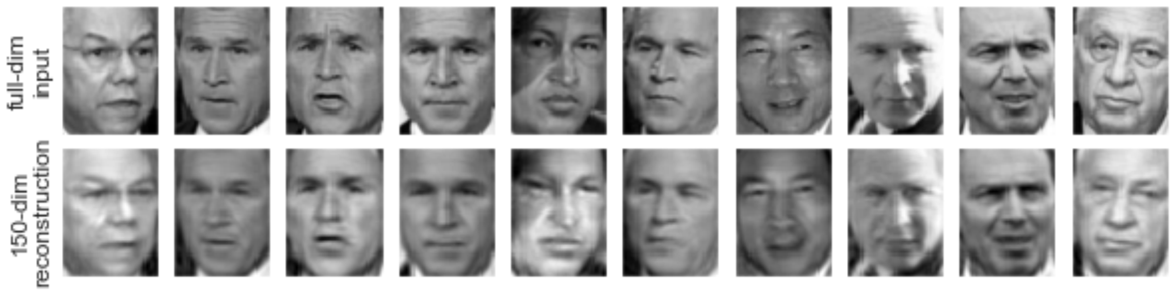


```
<Figure size 432x288 with 0 Axes>
```

We see that these 150 components account for just over 90% of the variance. That would lead us to believe that using these 150 components, we would recover most of the essential characteristics of the data. To make this more concrete, we can compare the input images with the images reconstructed from these 150 components:

In [60]:
```
# Compute the components and projected faces
# pca = RandomizedPCA(150).fit(faces.data)
pca = PCA(n_components=150,svd_solver='randomized').fit(faces.data)
components = pca.transform(faces.data)
projected = pca.inverse_transform(components)
```

In [61]:
```
# Plot the results
fig, ax = plt.subplots(2, 10, figsize=(10, 2.5),
                       subplot_kw={'xticks':[], 'yticks':[]},
                       gridspec_kw=dict(hspace=0.1, wspace=0.1))
for i in range(10):
    ax[0, i].imshow(faces.data[i].reshape(62, 47), cmap='binary_r')
    ax[1, i].imshow(projected[i].reshape(62, 47), cmap='binary_r')

ax[0, 0].set_ylabel('full-dim\ninput')
ax[1, 0].set_ylabel('150-dim\nreconstruction');
```



The top row here shows the input images, while the bottom row shows the reconstruction of the images from just 150 of the ~3,000 initial features. This visualization makes clear why the PCA feature selection can be so successful: although it reduces the dimensionality of the data by nearly a factor of 20, the projected images contain enough information that we might, by eye, recognize the individuals in the image. What this means is that following this dimensionality reduction a classification algorithm can be trained on 150-dimensional data rather than 3,000-dimensional data, which, depending on the particular algorithm we choose, can lead to a much more efficient classification.

### Principal Component Analysis Summary

In this section we have discussed the use of principal component analysis for dimensionality reduction, for visualization of high-dimensional data, for noise filtering, and for feature selection within high-dimensional data. Because of the versatility and interpretability of PCA, it has been shown to be effective in a wide variety of contexts and disciplines. Given any high-dimensional dataset, I tend to start with PCA in order to visualize the relationship between points (as we did with the digits), to understand the main variance in the data (as we did with the eigenfaces), and to understand the intrinsic dimensionality (by plotting the explained variance ratio). Certainly PCA is not useful for every high-dimensional dataset, but it offers a straightforward and efficient path to gaining insight into high-dimensional data.

PCA has two main weaknesses: first, it assumes that the principal components are linear combinations (which may not be appropriate if non-linear dimensions will be required) and second, it tends to be highly affected by outliers in the data. For these reasons, it may be necessary to use non-linear dimensionality reduction algorithms (such as *Isomap*, *LLE*, etc.) or robust PCA methods (such as *RandomizedPCA*, as used above).

# k-Means Clustering

Clustering algorithms seek to learn, from the properties of the data, an optimal division or discrete labeling of groups of points. Many clustering algorithms are available in Scikit-Learn and elsewhere, but perhaps the simplest to understand is an algorithm known as *k-means clustering*, which is implemented in `sklearn.cluster.KMeans` .

### Introducing k-Means

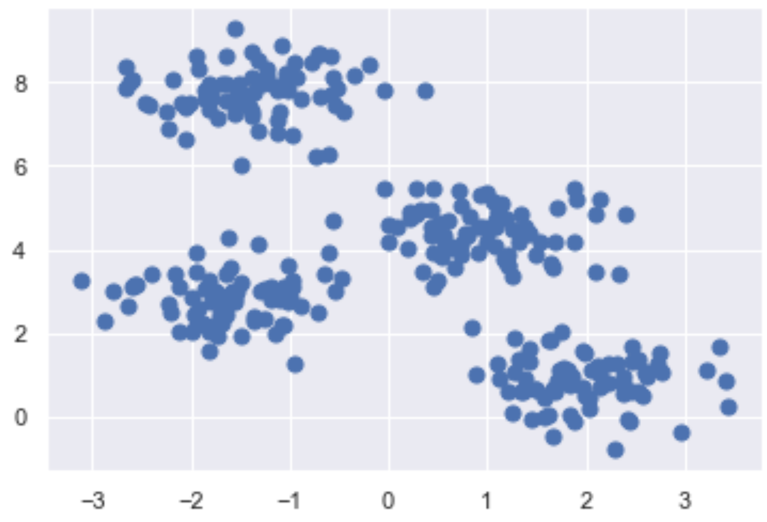
The *k*-means algorithm searches for a pre-determined number of clusters within an unlabeled multidimensional dataset. It accomplishes this using a simple conception of what the optimal clustering looks like:

- The "cluster center" is the arithmetic mean (centroid) of all the points belonging to the cluster.
- Each point is closer to its own cluster center than to other cluster centers.

Those two assumptions are the basis of the *k*-means model. We will soon dive into exactly *how* the algorithm reaches this solution, but for now let's take a look at a simple dataset and see the *k*-means result.

First, let's generate a two-dimensional dataset containing four distinct blobs. To emphasize that this is an unsupervised algorithm, we will leave the labels out of the visualization

In [62]:
```
from sklearn.datasets.samples_generator import make_blobs
X, y_true = make_blobs(n_samples=300, centers=4,
                       cluster_std=0.60, random_state=0)
plt.scatter(X[:, 0], X[:, 1], s=50);
```

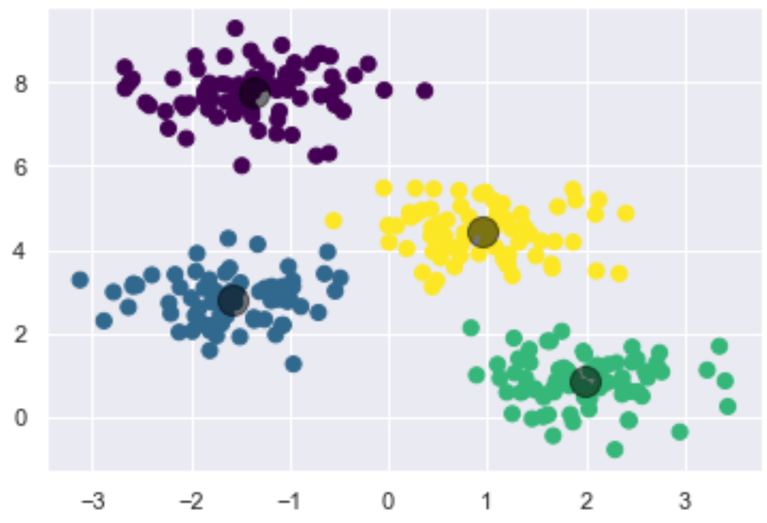


By eye, it is relatively easy to pick out the four clusters. The *k*-means algorithm does this automatically, and in Scikit-Learn uses the typical estimator API:

In [63]:
```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=4)
kmeans.fit(X)
y_kmeans = kmeans.predict(X)
# the following function combine the fit function and the predict f
y_kmeans1 = kmeans.fit_predict(X)
```

Let's visualize the results by plotting the data colored by these labels. We will also plot the cluster centers as determined by the *k*-means estimator:

In [64]:
```
plt.scatter(X[:, 0], X[:, 1], c=y_kmeans, s=50, cmap='viridis')

centers = kmeans.cluster_centers_
plt.scatter(centers[:, 0], centers[:, 1], c='black', s=200, alpha=0
```



The good news is that the *k*-means algorithm (at least in this simple case) assigns the points to clusters very similarly to how we might assign them by eye. But you might wonder how this algorithm finds these clusters so quickly! After all, the number of possible combinations of cluster assignments is exponential in the number of data points—an exhaustive search would be very, very costly. Fortunately for us, such an exhaustive search is not necessary: instead, the typical approach to *k*-means involves an intuitive iterative approach known as *expectation–maximization*.

## k-Means Algorithm: Expectation–Maximization

Expectation–maximization (E–M) is a powerful algorithm that comes up in a variety of contexts within data science. *k*-means is a particularly simple and easy-to-understand application of the algorithm, and we will walk through it briefly here. In short, the expectation–maximization approach here consists of the following procedure:

1. Guess some cluster centers
2. Repeat until converged
    A. *E-Step*: assign points to the nearest cluster center
    B. *M-Step*: set the cluster centers to the mean

Here the "E-step" or "Expectation step" is so-named because it involves updating our expectation of which cluster each point belongs to. The "M-step" or "Maximization step" is so-named because it involves maximizing some fitness function that defines the location of the cluster centers—in this case, that maximization is accomplished by taking a simple mean of the data in each cluster.

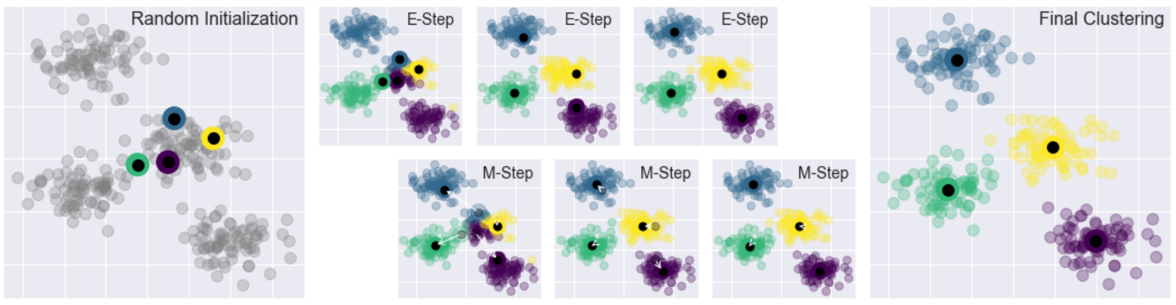
The literature about this algorithm is vast, but can be summarized as follows: under typical circumstances, each repetition of the E-step and M-step will always result in a better estimate of the cluster characteristics.

We can visualize the algorithm as shown in the following figure. For the particular initialization shown here, the clusters converge in just three iterations.

In [65]:
```
from sklearn.datasets.samples_generator import make_blobs
from sklearn.metrics import pairwise_distances_argmin

X, y_true = make_blobs(n_samples=300, centers=4,
                       cluster_std=0.60, random_state=0)

rng = np.random.RandomState(42)
centers = [0, 4] + rng.randn(4, 2)

def draw_points(ax, c, factor=1):
    ax.scatter(X[:, 0], X[:, 1], c=c, cmap='viridis',
               s=50 * factor, alpha=0.3)

def draw_centers(ax, centers, factor=1, alpha=1.0):
    ax.scatter(centers[:, 0], centers[:, 1],
               c=np.arange(4), cmap='viridis', s=200 * factor,
               alpha=alpha)
    ax.scatter(centers[:, 0], centers[:, 1],
               c='black', s=50 * factor, alpha=alpha)

def make_ax(fig, gs):
    ax = fig.add_subplot(gs)
    ax.xaxis.set_major_formatter(plt.NullFormatter())
    ax.yaxis.set_major_formatter(plt.NullFormatter())
    return ax

fig = plt.figure(figsize=(15, 4))
```

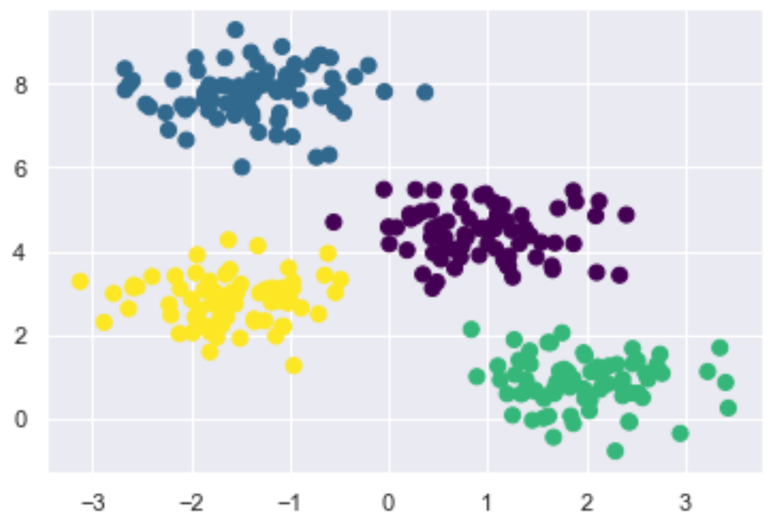
```
gs = plt.GridSpec(4, 15, left=0.02, right=0.98, bottom=0.05, top=0.
ax0 = make_ax(fig, gs[:4, :4])
ax0.text(0.98, 0.98, "Random Initialization", transform=ax0.transAx
         ha='right', va='top', size=16)
draw_points(ax0, 'gray', factor=2)
draw_centers(ax0, centers, factor=2)

for i in range(3):
    ax1 = make_ax(fig, gs[:2, 4 + 2 * i:6 + 2 * i])
    ax2 = make_ax(fig, gs[2:, 5 + 2 * i:7 + 2 * i])

    # E-step
    y_pred = pairwise_distances_argmin(X, centers)
    draw_points(ax1, y_pred)
    draw_centers(ax1, centers)

    # M-step
    new_centers = np.array([X[y_pred == i].mean(0) for i in range(4
    draw_points(ax2, y_pred)
    draw_centers(ax2, centers, alpha=0.3)
    draw_centers(ax2, new_centers)
    for i in range(4):
        ax2.annotate('', new_centers[i], centers[i],
                     arrowprops=dict(arrowstyle='->', linewidth=1))

    # Finish iteration
    centers = new_centers
    ax1.text(0.95, 0.95, "E-Step", transform=ax1.transAxes, ha='rig
    ax2.text(0.95, 0.95, "M-Step", transform=ax2.transAxes, ha='rig

# Final E-step
y_pred = pairwise_distances_argmin(X, centers)
axf = make_ax(fig, gs[:4, -4:])
draw_points(axf, y_pred, factor=2)
draw_centers(axf, centers, factor=2)
axf.text(0.98, 0.98, "Final Clustering", transform=axf.transAxes,
         ha='right', va='top', size=16)
```

Out[65]:
```
Text(0.98, 0.98, 'Final Clustering')
```



The *k*-Means algorithm is simple enough that we can write it in a few lines of code. The following is a very basic implementation:

In [66]:
```
from sklearn.metrics import pairwise_distances_argmin

def find_clusters(X, n_clusters, rseed=2):
    # 1. Randomly choose clusters
    rng = np.random.RandomState(rseed)
    i = rng.permutation(X.shape[0])[:n_clusters]
    centers = X[i]

    while True:
        # 2a. Assign labels based on closest center
        labels = pairwise_distances_argmin(X, centers)

        # 2b. Find new centers from means of points
        new_centers = np.array([X[labels == i].mean(0)
                                for i in range(n_clusters)])

        # 2c. Check for convergence
        if np.all(centers == new_centers):
            break
        centers = new_centers

    return centers, labels

centers, labels = find_clusters(X, 4)
plt.scatter(X[:, 0], X[:, 1], c=labels,
            s=50, cmap='viridis');
```



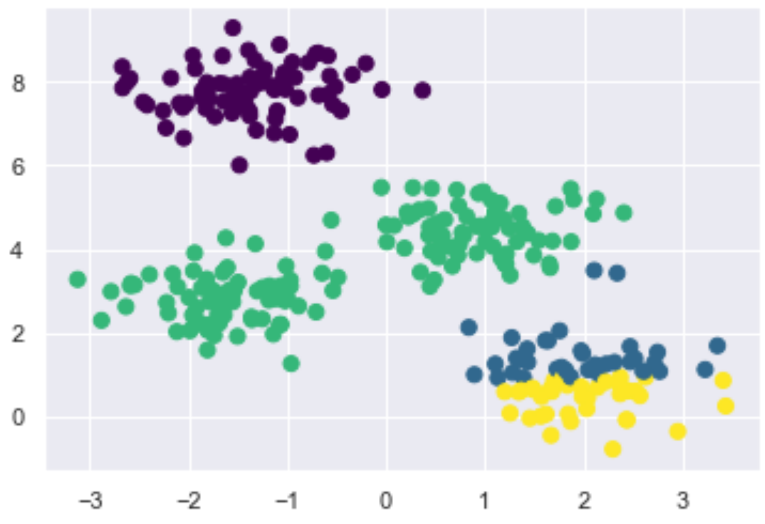
## Caveats of expectation–maximization

There are a few issues to be aware of when using the expectation–maximization algorithm.

### The globally optimal result may not be achieved

First, although the E–M procedure is guaranteed to improve the result in each step, there is no assurance that it will lead to the *global* best solution. For example, if we use a different random seed in our simple procedure, the particular starting guesses lead to poor results:

In [67]:
```
centers, labels = find_clusters(X, 4, rseed=0)
plt.scatter(X[:, 0], X[:, 1], c=labels,
            s=50, cmap='viridis');
```

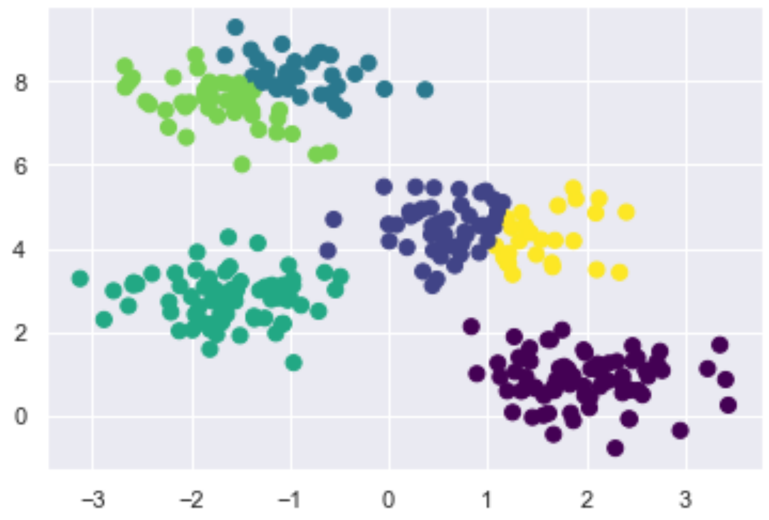


Here the E–M approach has converged, but has not converged to a globally optimal configuration. For this reason, it is common for the algorithm to be run for multiple starting guesses, as indeed Scikit-Learn does by default (set by the `n_init` parameter, which defaults to 10).

### The number of clusters must be selected beforehand

Another common challenge with *k*-means is that you must tell it how many clusters you expect: it cannot learn the number of clusters from the data. For example, if we ask the algorithm to identify six clusters, it will happily proceed and find the best six clusters:

In [68]:
```
labels = KMeans(6, random_state=0).fit_predict(X)
plt.scatter(X[:, 0], X[:, 1], c=labels,
            s=50, cmap='viridis');
```



Whether the result is meaningful is a question that is difficult to answer definitively; one approach that is rather intuitive, and that is discussed in the lecture notes, is called silhouette analysis (http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html).

Alternatively, you might use a more complicated clustering algorithm which has a better quantitative measure of the fitness per number of clusters (e.g., Gaussian mixture models) or which *can* choose a suitable number of clusters (e.g., DBSCAN, mean-shift, or affinity propagation, all available in the `sklearn.cluster` submodule)

**k-means is limited to linear cluster boundaries**

The fundamental model assumptions of *k*-means (points will be closer to their own cluster center than to others) means that the algorithm will often be ineffective if the clusters have complicated geometries.

In particular, the boundaries between *k*-means clusters will always be linear, which means that it will fail for more complicated boundaries.

#### k-means can be slow for large numbers of samples

Because each iteration of k-means must access every point in the dataset, the algorithm can be relatively slow as the number of samples grows. You might wonder if this requirement to use all data at each iteration can be relaxed; for example, you might just use a subset of the data to update the cluster centers at each step. This is the idea behind *batch-based* *k*-means algorithms, one form of which is implemented in `sklearn.cluster.MiniBatchKMeans`. The interface for this is the same as for standard `KMeans`; we will see an example of its use below.

### Example: k-means on digits

To start, let's take a look at applying *k*-means on the same simple digits data that we saw above.

Here we will attempt to use *k*-means to try to identify similar digits *without using the original label information*; this might be similar to a first step in extracting meaning from a new dataset about which you don't have any *a priori* label information.

We will start by loading the digits and then finding the `KMeans` clusters. Recall that the digits consist of 1,797 samples with 64 features, where each of the 64 features is the brightness of one pixel in an 8×8 image:

In [74]:
```python
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
```

Out[74]:
```
(1797, 64)
```

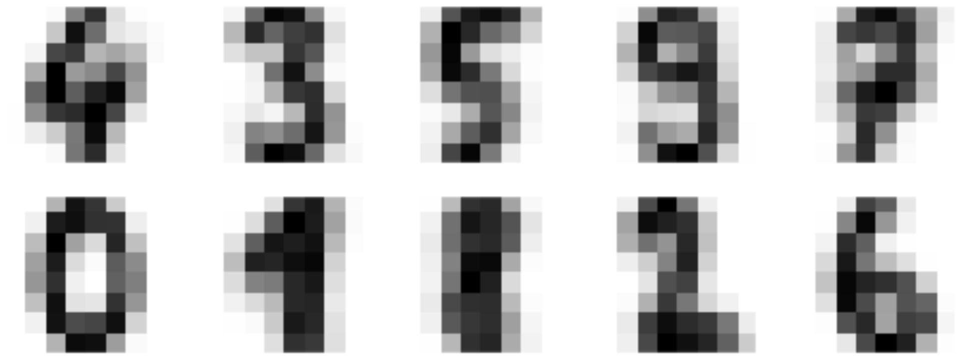
The clustering can be performed as we did before:

In [75]:
```python
kmeans = KMeans(n_clusters=10, random_state=0)
clusters = kmeans.fit_predict(digits.data)
kmeans.cluster_centers_.shape
```

Out[75]:
```
(10, 64)
```

The result is 10 clusters in 64 dimensions. Notice that the cluster centers themselves are 64-dimensional points, and can themselves be interpreted as the "typical" digit within the cluster (i.e., the centroid is a "digit"). Let's see what these cluster centers look like:

In [71]:
```
fig, ax = plt.subplots(2, 5, figsize=(8, 3))
centers = kmeans.cluster_centers_.reshape(10, 8, 8)
for axi, center in zip(ax.flat, centers):
    axi.set(xticks=[], yticks=[])
    axi.imshow(center, interpolation='nearest', cmap=plt.cm.binary)
```



We see that *even without the labels*, `KMeans` is able to find clusters whose centers are recognizable digits, with perhaps the exception of 1 and 8.

Because *k*-means knows nothing about the identity of the cluster, the 0–9 labels may be permuted. We can fix this by matching each learned cluster label with the true labels found in them:

In [72]:
```
from scipy.stats import mode

labels = np.zeros_like(clusters)
for i in range(10):
    mask = (clusters == i)
    labels[mask] = mode(digits.target[mask])[0]
```

Now we can check how accurate our unsupervised clustering was in finding similar digits within the data:

In [76]:
```
from sklearn.metrics import accuracy_score,adjusted_rand_score
print(accuracy_score(digits.target, labels))
print(adjusted_rand_score(digits.target, labels))
```

```
0.7935447968836951
0.6686991223627669
```

With just a simple k-means algorithm, we discovered the correct grouping for 80% of the input digits!

## Comparing different clustering algorithms on toy datasets

There *many* clustering algorithsm we did not cover. The following example aims at showing characteristics of some other clustering algorithms on datasets that are "interesting" but still in 2D. The last dataset is an example of a 'null' situation for clustering: the data is homogeneous, and there is no good clustering.

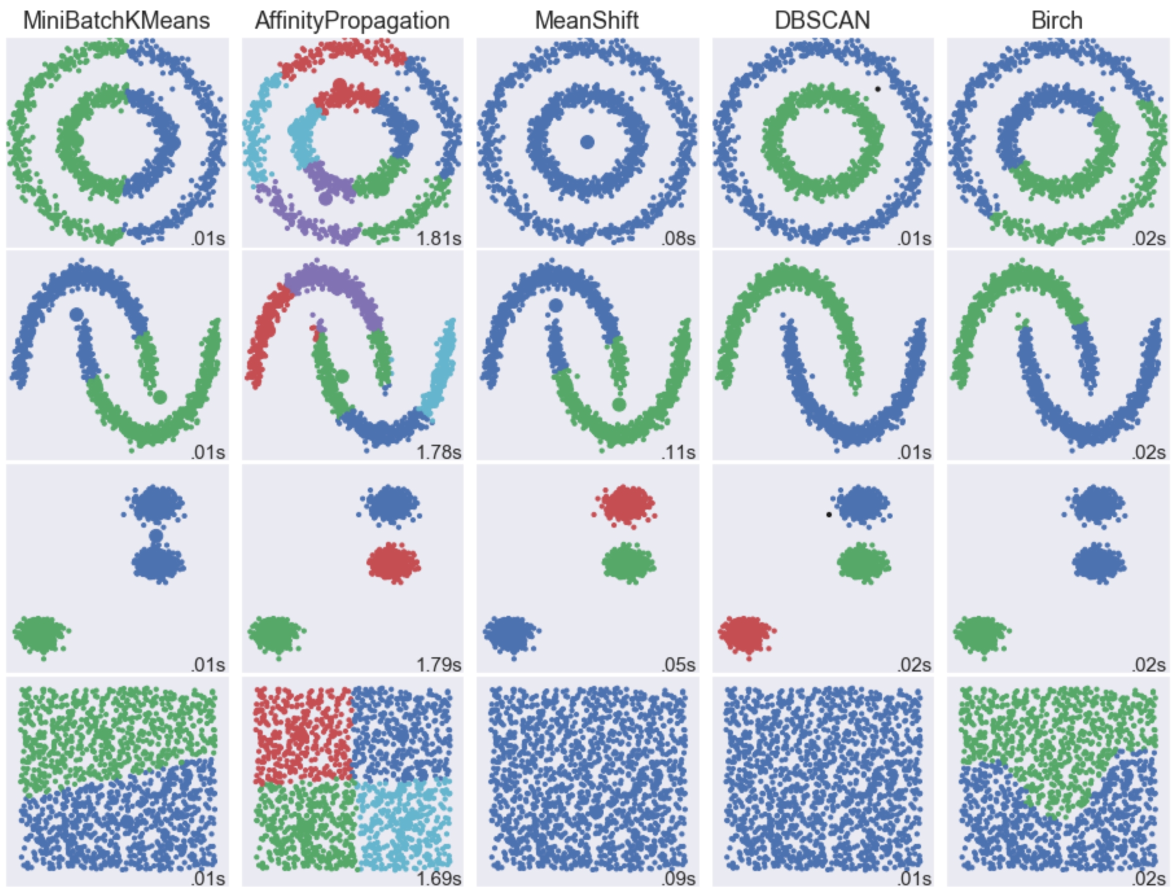
While these examples give some intuition about the algorithms, this intuition might not apply to very high dimensional data.

The results could be improved by tweaking the parameters for each clustering strategy, for instance, setting the number of clusters for the methods that need this parameter specified. Note that affinity propagation has a tendency to create many clusters. Thus in this example its two parameters (damping and per-point preference) were set to mitigate this behavior.

Run the code, inspect the visualizations, and read up a bit on the algorithms to try and understand what is going on!

In [77]:
```
print(__doc__)

import time

import numpy as np
import matplotlib.pyplot as plt

from sklearn import cluster, datasets
from sklearn.neighbors import kneighbors_graph
from sklearn.preprocessing import StandardScaler

np.random.seed(0)

# Generate datasets. We choose the size big enough to see the scala
# of the algorithms, but not too big to avoid too long running time
n_samples = 1500
noisy_circles = datasets.make_circles(n_samples=n_samples, factor=.
                                      noise=.05)
noisy_moons = datasets.make_moons(n_samples=n_samples, noise=.05)
blobs = datasets.make_blobs(n_samples=n_samples, random_state=8)
no_structure = np.random.rand(n_samples, 2), None

colors = np.array([x for x in 'bgrcmykbgrcmykbgrcmykbgrcmyk'])
colors = np.hstack([colors] * 20)

clustering_names = [
    'MiniBatchKMeans', 'AffinityPropagation', 'MeanShift',
    'DBSCAN', 'Birch']

plt.figure(figsize=(len(clustering_names) * 2 + 3, 9.5))
plt.subplots_adjust(left=.02, right=.98, bottom=.001, top=.96, wspa
                    hspace=.01)

plot_num = 1

datasets = [noisy_circles, noisy_moons, blobs, no_structure]
for i_dataset, dataset in enumerate(datasets):
    X, y = dataset
    # normalize dataset for easier parameter selection
    X = StandardScaler().fit_transform(X)

    # estimate bandwidth for mean shift
    bandwidth = cluster.estimate_bandwidth(X, quantile=0.3)

    # connectivity matrix for structured Ward
    connectivity = kneighbors_graph(X, n_neighbors=10, include_self
    # make connectivity symmetric
    connectivity = 0.5 * (connectivity + connectivity.T)

    # create clustering estimators
    ms = cluster.MeanShift(bandwidth=bandwidth, bin_seeding=True)

    two_means = cluster.MiniBatchKMeans(n_clusters=2)

    ward = cluster.AgglomerativeClustering(n_clusters=2, linkage='w
                                           connectivity=connectivit

    dbscan = cluster.DBSCAN(eps=.2)

    affinity_propagation = cluster.AffinityPropagation(damping=.9,
                                                       preference=-

    average_linkage = cluster.AgglomerativeClustering(
        linkage="average", affinity="cityblock", n_clusters=2,
        connectivity=connectivity)

    birch = cluster.Birch(n_clusters=2)

    clustering_algorithms = [
        two_means, affinity_propagation, ms,
        dbscan, birch]

    for name, algorithm in zip(clustering_names, clustering_algorit
        # predict cluster memberships
        t0 = time.time()
        algorithm.fit(X)
        t1 = time.time()
        if hasattr(algorithm, 'labels_'):
            y_pred = algorithm.labels_.astype(np.int)
        else:
            y_pred = algorithm.predict(X)

        # plot
        plt.subplot(4, len(clustering_algorithms), plot_num)
        plt.subplot(4, len(clustering_algorithms), plot_num)
        if i_dataset == 0:
            plt.title(name, size=18)
        plt.scatter(X[:, 0], X[:, 1], color=colors[y_pred].tolist()

        if hasattr(algorithm, 'cluster_centers_'):
            centers = algorithm.cluster_centers_
            center_colors = colors[:len(centers)]
            plt.scatter(centers[:, 0], centers[:, 1], s=100, c=cent
        plt.xlim(-2, 2)
        plt.ylim(-2, 2)
        plt.xticks(())
        plt.yticks(())
        plt.text(.99, .01, ('%.2fs' % (t1 - t0)).lstrip('0'),
                 transform=plt.gca().transAxes, size=15,
                 horizontalalignment='right')
        plot_num += 1

plt.show()
```

```
Automatically created module for IPython interactive environment
```



```
In [ ]:
```