demo12

April 21, 2020

In this lab, we will learn how to implement k-means and EM, and visualize some essential differences. Let us start with some synthetic data.

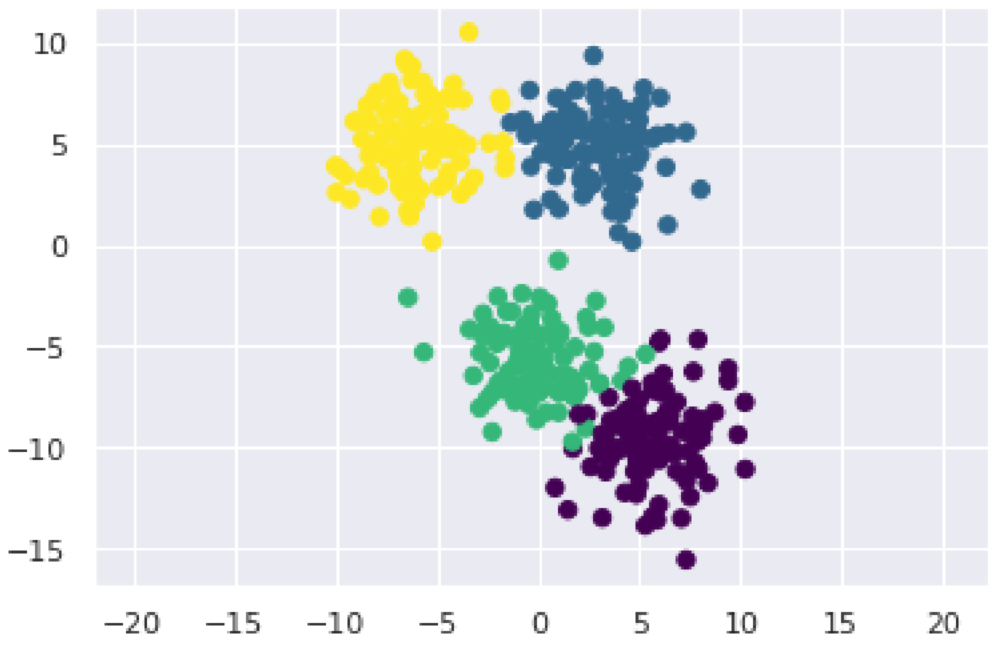
[1]:
```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
sns.set()
```

```
/usr/local/lib/python3.6/dist-packages/statsmodels/tools/_testing.py:19:
FutureWarning: pandas.util.testing is deprecated. Use the functions in the
public API at pandas.testing instead.
  import pandas.util.testing as tm
```

[0]:
```
from sklearn.datasets import make_blobs
X, y_true = make_blobs(n_samples=400,centers=4,cluster_std=2,random_state=10)
```

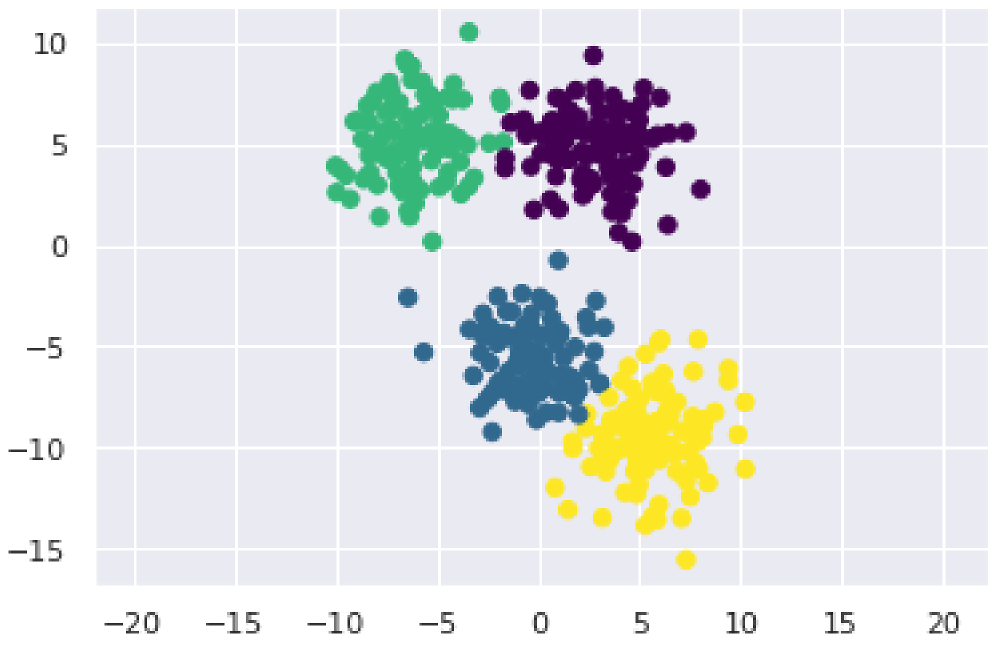
[3]:
```
plt.scatter(X[:, 0], X[:, 1], c=y_true, s=40, cmap='viridis');
ax = plt.gca()
ax.axis('equal')
```

[3]:
```
(-11.02535175761933,
 11.24746483124909,
 -16.848150742263016,
 11.839765378970164)
```



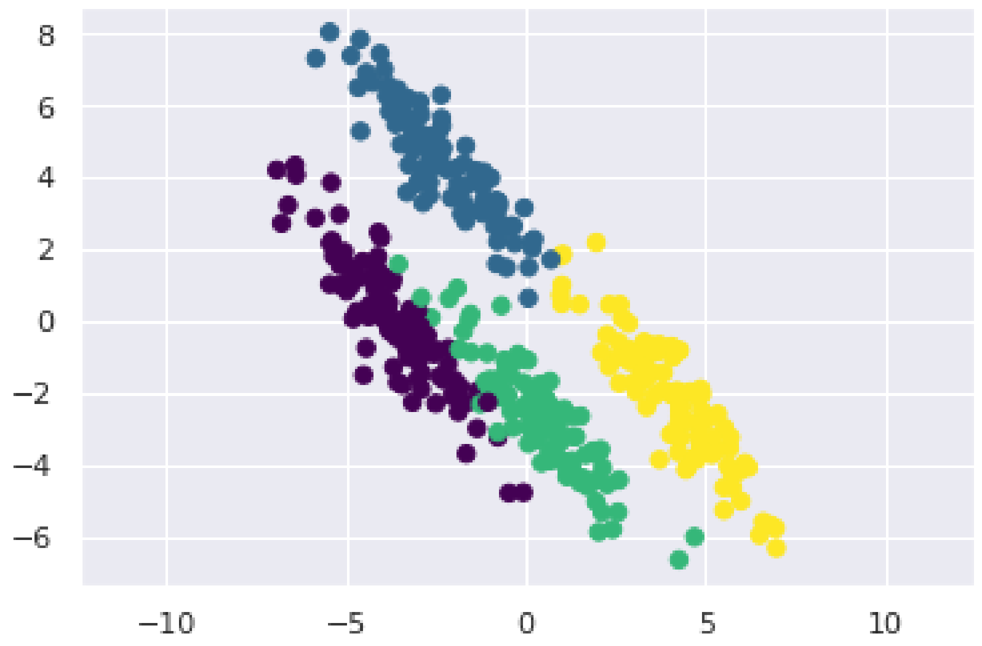
OK, let's now run KMeans.

[4]:
```
from sklearn.cluster import KMeans
kmeans = KMeans(4)
labels = kmeans.fit(X).predict(X)
plt.scatter(X[:, 0], X[:, 1], c=labels, s=40, cmap='viridis');
ax = plt.gca()
ax.axis('equal')
plt.show();
```

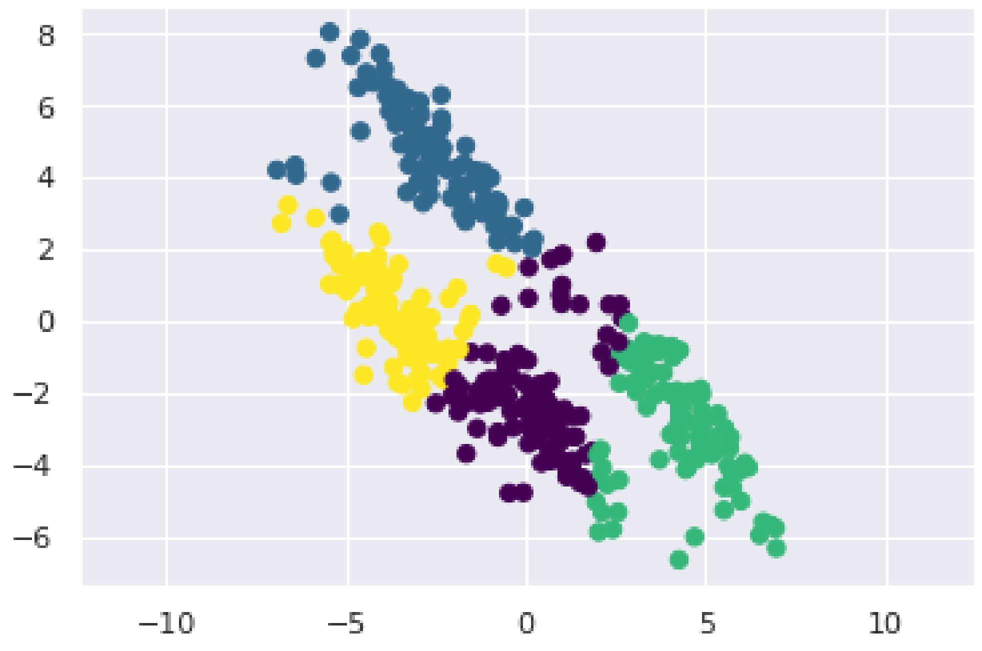


The first issue in k-means is that it does *hard* clustering: points at the borders between clusters get somewhat arbitrarily assigned, and there is no way to declare low cluster confidence. The seond issue is that clusters are necessarily circular/spherical.

[5]:
```
rng = np.random.RandomState(13)
X_stretched = np.dot(X, rng.randn(2, 2))
plt.scatter(X_stretched[:, 0], X_stretched[:, 1], c=y_true, s=40,␣
 ↪cmap='viridis');
ax = plt.gca()
ax.axis('equal')
plt.show();
```

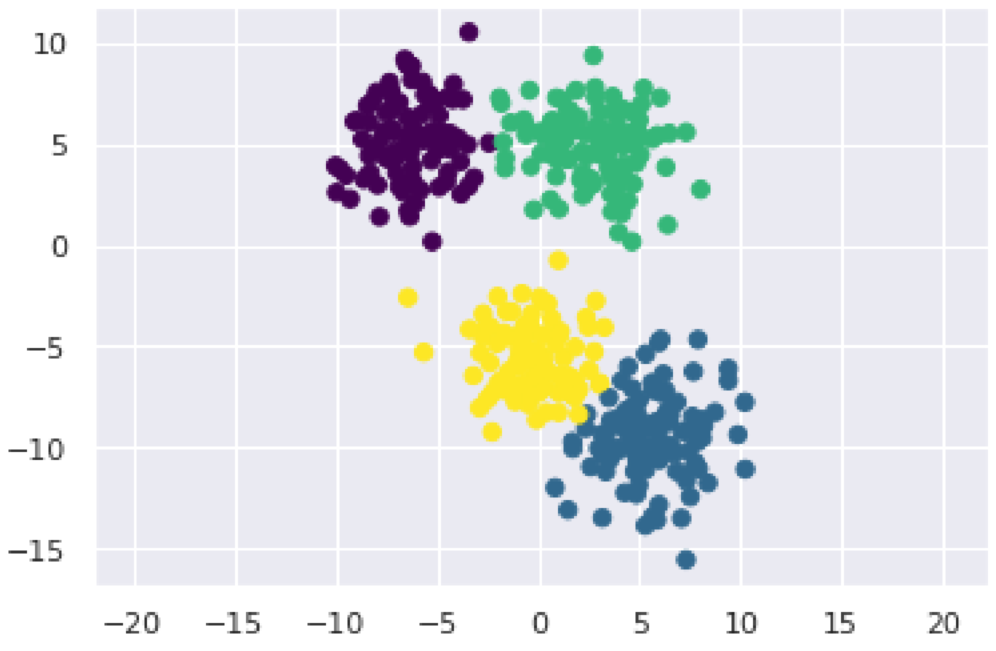


```
[6]: kmeans = KMeans(n_clusters=4, random_state=0)
     labels = kmeans.fit(X_stretched).predict(X_stretched)
     plt.scatter(X_stretched[:, 0], X_stretched[:, 1], c=labels, s=40,␣
      ↪cmap='viridis');
     ax = plt.gca()
     ax.axis('equal')
     plt.show();
```



Interesting. Because output cluster labels are forced to be circular, kmeans is picking up data points for different "true clusters". This can be fixed via EM using a GMM model.

[7]:
```
from sklearn.mixture import GaussianMixture as GMM
gmm = GMM(n_components=4)
labels = gmm.fit(X).predict(X)
plt.scatter(X[:, 0], X[:, 1], c=labels, s=40, cmap='viridis');
ax = plt.gca()
ax.axis('equal')
plt.show();
```



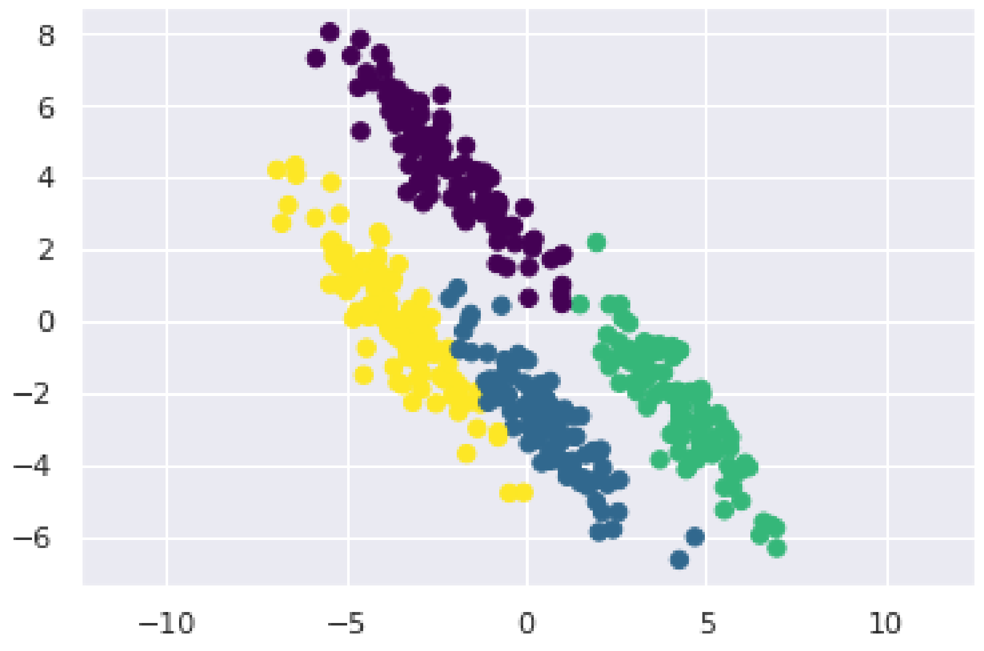
Slightly better clustering results, especially at the border. EM does “soft” clustering, so we can actually examine each point’s posterior probability.

[8]:
```
probs = gmm.predict_proba(X)
print(probs[:10].round(3))
```

```
[[0.    0.    0.    1.   ]
 [0.    1.    0.    0.   ]
 [0.    0.    0.    1.   ]
 [0.    0.    1.    0.   ]
 [0.    0.    1.    0.   ]
 [1.    0.    0.    0.   ]
 [1.    0.    0.    0.   ]
 [0.    0.996 0.    0.004]
 [0.    0.974 0.    0.026]
 [0.    0.999 0.    0.001]]
```

Let’s now test it on the stretched dataset.

[9]:
```
labels = gmm.fit(X_stretched).predict(X_stretched)
plt.scatter(X_stretched[:, 0], X_stretched[:, 1], c=labels, s=40,␣
 ↪cmap='viridis');
ax = plt.gca()
ax.axis('equal')
plt.show();
```

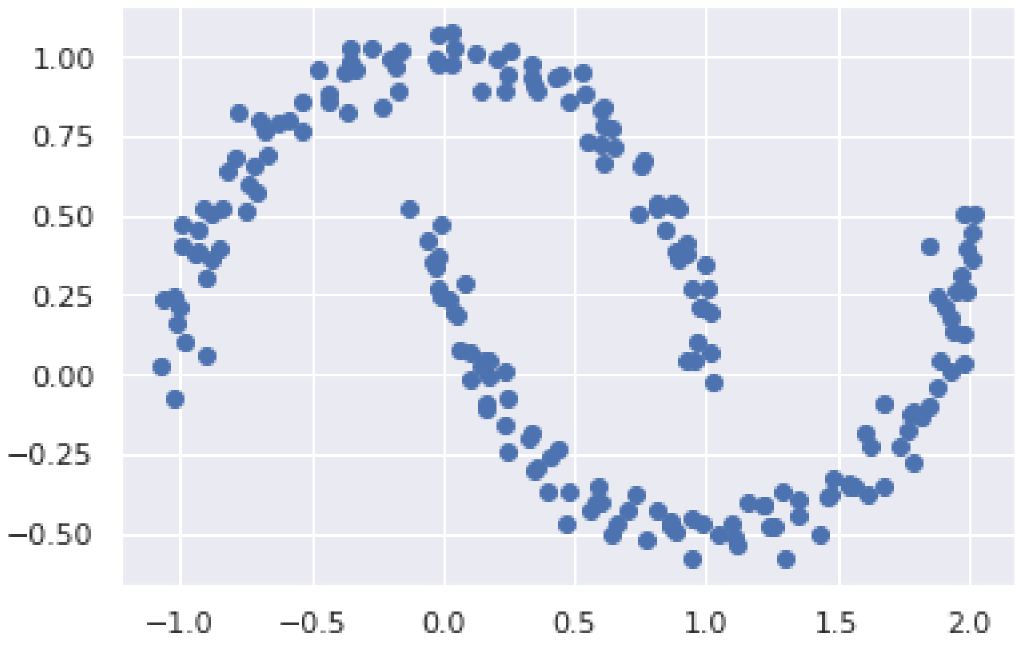


Nice! The clusters have been currently identified.

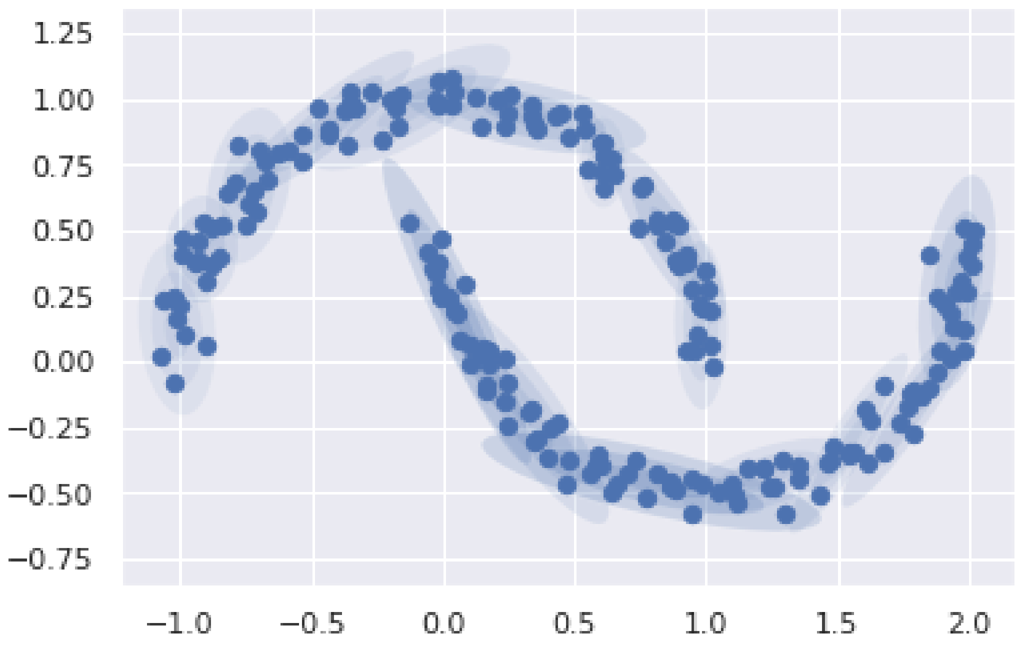
(This part is optional). We can actually use GMM to fit lots of tiny clusters – this helps us to model non-spherical/elliptical datasets too.

[0]:
```python
from matplotlib.patches import Ellipse

def draw_ellipse(position, covariance, ax=None, **kwargs):
    """Draw an ellipse with a given position and covariance"""
    ax = ax or plt.gca()

    # Convert covariance to principal axes
    if covariance.shape == (2, 2):
        U, s, Vt = np.linalg.svd(covariance)
        angle = np.degrees(np.arctan2(U[1, 0], U[0, 0]))
        width, height = 2 * np.sqrt(s)
    else:
        angle = 0
        width, height = 2 * np.sqrt(covariance)

    # Draw the Ellipse
    for nsig in range(1, 4):
        ax.add_patch(Ellipse(position, nsig * width, nsig * height,
                             angle, **kwargs))

def plot_gmm(gmm, X, label=True, ax=None):
    ax = ax or plt.gca()
    labels = gmm.fit(X).predict(X)
    if label:
        ax.scatter(X[:, 0], X[:, 1], c=labels, s=40, cmap='viridis', zorder=2)
    else:
        ax.scatter(X[:, 0], X[:, 1], s=40, zorder=2)
    ax.axis('equal')

    w_factor = 0.2 / gmm.weights_.max()
    for pos, covar, w in zip(gmm.means_, gmm.covariances_, gmm.weights_):
        draw_ellipse(pos, covar, alpha=w * w_factor)
```

[11]:
```
from sklearn.datasets import make_moons
Xmoon, ymoon = make_moons(200, noise=.05, random_state=0)
plt.scatter(Xmoon[:, 0], Xmoon[:, 1]);
```



[12]:
```
gmm16 = GMM(n_components=16, covariance_type='full', random_state=0)
plot_gmm(gmm16, Xmoon, label=False)
```



OK, let's do a real(istic) data experiment. Let's now use k-means to *automatically learn* MNIST digit classes without training labels.

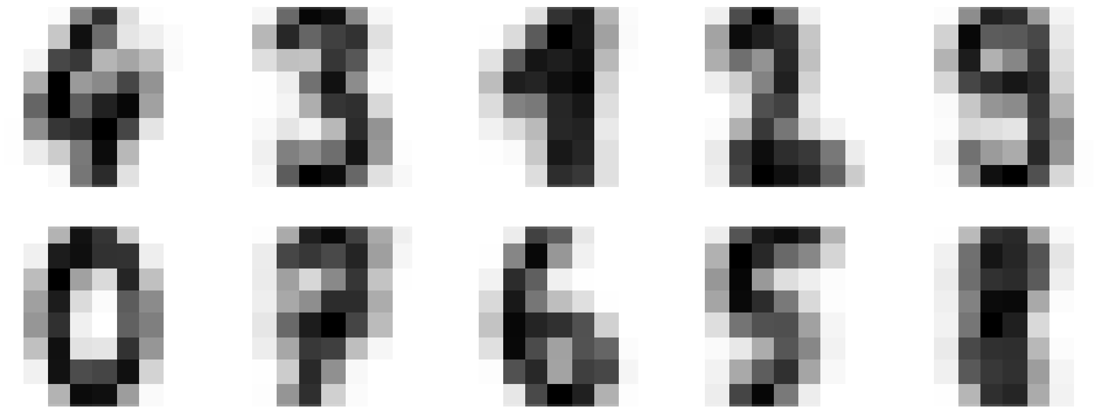
[13]:
```
from sklearn.datasets import load_digits
digits = load_digits()
digits.data.shape
```

[13]:
```
(1797, 64)
```

[14]:
```
kmeans = KMeans(n_clusters=10, random_state=0)
clusters = kmeans.fit_predict(digits.data)
kmeans.cluster_centers_.shape
```

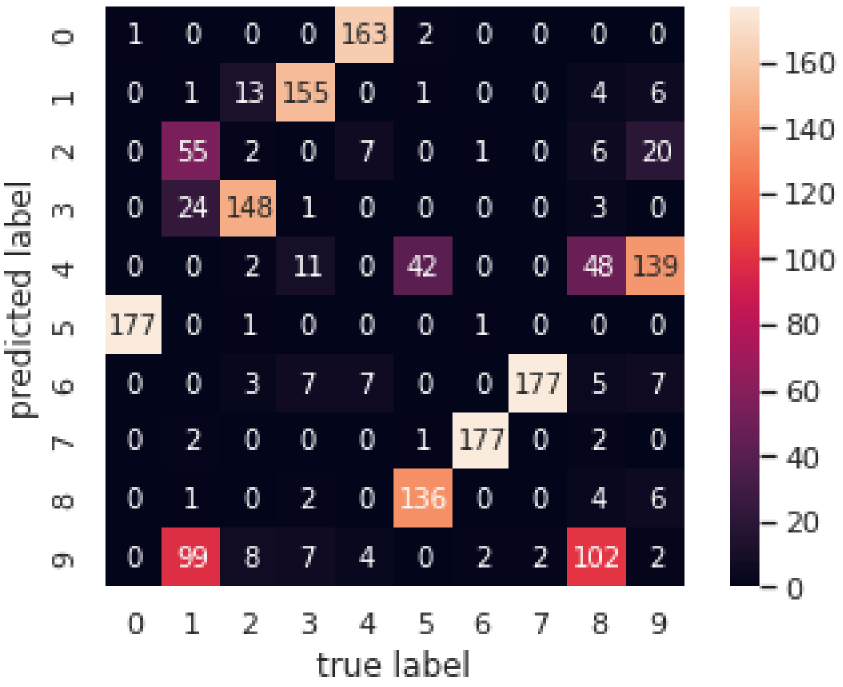
[14]:
```
(10, 64)
```

[15]:
```
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)
```



Quite remarkably, the cluster centers recover the digits (without ever telling the algorithm what they are). The digit “8” is a bit blurred out though.

```
[16]: from sklearn.metrics import confusion_matrix
      mat = confusion_matrix(digits.target, clusters)
      sns.heatmap(mat.T, square=True, annot=True, fmt='d',
                  xticklabels=digits.target_names,
                  yticklabels=digits.target_names)
      plt.xlabel('true label')
      plt.ylabel('predicted label');
```



	0	1	2	3	4	5	6	7	8	9
0	1	0	0	0	163	2	0	0	0	0
1	0	1	13	155	0	1	0	0	4	6
2	0	55	2	0	7	0	1	0	6	20
3	0	24	148	1	0	0	0	0	3	0
4	0	0	2	11	0	42	0	0	48	139
5	177	0	1	0	0	0	1	0	0	0
6	0	0	3	7	7	0	0	177	5	7
7	0	2	0	0	0	1	177	0	2	0
8	0	1	0	2	0	136	0	0	4	6
9	0	99	8	7	4	0	2	2	102	2

Fairly accurate! We can compute accuracy by permuting the rows of the above matrix to match the max values of each row and column.

```
[17]: from scipy.stats import mode
corrected_labels = np.zeros_like(clusters)
for i in range(10):
  mask = (clusters == i)
  corrected_labels[mask] = mode(digits.target[mask])[0]

from sklearn.metrics import accuracy_score
accuracy_score(digits.target, corrected_labels)
```

```
[17]: 0.7952142459654981
```

Great! ~80% accuracy with no labels whatsoever!

Actually – if we do a bit more pre-processing, we can get even better results. There is a nonlinear dimensionality algorithm called (tSNE) which we don't discuss – but which is very good at retaining "cluster" information. If we fit kmeans to a tSNE-reduced version of the dataset, we can improve performance all the way to 93% (which is even better than logistic regression/shallow neural nets) on MNIST. This example illustrates the power of unsupervised learning when used carefully.

```
[18]: from sklearn.manifold import TSNE

tsne = TSNE(n_components=2, init='random', random_state=0)
digits_proj = tsne.fit_transform(digits.data)

kmeans = KMeans(n_clusters=10, random_state=0)
clusters = kmeans.fit_predict(digits_proj)

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

accuracy_score(digits.target, labels)
```

```
[18]: 0.9371174179187535
```