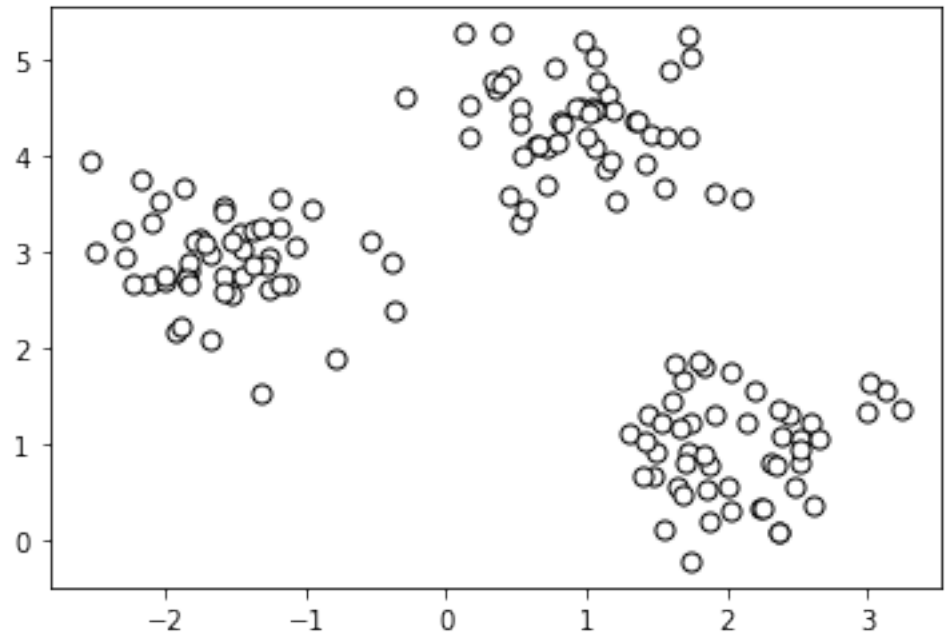
k_means_skl

September 10, 2023

[6]:
```
%matplotlib inline
import matplotlib.pyplot as plt
from sklearn.datasets import make_blobs

# create dataset
X, y = make_blobs(
   n_samples=150, n_features=2,
   centers=3, cluster_std=0.5,
   shuffle=True, random_state=0
)

# plot
plt.scatter(
   X[:, 0], X[:, 1],
   c='white', marker='o',
   edgecolor='black', s=50
)
plt.show()
```



Apply k-means clustering

[2]:
```
from sklearn.cluster import KMeans

km = KMeans(
    n_clusters=3, init='random',
    n_init=10, max_iter=300,
    tol=1e-04, random_state=0
)
y_km = km.fit_predict(X)
```

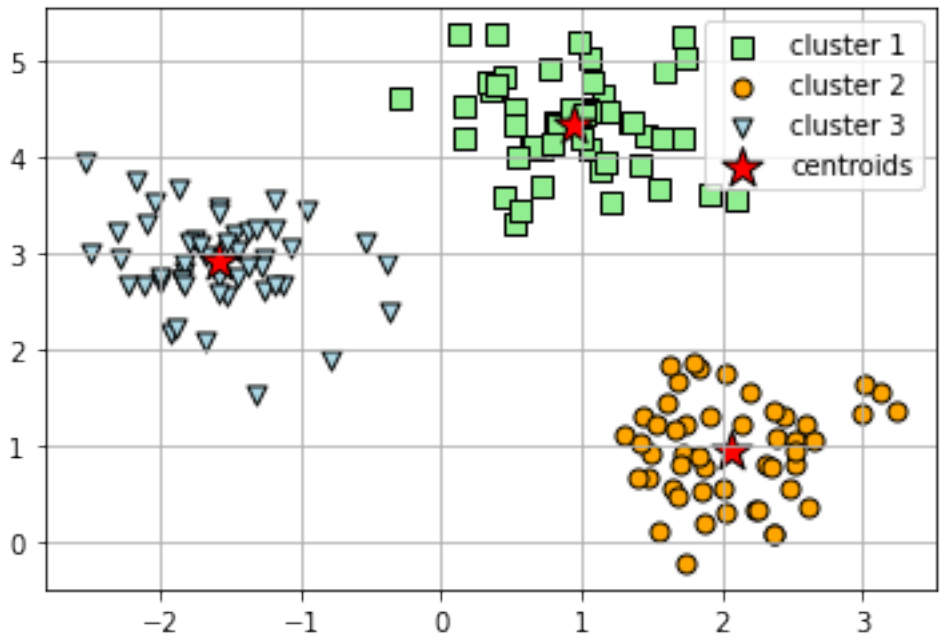
Plot the results.

[3]:
```
# plot the 3 clusters
plt.scatter(
    X[y_km == 0, 0], X[y_km == 0, 1],
    s=50, c='lightgreen',
    marker='s', edgecolor='black',
    label='cluster 1'
)

plt.scatter(
    X[y_km == 1, 0], X[y_km == 1, 1],
    s=50, c='orange',
    marker='o', edgecolor='black',
    label='cluster 2'
)

plt.scatter(
    X[y_km == 2, 0], X[y_km == 2, 1],
    s=50, c='lightblue',
    marker='v', edgecolor='black',
    label='cluster 3'
)

# plot the centroids
plt.scatter(
    km.cluster_centers_[:, 0], km.cluster_centers_[:, 1],
    s=250, marker='*',
    c='red', edgecolor='black',
    label='centroids'
)
plt.legend(scatterpoints=1)
plt.grid()
```



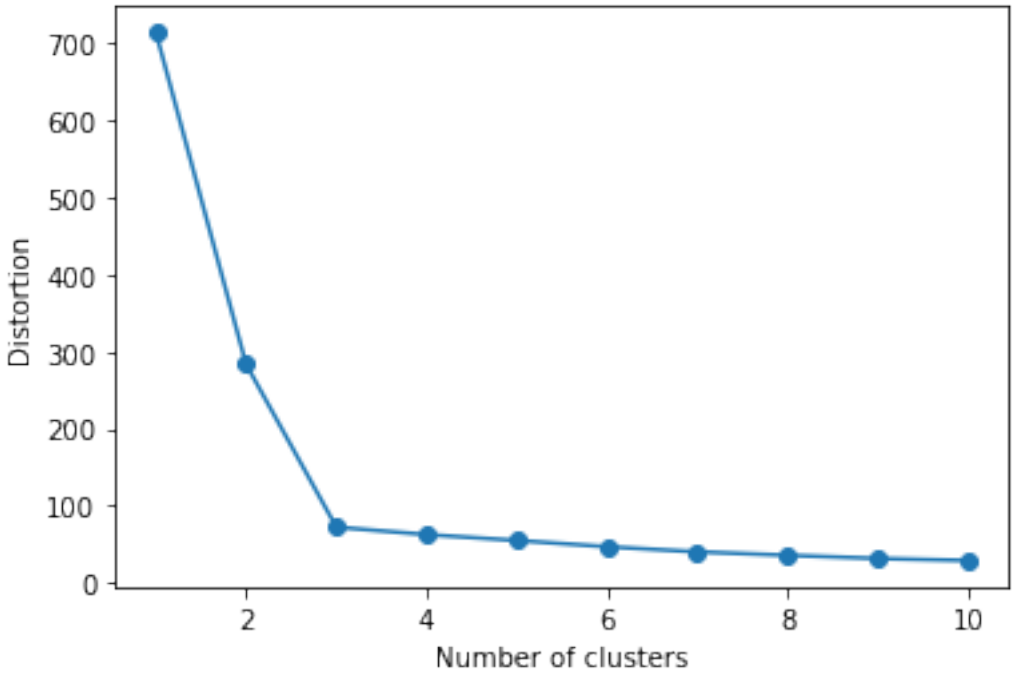
This looks very good. But in real-life, we do not know how many clusters to seek. This is particularly true in higher dimensions.

The elbow method is a useful graphical tool to estimate the optimal number of clusters k for a given dataset. If k increases, we expect the intra-cluster SSE—the distortion—to decrease. This is because the samples will be closer to the centroids that they are assigned to.

The idea behind the elbow method is to identify the value of k where the distortion begins to decrease most rapidly, which will become clearer if we plot the distortion for different values of k.

[5]:
```
# calculate distortion for a range of number of cluster
distortions = []
for i in range(1, 11):
    km = KMeans(
        n_clusters=i, init='random',
        n_init=10, max_iter=300,
        tol=1e-04, random_state=0
    )
    km.fit(X)
    distortions.append(km.inertia_)

# plot
plt.plot(range(1, 11), distortions, marker='o')
plt.xlabel('Number of clusters')
plt.ylabel('Distortion')
plt.show()
```



The elbow is located at $k = 3$, which is evidence that it is indeed a good choice for this dataset.

[ ]: