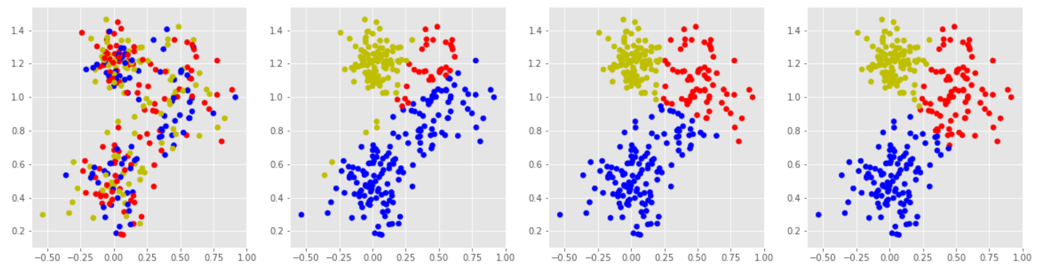
CSCI 303

Introduction to Data Science

19-Clustering



This Lecture

- Clustering

Setup

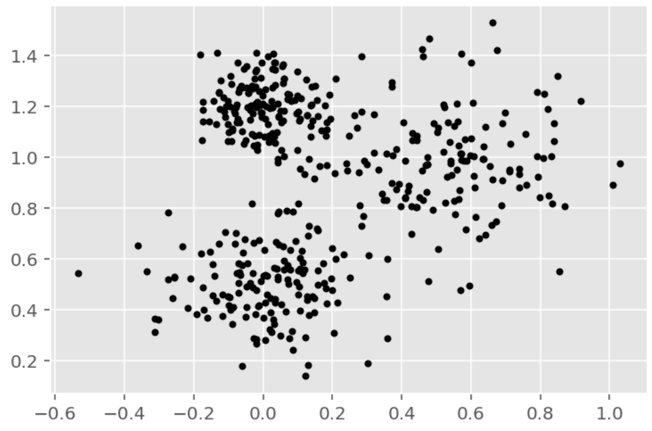
The obligatory setup code.

In [1]:
```python
import numpy as np
import pandas as pd
import sklearn as sk
import matplotlib.pyplot as plt

from pandas import DataFrame

plt.style.use("ggplot")

%matplotlib inline
%config InlineBackend.figure_format = 'retina'
```

In [2]:
```python
# function for generating normally distributed data
def sample_cluster(n, x, y, sigma):
    x = np.random.randn(n) * sigma + x;
    y = np.random.randn(n) * sigma + y;
    return np.array([x, y]).T

```

Synthetic Clustering Example

In [3]:
```python
np.random.seed(1234)
n = 150

# create three 'sets' of 150 random data
c1 = sample_cluster(n, 0, 0.5, 0.15)
c2 = sample_cluster(n, 0, 1.2, 0.1)
c3 = sample_cluster(n, 0.5, 1, 0.2)

# put all of that data into one and plot it
data = np.concatenate((c1, c2, c3))
plt.plot(data[:,0], data[:,1], 'k.')
plt.show()
```



Clustering

Simple idea:

- Choose [Math Processing Error] (decide how many clusters you *think* there ought to be)
- Partition the data into [Math Processing Error] disjoint clusters such that [Math Processing Error] is minimized.
    - W(C) is some measure of within-cluster variation
    - Common choice for W is the sum of Euclidean distances between pairs of points:

  [Math Processing Error]

Solution Approaches

- Brute force: try every possible partitions of the data
    - Advantage: globally optimal
    - Disadvantage: [Math Processing Error] different partitions (given [Math Processing Error] data points)
- K-Means algorithm: iterative improvement
    - Advantage: efficient
    - Disadvantage: locally optimal, result depends on initialization

K-Means Algorithm

- Various initialization schemes

    - One way is to assign each point a cluster identity at random
    - Another is to choose K points to serve as initial cluster centers at random
- Iterate until cluster assignments stop changing:
    - Compute the cluster *centroids*. The centroid is the mean point (vector of means of all features) for all points in the cluster
    - Re-assign each data point to the cluster associated with the nearest centroid

This algorithm is ridiculously easy to code up.

In [5]:
```
# a simple k-means implementation
# input: integer K, ndarray data
def KMeans(K, data):
    n = data.shape[0]
    # intialize data into random clusters
    c = np.random.randint(low=0, high=K, size=n)
    C = [c]
    changed = True
    centroid = lambda k: np.mean(np.array([d for c,d in zip(c,data) if c == k]), a
    while changed:
        centroids = np.array([centroid(k) for k in range(K)])
        dists = [[np.linalg.norm(d - centroids[k]) for k in range(K)] for d in data
        newc = np.argmin(np.array(dists), axis=1)
        changed = np.any(c != newc)
        C.append(newc)
        c = newc
    return C
```

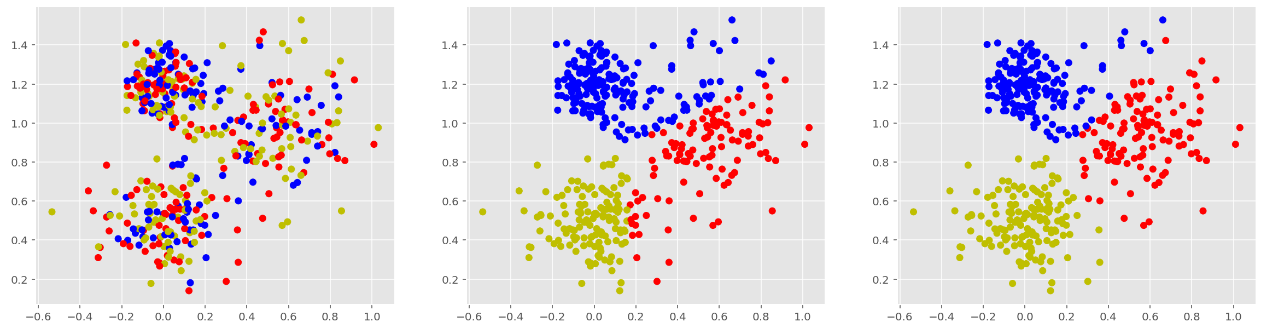
Let's give it a spin:

In [6]:
```
C = KMeans(3, data)
print("Iterations:", len(C))
```

```
Iterations: 7
```

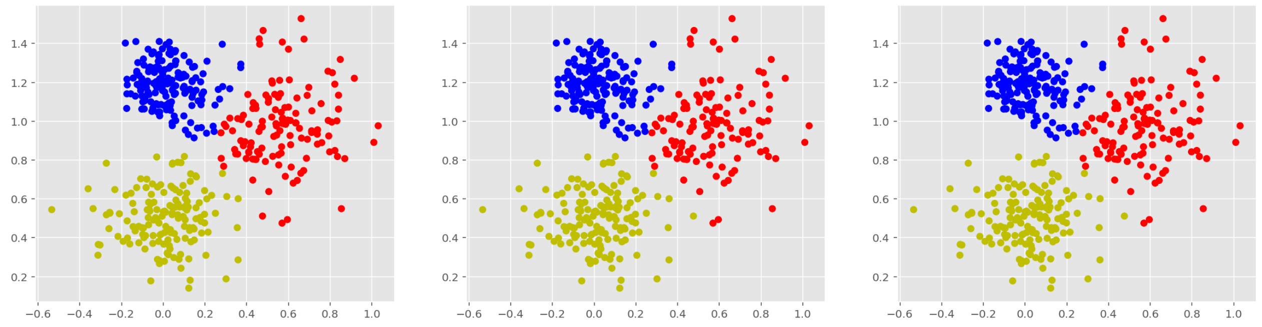
Let's look at the first few iterations:

In [7]:
```
from matplotlib.colors import ListedColormap
cmap = ListedColormap(['r', 'y', 'b'])
plt.figure(figsize=[20,5])
for i in range(3):
    plt.subplot(1,3,i+1)
    plt.scatter(data[:,0], data[:,1], c=C[i], cmap=cmap)
```



Look at the final four:

In [8]:
```python
plt.figure(figsize=[20,5])
for i in range(3):
    plt.subplot(1,3,i+1)
    plt.scatter(data[:,0], data[:,1], c=C[-(3-i)], cmap=cmap)
```



Here's an implementation that picks K points at random and clusters on those points initially:

In [4]:
```python
# a simple k-means implementation
# input: integer K, ndarray data
def KMeans2(K, data):
    n = data.shape[0]
    # intialize data using normally distributed random centers
    centroids = data[np.random.randint(low=0, high=n, size=3)]
    dists = [[np.linalg.norm(d - centroids[k]) for k in range(K)] for d in data]
    c = np.argmin(np.array(dists), axis=1)
    C = [c]
    changed = True
    centroid = lambda k: np.mean(np.array([d for c,d in zip(c,data) if c == k]), a
    while changed:
        centroids = np.array([centroid(k) for k in range(K)])
        dists = [[np.linalg.norm(d - centroids[k]) for k in range(K)] for d in data
        newc = np.argmin(np.array(dists), axis=1)
        changed = np.any(c != newc)
        C.append(newc)
        c = newc
    return C
```

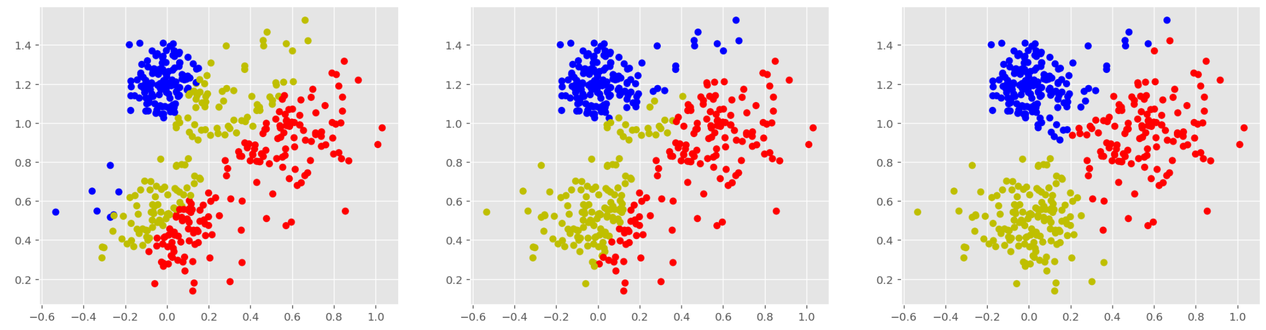
In [5]:
```python
C = KMeans2(3, data)
print("Iterations:", len(C))
```

```
Iterations: 5
```

First few interations:

In [11]:

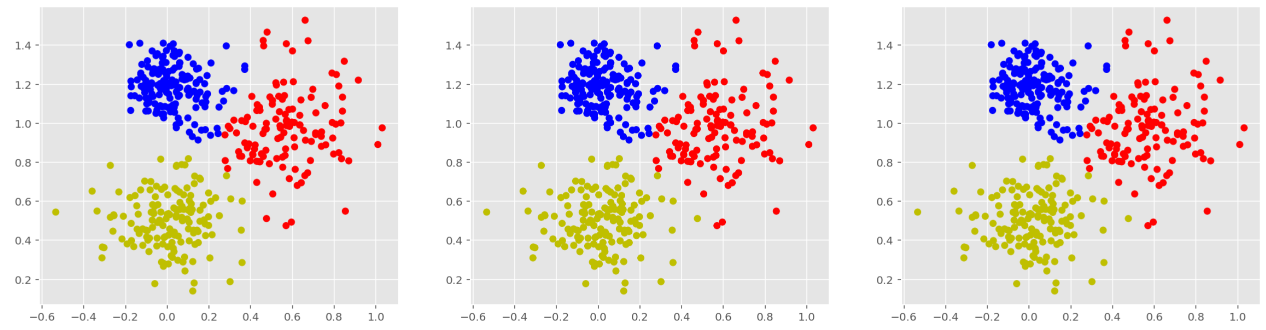
```python
plt.figure(figsize=[20,5])
for i in range(3):
    plt.subplot(1,3,i+1)
    plt.scatter(data[:,0], data[:,1], c=C[i], cmap=cmap)
```



Final four:

In [12]:

```python
plt.figure(figsize=[20,5])
for i in range(3):
    plt.subplot(1,3,i+1)
    plt.scatter(data[:,0], data[:,1], c=C[-(3-i)], cmap=cmap)
```



Of course, scikit-learn gives us a robust KMeans object.

It behaves just like a classifier, except that you only give it inputs (no class labels).

The scikit-learn KMeans clusterer will actually try several random starts, and pick the "best" result.

Unfortunately, it doesn't give us a way to visualize the steps it went through.

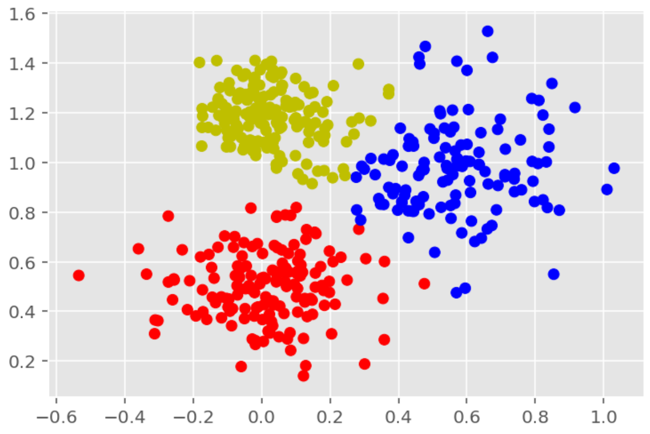
In [13]:

```python
from sklearn.cluster import KMeans
km = KMeans(3)
km.fit(data)
```

Out[13]:

```
KMeans(n_clusters=3)
```

In [13]:
```
plt.scatter(data[:,0], data[:,1], c=km.predict(data), cmap=cmap)
plt.show()
```



Guessing K

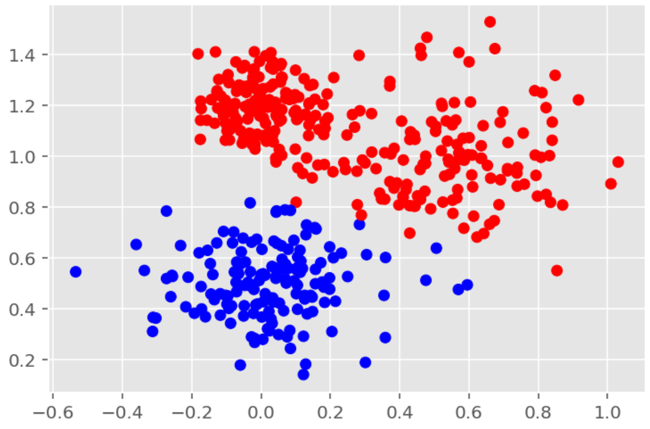
I know the data used above was generated from 3 Gaussian blobs, so we've been using K.

In general, though, how many clusters should there be?

How can we guess?

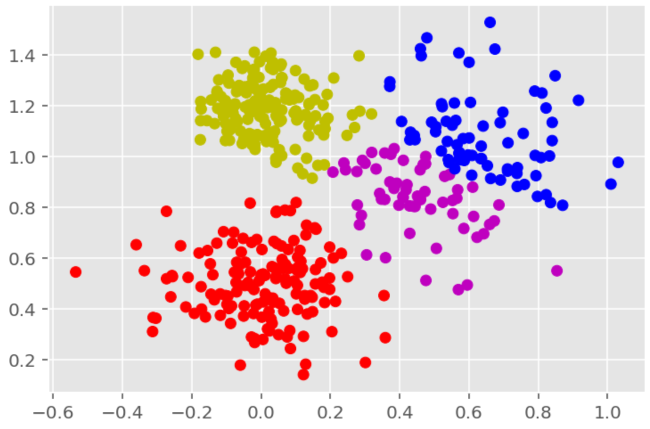
Let's try K=2:

In [14]:
```python
km2 = KMeans(2) # uses two clusters
km2.fit(data)
plt.scatter(data[:,0], data[:,1], c=km2.predict(data), cmap=cmap)
plt.show()
```



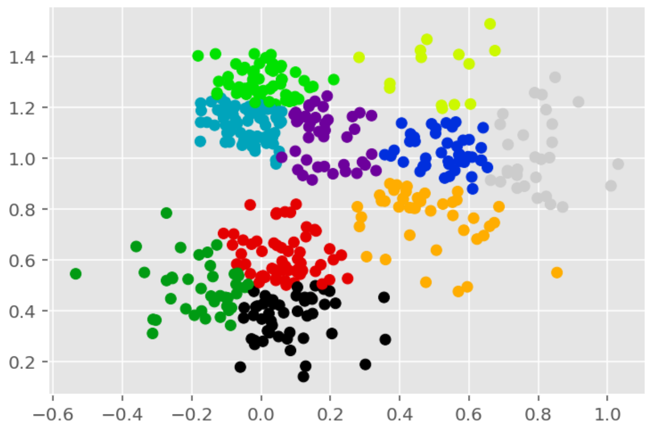
Or K=4:

In [20]:
```python
cmap = ListedColormap(['r','y','b','m'])
km4 = KMeans(4) # uses two clusters
km4.fit(data)
plt.scatter(data[:,0], data[:,1], c=km4.predict(data), cmap=cmap)
plt.show()
```



Or K=10:

In [21]:
```python
km10 = KMeans(10) # uses ten clusters
km10.fit(data)
plt.scatter(data[:,0], data[:,1], c=km10.predict(data), cmap='nipy_spectral')
plt.show()
```



Hierarchical Clustering

One answer to the problem of "how many clusters":

Try all of them!

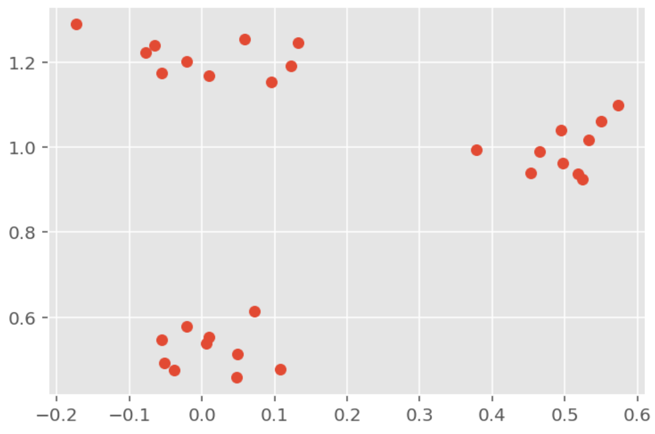
Hierarchical algorithms are either top down or bottom up.

The bottom up algorithms (agglomerative) are the most popular.

The result of hierarchical clustering is a *dendrogram* plot, showing how the clusters break down (or build up, if you prefer).

Let's first get a smaller dataset to illustrate.

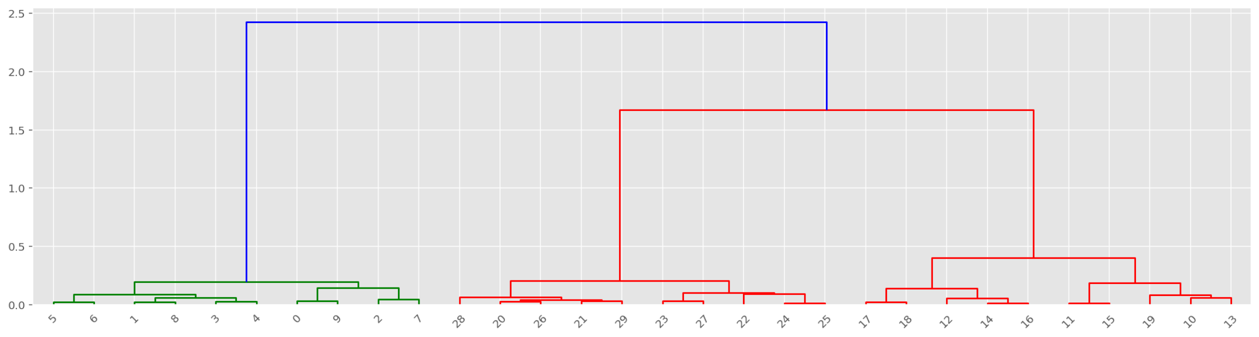
In [22]:
```python
c1 = sample_cluster(10, 0, 0.5, 0.05)
c2 = sample_cluster(10, 0, 1.2, 0.1)
c3 = sample_cluster(10, 0.5, 1, 0.05)
data = np.concatenate((c1, c2, c3))
plt.scatter(data[:,0], data[:,1])
plt.show()
```



While scikit-learn has agglomerative clustering, it isn't capable of showing us a dendrogram.

We'll use SciPy instead for this example.

In [18]:
```python
from scipy.cluster.hierarchy import dendrogram, ward
linkage_array = ward(data)
plt.figure(figsize=[20,5])
dendrogram(linkage_array)
plt.show()
```


2.5
2.0
1.5
1.0
0.5
0.0
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3
4
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