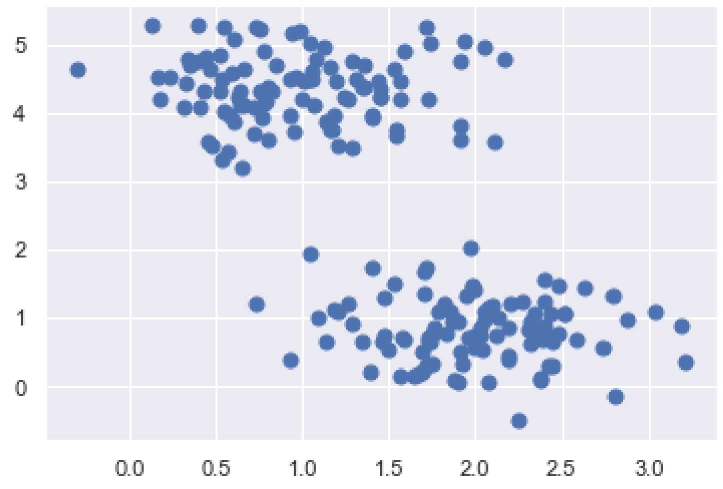
```
In [1]: import numpy as np
        import matplotlib.pyplot as plt
        import seaborn as sns
        sns.set()
```

Consider a small "city" of people.

- Each point represents a person
- Friendships are formed entirely based on how close they live to each other

Could you put these people into communities?

```
In [2]: from sklearn.datasets.samples_generator import make_blobs
        X, y_true = make_blobs(n_samples=200, centers=2,
                               cluster_std=0.50, random_state=0)
        plt.scatter(X[:, 0], X[:, 1], s=50);
```



How would you tell a program to do what you did visually?

Remember how the computer "sees" these points

In [3]:
```
# Print first 15 points
print(X[:15, :])
```

```
[[2.43859911 1.07581007]
 [1.85554301 1.0826916 ]
 [2.58952222 0.67097076]
 [1.73654901 0.69902775]
 [1.74265969 5.03846671]
 [0.64003985 4.12401075]
 [1.04829186 5.03092408]
 [0.5323772  3.31338909]
 [1.98882723 0.74876822]
 [0.16117091 4.53517846]
 [1.7571105  0.87138001]
 [1.28486901 0.92929466]
 [1.16448284 3.75408693]
 [0.3498724  4.69253251]
 [2.10413001 1.1891405 ]]
```

Brief aside on multi-dimensional numpy arrays

- Shape
- Indexing
- Boolean indexing
- Slicing

In [4]:
```
# Shape
print('The shape of the array is %s' % (str(X.shape)))
print('The number of samples is %d' % X.shape[0])
print('The number of dimensions is %d' % X.shape[1])
```

```
The shape of the array is (200, 2)
The number of samples is 200
The number of dimensions is 2
```

In [5]:
```
# Indexing
i = 4
j = 1
print('The %d-th dimension of sample %d is %g' % (j+1, i+1, X[i, j]))

temp = -10*np.arange(10) # numbers 0-9
print('Selecting 1st 3rd and 8th part of array')
print(temp[[1,3,8]])
```

```
The 2-th dimension of sample 5 is 5.03847
Selecting 1st 3rd and 8th part of array
[-10 -30 -80]
```

In [6]:
```
# Boolean indexing
temp = -10*np.arange(10) # numbers 0-9
selection = np.zeros(temp.shape[0], dtype=bool)
print('Boolean array')
print(selection)
selection[1] = True
selection[3] = True
selection[8] = True
# Or equivalently selection[[1,3,8]] = True

print('Selecting 1st 3rd and 8th part of array via boolean array')
print(temp[selection])
```

```
Boolean array
[False False False False False False False False False False]
Selecting 1st 3rd and 8th part of array via boolean array
[-10 -30 -80]
```

In [7]:
```
# Slicing
print('The first 10 samples with all dimensions')
print(X[:10, :])
```

```
The first 10 samples with all dimensions
[[2.43859911 1.07581007]
 [1.85554301 1.0826916 ]
 [2.58952222 0.67097076]
 [1.73654901 0.69902775]
 [1.74265969 5.03846671]
 [0.64003985 4.12401075]
 [1.04829186 5.03092408]
 [0.5323772  3.31338909]
 [1.98882723 0.74876822]
 [0.16117091 4.53517846]]
```

In [8]:
```
print('The %d-th sample is:' % (i+1))
print(str(X[i, :]))
```

```
The 5-th sample is:
[1.74265969 5.03846671]
```

In [9]:
```
print('The first 10 samples for the dimension %d' % (j+1))
print(X[:10, j])
```

```
The first 10 samples for the dimension 2
[1.07581007 1.0826916  0.67097076 0.69902775 5.03846671 4.12401075
 5.03092408 3.31338909 0.74876822 4.53517846]
```

In [10]:
```
print('The last 10 samples for the dimension %d' % (j+1))
print(X[-10:, j])
```

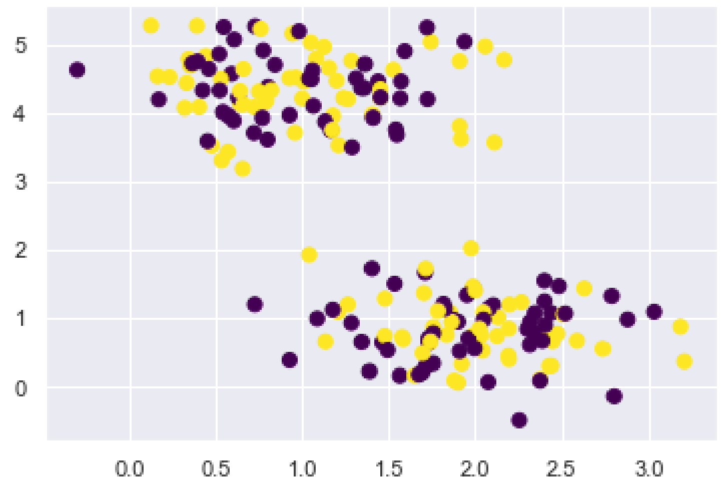
```
The last 10 samples for the dimension 2
[1.10568868 3.97204818 1.12313089 0.84858847 1.46821459 1.24503823
 4.2012082  3.57660449 4.22810872 4.75420057]
```

How do we formalize what we did visually?

- Let's assume for now that we know there are exactly *two* communities
- How can we assign each person to a community?
- Naive idea: Randomly assign points to each community

In [11]:
```python
from sklearn.utils import check_random_state
def get_random_assignment(random_state=None):
    rng = check_random_state(random_state)
    y = rng.randint(2, size=X.shape[0])
    return y
y_rand = get_random_assignment(random_state=0)
plt.scatter(X[:, 0], X[:, 1], c=y_rand, s=50, cmap='viridis')
```

Out[11]:
```
<matplotlib.collections.PathCollection at 0x1a1ac60ac8>
```



This clustering "looks" quite bad.

How can we formalize whether a particular assignment is good or bad?

- One intuition: People in a communities will be as close to each other as possible.
- Take average distance between each person in a community to every other person in the **same** community.
- Sum over all communities.

(Derive on board)

Implement (Euclidean) distance function

$$\mathrm{dist}(x, z) = \sqrt{(x_1 - z_1)^2 + (x_2 - z_2)^2}$$

In [12]:
```
# Euclidean distance function
def distance(xvec, zvec, show=False):
    diff = xvec - zvec
    squared = diff * diff
    sum_squared = np.sum(squared)
    d = np.sqrt(sum_squared)
    if show:
        print('xvec', xvec)
        print('zvec', zvec)
        print('diff', diff)
        print('squared', squared)
        print('sum_squared', sum_squared)
        print('distance', d)
    return d

print('Simple')
distance(np.array([0, 1]), np.array([1, 0]), show=True)
print()
print('Real example')
distance(X[0, :], X[1, :], show=True)
```

```
Simple
xvec [0 1]
zvec [1 0]
diff [-1  1]
squared [1 1]
sum_squared 2
distance 1.4142135623730951

Real example
xvec [2.43859911 1.07581007]
zvec [1.85554301 1.0826916 ]
diff [ 0.58305611 -0.00688154]
squared [3.39954422e-01 4.73555265e-05]
sum_squared 0.3400017776337018
distance 0.5830967137908615
```

Out[12]:
```
0.5830967137908615
```

Programming: `zip(a,b)` - Your looping friend, generally much better than indices like `i` or `j` if possible

In [13]:
```
num_arr = 10*np.arange(10)
char_list = ['a','b','c','d']

for n, c in zip(num_arr, char_list):
    print('n=', n, 'c=', c)

for n, c, xvec in zip(num_arr, char_list, X):
    print('n=', n, 'c=', c, 'xvec=', xvec)
```

```
n= 0 c= a
n= 10 c= b
n= 20 c= c
n= 30 c= d
n= 0 c= a xvec= [2.43859911 1.07581007]
n= 10 c= b xvec= [1.85554301 1.0826916 ]
n= 20 c= c xvec= [2.58952222 0.67097076]
n= 30 c= d xvec= [1.73654901 0.69902775]
```

In [14]:
```
# Loop through first 10 x-y pairs
for xvec, yy in zip(X[:10], y_true[:10]):
    print('xvec=', xvec, 'y=', yy)
```

```
xvec= [2.43859911 1.07581007] y= 1
xvec= [1.85554301 1.0826916 ] y= 1
xvec= [2.58952222 0.67097076] y= 1
xvec= [1.73654901 0.69902775] y= 1
xvec= [1.74265969 5.03846671] y= 0
xvec= [0.64003985 4.12401075] y= 0
xvec= [1.04829186 5.03092408] y= 0
xvec= [0.5323772  3.31338909] y= 0
xvec= [1.98882723 0.74876822] y= 1
xvec= [0.16117091 4.53517846] y= 0
```

In [15]:
```
# Loop through columns of data matrix
for xcol in X.transpose():
    print(xcol[:10]) # Only show first 10 elements of column
```

```
[2.43859911 1.85554301 2.58952222 1.73654901 1.74265969 0.64003985
 1.04829186 0.5323772  1.98882723 0.16117091]
[1.07581007 1.0826916  0.67097076 0.69902775 5.03846671 4.12401075
 5.03092408 3.31338909 0.74876822 4.53517846]
```

Note: `zip` will only match elements up to the shortest iterable

Implement objective with loop

$$\mathcal{C}_j = \{x \in \mathcal{X} : y = j\}$$

$$\sum_{j=1}^{k} \frac{1}{2|\mathcal{C}_j|} \sum_{x \in \mathcal{C}_j, z \in \mathcal{C}_j} \mathrm{dist}(x, z)^2$$

In [16]:
```
def objective_loop(X, y):
    k = len(np.unique(y))
    out = 0
    for j in range(k):
        n_community = 0
        community_sum = 0
        for xvec, y1 in zip(X, y):
            if y1 != j:
                continue
            n_community += 1
            for zvec, y2 in zip(X, y):
                if y2 != j:
                    continue
                dist = distance(xvec, zvec)
                community_sum += dist**2
        out += community_sum / (2*n_community)
    return out

print(objective_loop(X, y_rand))
```

```
767.2572924351306
```

Implement objective in via vectorized calls

$$\mathcal{C}_j = \{x \in \mathcal{X} : y = j\}$$

$$\sum_{j=1}^{k} \frac{1}{2|\mathcal{C}_j|} \sum_{x \in \mathcal{C}_j, z \in \mathcal{C}_j} \text{dist}(x, z)^2$$

In [17]:
```
from sklearn.metrics import pairwise_distances
# Using vectorized computation
def objective(X, y):
    y_vals = np.unique(y)
    out = 0
    for yv in y_vals:
        sel = (y==yv)  # boolean array
        Xj = X[sel, :]
        n_community = np.sum(sel)
        community_sum = np.sum(pairwise_distances(Xj, Xj)**2)
        out += community_sum / (2*n_community)
    return out

print(objective(X, y_rand))
print('Difference from loop version = %g' % (objective(X, y_rand) - obje
ctive_loop(X, y_rand)))
```

```
767.2572924351311
Difference from loop version = 5.68434e-13
```

Programming: *List Comprehensions*, also your friend, MAP and FILTER operations

- Suppose you want to map a list of numbers to a list of strings
- Suppose you only want to map odd numbers
- Syntax `[<expression> for <item> in <iterable> if <condition>]`

In [18]:
```
num_list = [1, 2, 3, 4, 5]
str_list = []
for i in range(len(num_list)):
    str_list.append('Num:' + str(num_list[i]))
print('With index loops')
print(str_list)

# Use iterators
str_list = []
for n in num_list:
    str_list.append('Num:' + str(n))
print('With iterator loops')
print(str_list)

# Use list comprehension
str_list = ['Num:' + str(n) for n in num_list]
print('With list comprehension')
print(str_list)

# Use list comprehension
str_list = ['Num:' + str(n) for n in num_list if np.mod(n, 2) == 1]
print('Odd numbers only with list comprehension')
print(str_list)
```

```
With index loops
['Num:1', 'Num:2', 'Num:3', 'Num:4', 'Num:5']
With iterator loops
['Num:1', 'Num:2', 'Num:3', 'Num:4', 'Num:5']
With list comprehension
['Num:1', 'Num:2', 'Num:3', 'Num:4', 'Num:5']
Odd numbers only with list comprehension
['Num:1', 'Num:3', 'Num:5']
```

In [19]:
```
from sklearn.metrics import pairwise_distances
# Using vectorized and list comprehensions computation
def objective(X, y):
    y_vals = np.unique(y)
    def inner(yv):
        sel = (y==yv)  # boolean array
        Xj = X[sel, :]
        n_community = np.sum(sel)
        community_sum = np.sum(pairwise_distances(Xj, Xj)**2)
        return community_sum / (2*n_community)
    return np.sum([inner(yv) for yv in y_vals])

print(objective(X, y_rand))
print('Difference from loop version = %g' % (objective(X, y_rand) - obje
ctive_loop(X, y_rand)))
```

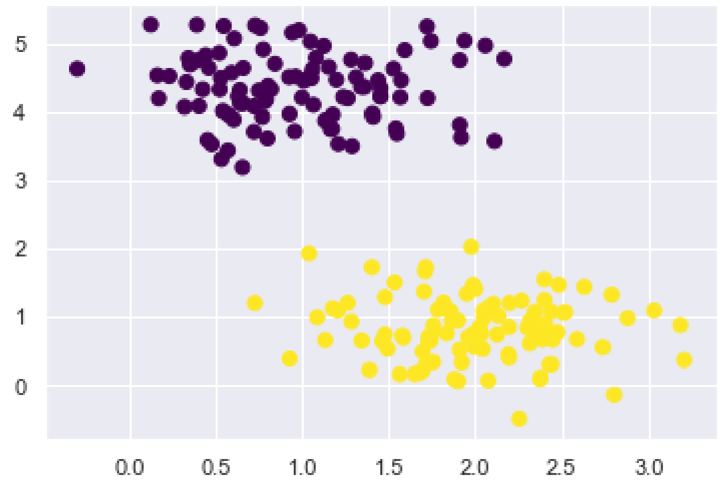
```
767.2572924351311
Difference from loop version = 5.68434e-13
```

Intuition sanity check, does visual clustering solution have a low value?

In [20]:
```
print(objective(X, y_true))
plt.scatter(X[:, 0], X[:, 1], c=y_true, s=50, cmap='viridis')
```

```
94.67363954089785
```

Out[20]:
```
<matplotlib.collections.PathCollection at 0x1a1ae45e10>
```



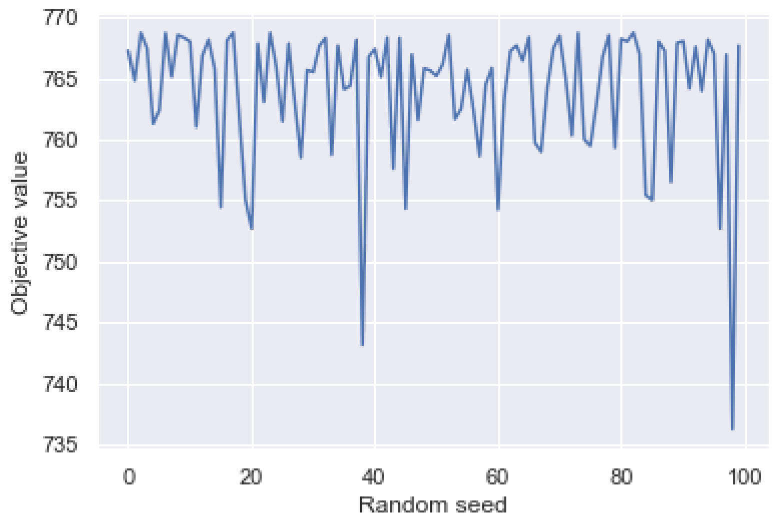
Clustering goal: Minimize objective over possible community assignments

$$\arg\min_{C_1, C_2} \sum_{j=1}^{k} \frac{1}{2|C_j|} \sum_{x \in C_j, z \in C_j} \text{dist}(x, z)^2$$

- Naively, we could just enumerate all possibilities
- Let's try several random combinations

In [21]:
```
rand_obj = np.nan * np.ones(100)
for seed in range(rand_obj.shape[0]):
    y_rand = get_random_assignment(random_state=seed)
    rand_obj[seed] = objective(X, y_rand)
    #print('Seed = %2d, Objective = %g' % (seed, obj))
plt.plot(rand_obj)
plt.xlabel('Random seed')
plt.ylabel('Objective value')
#plt.scatter(X[:, 0], X[:, 1], c=y_rand, s=50, cmap='viridis')
```

Out[21]:
```
Text(0, 0.5, 'Objective value')
```



How many possible assignments are there?

In terms of the number of samples n and the number of communities k

In [22]:
```
n_samples = X.shape[0]
n_communities = 2
n_assignments = n_communities ** (n_samples-1)
print('For %d samples and %d communities, there are %d possible assignme
nts'
      % (n_samples, n_communities, n_assignments))
print('Or in exponential notation: %g possible assignments' % n_assignme
nts)
```

```
For 200 samples and 2 communities, there are 803469022129495137770981046
170581301261101496891396417650688 possible assignments
Or in exponential notation: 8.03469e+59 possible assignments
```

Some perspective: Fastest super computer is 200 petaflops = 2 * 10^17 operations per second

In [23]:
```
ops = 2 * (10 ** 17)
print(ops)
compute_time = n_assignments / ops
compute_time_years = compute_time / 60 / 60 / 24 / 365
print('Years of compute time: %d' % compute_time_years)
```

```
200000000000000000
Years of compute time: 127389177785625178899305200808361984
```

Clearly, not a good way to optimize

Let's consider a *equivalent* optimization

Can you figure out what these two equations mean?

$$\mu_j \equiv \frac{1}{|C_j|} \sum_{x \in C_j} x_i$$

$$\arg \min_{C_1, C_2, \ldots, C_k} \sum_{j=1}^{k} \sum_{x \in C_j} \text{dist}(x, \mu_j)^2$$

In [24]:
```
# Just space holder
```

Consider an equivalent optimization via community *representatives*

- Intuition: Instead of measuring from each person to every other person in the same community, measure between a person and an ideal "representative" of each community, who is at the center of everyone.
- Representative can move freely.
- If the community assignments $\mathcal{C}_j$ are fixed, then the position of the "representative", denoted by μ_j is defines as the mean/average point:

$$\mu_j \equiv \frac{1}{|\mathcal{C}_j|} \sum_{x \in \mathcal{C}_j} x_i$$

- Given this definition of the representative, this leads to the following equivalent minimization:

$$\arg \min_{\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k} \sum_{j=1}^{k} \sum_{x \in \mathcal{C}_j} \text{dist}(x, \mu_j)^2$$

$$\arg \min_{\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k} \sum_{j=1}^{k} \sum_{x \in \mathcal{C}_j} \text{dist}\left(x, \frac{1}{|\mathcal{C}_j|} \sum_{x \in \mathcal{C}_j} x_i\right)^2$$

(Derivation of equivalence can be seen at https://www.math.ucdavis.edu/~strohmer/courses/180BigData/180lecture_kmeans.pdf (https://www.math.ucdavis.edu/~strohmer/courses/180BigData/180lecture_kmeans.pdf))

Programming: Numpy reduction functions

- Many useful **reduction** functions such as `np.sum` , `np.mean` , `np.prod` , `np.min` , `np.max` , etc. are interpreted as follows:

  1. If no axis argument, then just apply to all numbers in all dimensions.
  2. If axis argument given, then apply the reduction along that dimension and leave other dimensions alone.

In [25]:
```
A = np.arange(3*4).reshape(3, 4)
print(A)

print('With no argument, it is the total sum', np.sum(A))
print('With axis=0, it sums along the first dimension (i.e. along the ro
ws)')
print(np.sum(A, axis=0))
print('With axis=1, it sums along the second dimension (i.e. along the c
olumns)')
print(np.sum(A, axis=1))
```

```
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]
With no argument, it is the total sum 66
With axis=0, it sums along the first dimension (i.e. along the rows)
[12 15 18 21]
With axis=1, it sums along the second dimension (i.e. along the column
s)
[ 6 22 38]
```

Implement the objective of the equivalent optimization

$$\arg \min_{C_1, C_2, \ldots, C_k} \sum_{j=1}^{k} \sum_{x \in C_j} \text{dist}(x, \mu_j)^2$$

In [26]:
```
def objective2(X, y):
    k = len(np.unique(y))
    out = 0
    for j in range(k):
        sel = (y==j)  # boolean array
        Xj = X[sel, :]
        mu_j = np.mean(Xj, axis=0)
        dist_to_mu = np.sqrt(np.sum((Xj - mu_j)**2, axis=0))
        out += np.sum(dist_to_mu**2)
    return out

print('Quick sanity check that objective corresponds to visual understan
ding')
print('Objective random', objective2(X, y_rand))
print('Objective visual', objective2(X, y_true))
```

```
Quick sanity check that objective corresponds to visual understanding
Objective random 767.679899871254
Objective visual 94.67363954089788
```

Let's suppose the representative can move around and the communities haven't settled yet

$$\arg \min_{C_1,\ldots,C_k,\mu_1,\ldots,\mu_k} \sum_{j=1}^{k} \sum_{x \in C_j} \text{dist}(x, \mu_j)^2$$

- Two intuitive ideas in this "unsettled" state

   1. People will join the community of their closest *representative* μ_j.
   $$y_i = \arg \min_{j=\{1,2,\ldots,k\}} \text{dist}(x_i, \mu_j)$$
   2. The representative will move to the center of it's current community.
   $$\mu_j = \frac{1}{|C_j|} \sum_{x \in C_j} x_i$$

In [27]:
```
def objective3(X, y, mu_array):
    k = len(np.unique(y))
    out = 0
    for j in range(k):
        sel = (y==j)  # boolean array
        Xj = X[sel, :]
        mu_j = mu_array[j, :]
        dist_to_mu = np.sqrt(np.sum((Xj - mu_j)**2, axis=0))
        out += np.sum(dist_to_mu**2)
    return out
```

Two intuitive ideas in this "unsettled" state

1. People will join the community of their closest *representative* μ_j.
$$y_i = \arg \min_{j=\{1,2,\ldots,k\}} \text{dist}(x_i, \mu_j)$$
2. The representative will move to the center of it's current community.
$$\mu_j = \frac{1}{|C_j|} \sum_{x \in C_j} x_i$$

Let's assume the representatives don't know anything about the community so they just randomly choose to start in one house

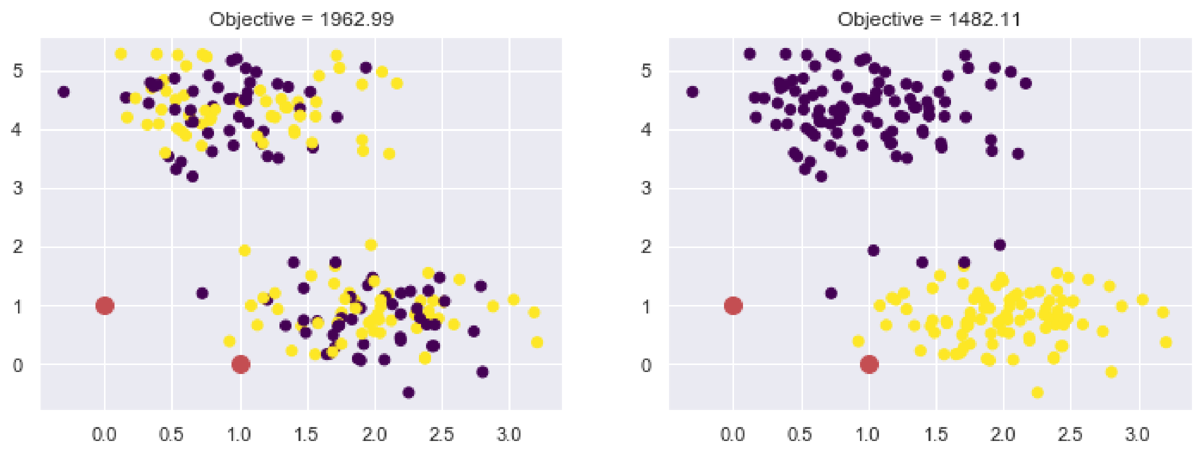
(1) Assign people to their communities based on the representatives

In [28]:
```
mu_array = np.array([[0, 1], [1, 0]])
print(objective3(X, y_rand, mu_array))

# Assign people
def best_assignment(X, mu_array):
    y_best = np.argmin(pairwise_distances(X, mu_array), axis=1)
    return y_best

y_new = best_assignment(X, mu_array)
print(objective3(X, y_new, mu_array))
```

```
1962.992539917816
1482.1076321431726
```

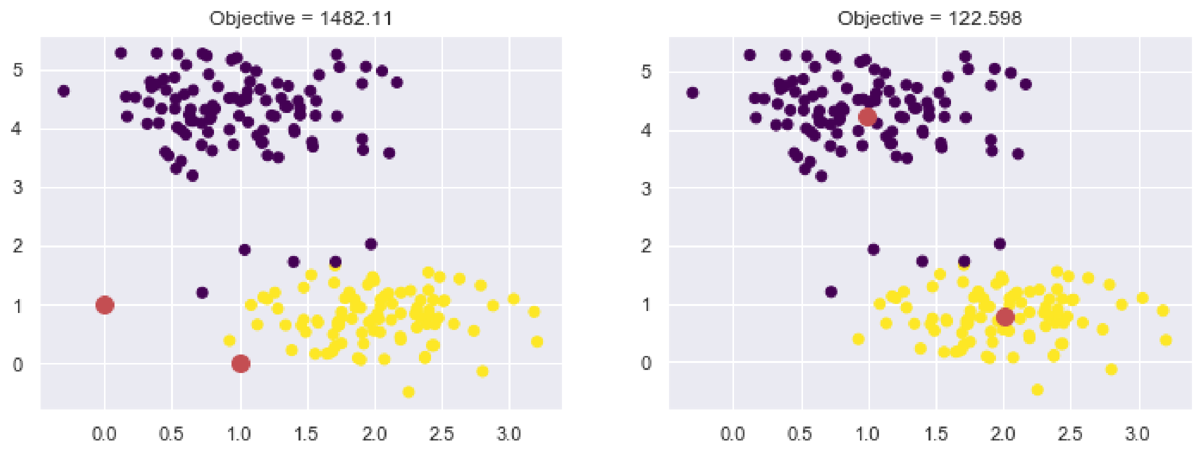
Programming: Make simple function for plotting (use ax as argument)

In [29]:
```
def plot_clustering(X, y, mu_array, ax=None):
    if ax is None:
        ax = plt.gca()
    ax.plot(mu_array[:, 0], mu_array[:, 1], 'ro', markersize=10)
    ax.scatter(X[:, 0], X[:, 1], c=y, cmap='viridis')
    ax.set_title('Objective = %g' % objective3(X, y, mu_array))

fig, axes = plt.subplots(1, 2, figsize=(12, 4))
for ycur, ax in zip([y_rand, y_new], axes):
    plot_clustering(X, ycur, mu_array, ax=ax)
```



(2) Now let's move the representative to the center of its community

In [30]:
```
def recenter(X, y):
    return np.array([
        np.mean(X[y==yv, :], axis=0)
        for yv in np.unique(y)
    ])
mu_array_new = recenter(X, y_new)

fig, axes = plt.subplots(1, 2, figsize=(12, 4))
for m, ax in zip([mu_array, mu_array_new], axes):
    plot_clustering(X, y_new, m, ax=ax)
```



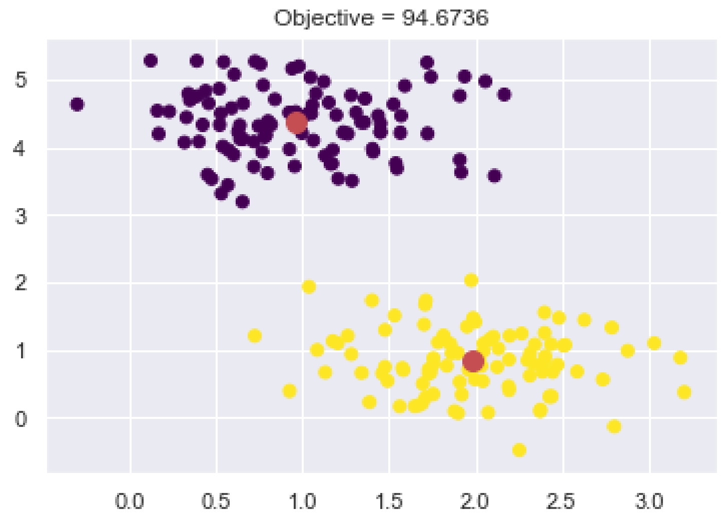
What do you think you should do next?

In [31]:
```
# Program kmeans
def kmeans_alg(X, maxiter=100, random_state=None):
    rng = check_random_state(random_state)

    # Initialize with random points in X
    rand_idx = rng.permutation(X.shape[0])
    mu_array = X[rand_idx[:2], :]
    y = get_random_assignment(random_state=rng)

    for i in range(maxiter):
        # Get new best assignment
        y_old = y  # Save old assignment matrix
        y = best_assignment(X, mu_array)

        # Recenter / compute cluster mean
        mu_array = recenter(X, y)

        # Check convergence
        if y_old is not None and np.all(y == y_old):
            print('Converged after %d iteration' % i)
            break
    return y, mu_array
```

In [48]:
```
y_kmeans, mu_kmeans = kmeans_alg(X, maxiter=100, random_state=0)

plt.plot(mu_kmeans[:, 0], mu_kmeans[:, 1], 'ro', markersize=10)
plt.scatter(X[:, 0], X[:, 1], c=y_kmeans, cmap='viridis')
plt.title('Objective = %g' % objective3(X, y_kmeans, mu_kmeans))
```

```
Converged after 3 iteration
```

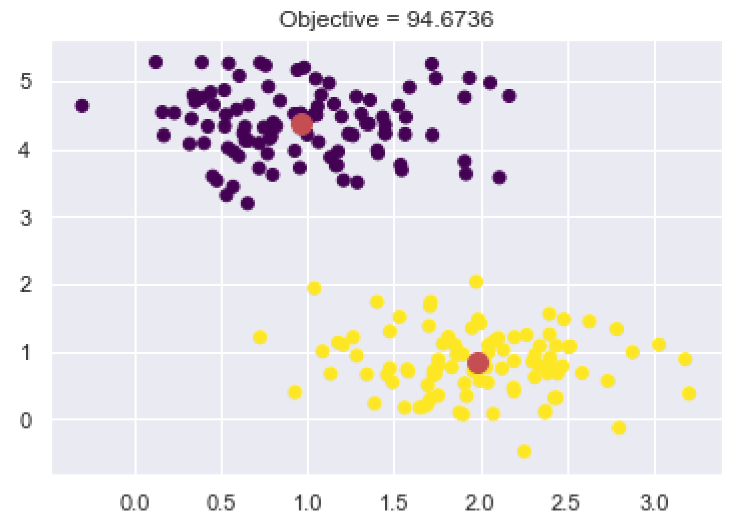
Out[48]:
```
Text(0.5, 1.0, 'Objective = 94.6736')
```



Let's inspect the underlying operation by splitting the iteration

In [33]:
```
# Program kmeans
def kmeans_alg(X, maxiter=100, random_state=None):
    rng = check_random_state(random_state)

    # Initialize with random points in X
    rand_idx = rng.permutation(X.shape[0])
    mu_array = X[rand_idx[:2], :]
    y = get_random_assignment(random_state=rng)

    for i in range(int(2*maxiter)): #CHANGED
        if i % 2 == 0: #CHANGED
            # Get new best assignment
            y_old = y  # Save old assignment matrix
            y = best_assignment(X, mu_array)
        else: #CHANGED
            # Recenter / compute cluster mean
            mu_array = recenter(X, y)

            # Check convergence
            if y_old is not None and np.all(y == y_old):
                print('Converged after %d iteration' % (i/2)) #CHANGED
                break
    return y, mu_array
```

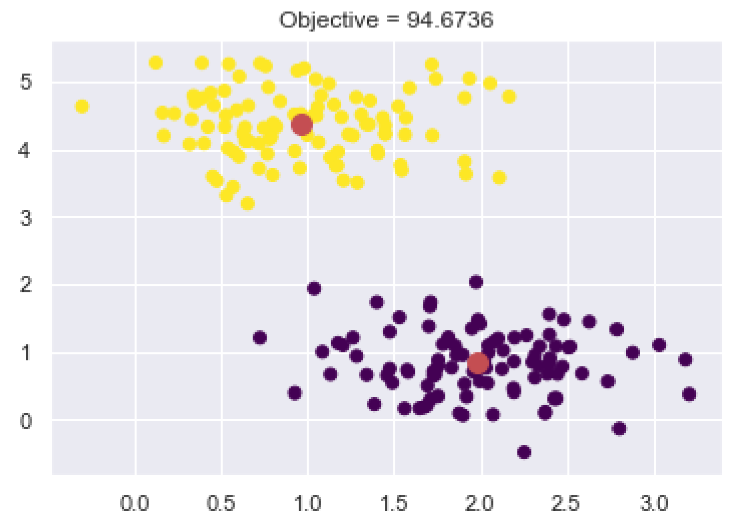
```
In [34]: y_kmeans, mu_kmeans = kmeans_alg(X, maxiter=4, random_state=0)

         plt.plot(mu_kmeans[:, 0], mu_kmeans[:, 1], 'ro', markersize=10)
         plt.scatter(X[:, 0], X[:, 1], c=y_kmeans, cmap='viridis')
         plt.title('Objective = %g' % objective3(X, y_kmeans, mu_kmeans))

         Converged after 3 iteration

Out[34]: Text(0.5, 1.0, 'Objective = 94.6736')
```



Introducing scikit-learn's `sklearn.cluster.KMeans`

- Documentation: [https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html (https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html)](https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html) (some nice examples at the bottom of the documentation)
- See Python handbook for nice examples of kmeans [https://jakevdp.github.io/PythonDataScienceHandbook/05.11-k-means.html (https://jakevdp.github.io/PythonDataScienceHandbook/05.11-k-means.html)](https://jakevdp.github.io/PythonDataScienceHandbook/05.11-k-means.html)

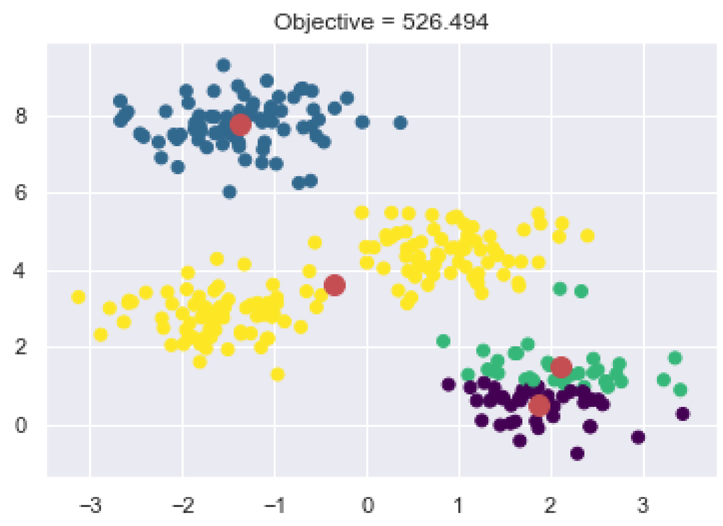
In [42]:
```
from sklearn.datasets.samples_generator import make_blobs
X, y_true = make_blobs(n_samples=200, centers=2,
                       cluster_std=0.50, random_state=0)

from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=2, random_state=0) # 0 and 2 give opposite cl
usterings

kmeans.fit(X)
y_kmeans = kmeans.labels_
mu_array = kmeans.cluster_centers_
plot_clustering(X, y_kmeans, mu_array)
```



This looks great! But isn't this an NP-Hard problem?

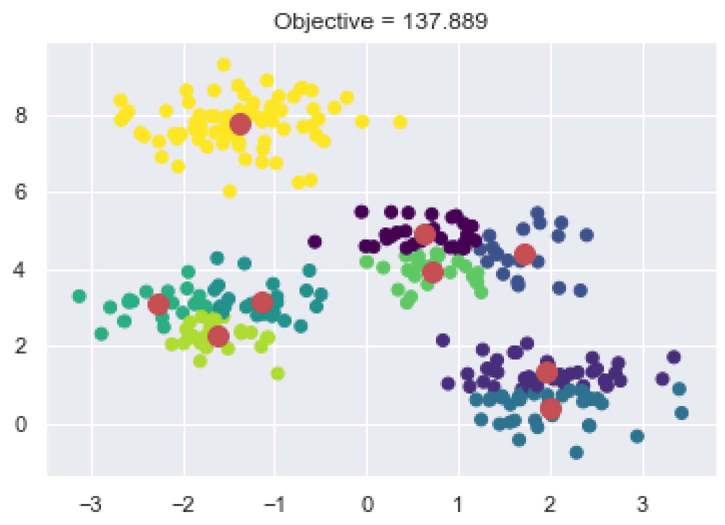
First caveat: Does not always converge to the optimal/best solution.

In [43]:
```
# Example from Python handbook
from sklearn.datasets.samples_generator import make_blobs
X2, y_true2 = make_blobs(n_samples=300, centers=4,
                       cluster_std=0.60, random_state=0)

kmeans = KMeans(n_clusters=4, init='random', n_init=1, random_state=104)
# 104 gives bad seeding
kmeans.fit(X2)
plot_clustering(X2, kmeans.labels_, kmeans.cluster_centers_)
```



Second caveat: Choosing the number of clusters is not obvious

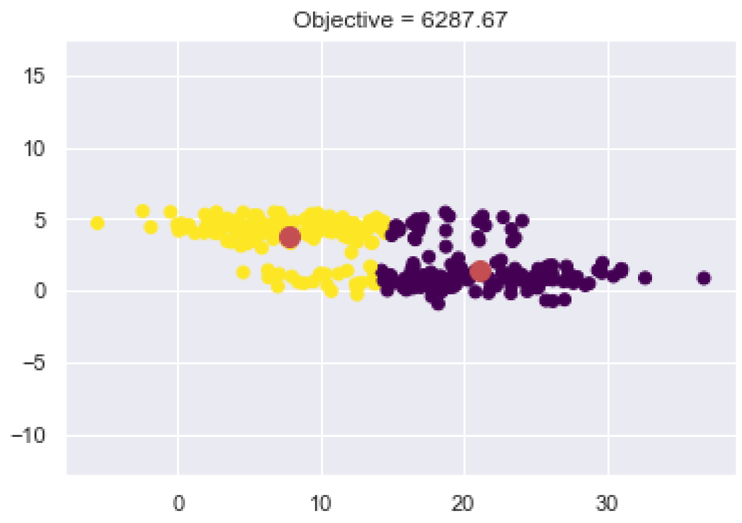
In [44]:
```python
# Example from Python handbook
from sklearn.datasets.samples_generator import make_blobs
X2, y_true2 = make_blobs(n_samples=300, centers=4,
                         cluster_std=0.60, random_state=0)

kmeans = KMeans(n_clusters=9, init='random', n_init=1, random_state=0)
kmeans.fit(X2)
plot_clustering(X2, kmeans.labels_, kmeans.cluster_centers_)
```



Third caveat: Scaling of variables and clusters matters

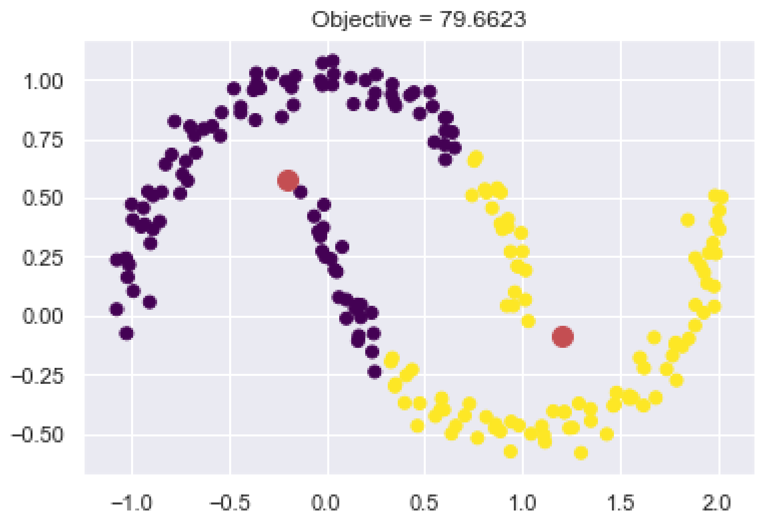
In [46]:
```
from sklearn.datasets import make_moons
X3, y_true = make_blobs(n_samples=300, centers=2,
                        cluster_std=0.60, random_state=0)
X3[:, 0] = X3[:, 0]*10

kmeans = KMeans(n_clusters=2, random_state=0).fit(X3)

plot_clustering(X3, kmeans.labels_, kmeans.cluster_centers_)
plt.axis('equal')
```

Out[46]:
```
(-7.813474526935023,
 38.988255947105756,
 -1.2918715239530854,
 5.9043323952750475)
```



Fourth caveat: Only linear boundaries between clusters

In [47]:
```
from sklearn.datasets import make_moons
X4, y_true4 = make_moons(200, noise=.05, random_state=0)

kmeans = KMeans(n_clusters=2, random_state=0).fit(X4)
plot_clustering(X4, kmeans.labels_, kmeans.cluster_centers_)
```



In [ ]:
```
```