Sample solutions

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main (Score: 14.0 / 14.0)

1. Test cell (Score: 2.0 / 2.0)
2. Test cell (Score: 3.0 / 3.0)
3. Test cell (Score: 2.0 / 2.0)
4. Test cell (Score: 2.0 / 2.0)
5. Test cell (Score: 2.0 / 2.0)
6. Test cell (Score: 3.0 / 3.0)

Important note! Before you turn in this lab notebook, make sure everything runs as expected:

- First, **restart the kernel** -- in the menubar, select Kernel→Restart.
- Then **run all cells** -- in the menubar, select Cell→Run All.

Make sure you fill in any place that says `YOUR CODE HERE` or "YOUR ANSWER HERE."

Clustering via k-means

We previously studied the classification problem using the logistic regression algorithm. Since we had labels for each data point, we may regard the problem as one of *supervised learning*. However, in many applications, the data have no labels but we wish to discover possible labels (or other hidden patterns or structures). This problem is one of *unsupervised learning*. How can we approach such problems?

Clustering is one class of unsupervised learning methods. In this lab, we'll consider the following form of the clustering task. Suppose you are given

- a set of observations, $X \equiv \{\hat{x_i} \mid 0 \leq i < n\}$, and
- a target number of *clusters*, k.

Your goal is to partition the points into k subsets, $C_0, \ldots, C_{k-1} \subseteq X$, which are

- disjoint, i.e., $i \neq j \implies C_i \cap C_j = \emptyset$;
- but also complete, i.e., $C_0 \cup C_1 \cup \cdots \cup C_{k-1} = X$.

Intuitively, each cluster should reflect some "sensible" grouping. Thus, we need to specify what constitutes such a grouping.

Setup: Dataset

The following cell will download the data you'll need for this lab. Run it now.

In [1]:
```
import requests
import os
import hashlib
import io

def on_vocareum():
    return os.path.exists('.voc')
```

```
    return os.path.exists('.voc')

def download(file, local_dir="", url_base=None, checksum=None):
    local_file = "{}{}".format(local_dir, file)
    if not os.path.exists(local_file):
        if url_base is None:
            url_base = "https://cse6040.gatech.edu/datasets/"
        url = "{}{}".format(url_base, file)
        print("Downloading: {} ...".format(url))
        r = requests.get(url)
        with open(local_file, 'wb') as f:
            f.write(r.content)

    if checksum is not None:
        with io.open(local_file, 'rb') as f:
            body = f.read()
            body_checksum = hashlib.md5(body).hexdigest()
            assert body_checksum == checksum, \
                "Downloaded file '{}' has incorrect checksum: '{}' instead of '{}'".forma
t(local_file,

body_checksum,

checksum)
    print("'{}' is ready!".format(file))

if on_vocareum():
    URL_BASE = "https://cse6040.gatech.edu/datasets/kmeans/"
    DATA_PATH = "../resource/lib/publicdata/kmeans/"
else:
    URL_BASE = "https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/"
    DATA_PATH = ""

datasets = {'logreg_points_train.csv': '9d1e42f49a719da43113678732491c6d',
            'centers_initial_testing.npy': '8884b4af540c1d5119e6e8980da43f04',
            'compute_d2_soln.npy': '980fe348b6cba23cb81ddf703494fb4c',
            'y_test3.npy': 'df322037ea9c523564a5018ea0a70fbf',
            'centers_test3_soln.npy': '0c594b28e512a532a2ef4201535868b5',
            'assign_cluster_labels_S.npy': '37e464f2b79dc1d59f5ec31eaefe4161',
            'assign_cluster_labels_soln.npy': 'fc0e084ac000f30948946d097ed85ebc'}

for filename, checksum in datasets.items():
    download(filename, local_dir=DATA_PATH, url_base=URL_BASE, checksum=checksum)

print("\n(All data appears to be ready.)")
```

```
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/logreg_point
s_train.csv ...

'logreg_points_train.csv' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/assign_clust
er_labels_soln.npy ...

'assign_cluster_labels_soln.npy' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/assign_clust
er_labels_S.npy ...

'assign_cluster_labels_S.npy' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/centers_init
ial_testing.npy ...

'centers_initial_testing.npy' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/centers_test
3_soln.npy ...

'centers_test3_soln.npy' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/compute_d2_s
oln.npy ...

'compute_d2_soln.npy' is ready!
Downloading: https://github.com/cse6040/labs-fa17/raw/master/datasets/kmeans/y_test3.npy
...

'y_test3.npy' is ready!

(All data appears to be ready.)
```

The k-means clustering criterion

Here is one way to measure the quality of a set of clusters. For each cluster C, consider its center μ and measure the distance $\|x - \mu\|$ of each observation $x \in C$ to the center. Add these up for all points in the cluster; call this sum is the *within-cluster sum-of-squares (WCSS)*. Then, set as our goal to choose clusters that minimize the total WCSS over *all* clusters.

More formally, given a clustering $C = \{C_0, C_1, \ldots, C_{k-1}\}$, let

$$\mathrm{WCSS}(C) \equiv \sum_{i=0}^{k-1} \sum_{x \in C_i} \|x - \mu_i\|^2,$$

where μ_i is the center of C_i. This center may be computed simply as the mean of all points in C_i, i.e.,

$$\mu_i \equiv \frac{1}{|C_i|} \sum_{x \in C_i} x.$$

Then, our objective is to find the "best" clustering, C_*, which is the one that has a minimum WCSS.

$$C_* = \arg\min_C \mathrm{WCSS}(C).$$

The standard k-means algorithm (Lloyd's algorithm)

Finding the global optimum is NP-hard (https://en.wikipedia.org/wiki/NP-hardness), which is computer science mumbo jumbo for "we don't know whether there is an algorithm to calculate the exact answer in fewer steps than exponential in the size of the input." Nevertheless, there is an iterative method, Lloyd's algorithm, that can quickly converge to a *local* (as opposed to *global*) minimum. The procedure alternates between two operations: *assignment* and *update*.

Step 1: Assignment. Given a fixed set of k centers, assign each point to the nearest center:

$$C_i = \{\hat{x} : \|\hat{x} - \mu_i\| \leq \|\hat{x} - \mu_j\|, 1 \leq j \leq k\}.$$

Step 2: Update. Recompute the k centers ("centroids") by averaging all the data points belonging to each cluster, i.e., taking their mean:

$$\mu_i = \frac{1}{|C_i|} \sum_{\hat{x} \in C_i} \hat{x}$$

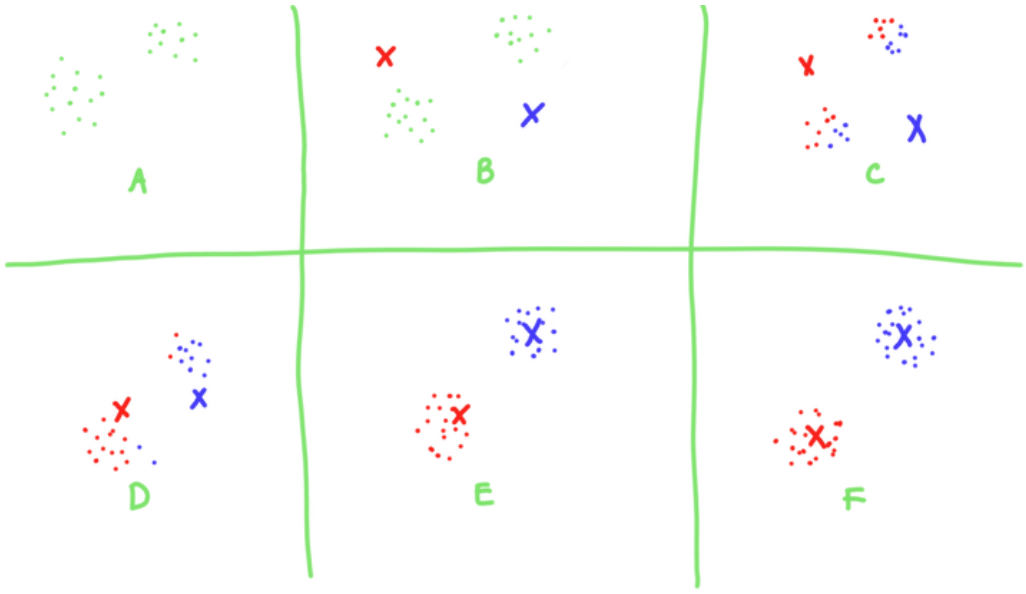


Figure adapted from: http://stanford.edu/~cpiech/cs221/img/kmeansViz.png (http://stanford.edu/~cpiech/cs221/img/kmeansViz.png)

In the code that follows, it will be convenient to use our usual "data matrix" convention, that is, each row of a data matrix X is one of m observations and each column (coordinate) is one of d predictors. However, we will *not* need a dummy column of ones since we are not fitting a function.

fitting a function.

$$X \equiv \begin{pmatrix} x_0^T \\ \vdots \\ x_m^T \end{pmatrix} = \begin{pmatrix} x_0 & \cdots & x_{d-1} \end{pmatrix}.$$

In [2]:
```
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

%matplotlib inline

import matplotlib as mpl
mpl.rc("savefig", dpi=100) # Adjust for higher-resolution figures
```

We will use the following data set which some of you may have seen previously.

In [3]:
```
df = pd.read_csv('{}logreg_points_train.csv'.format(DATA_PATH))
df.head()
```

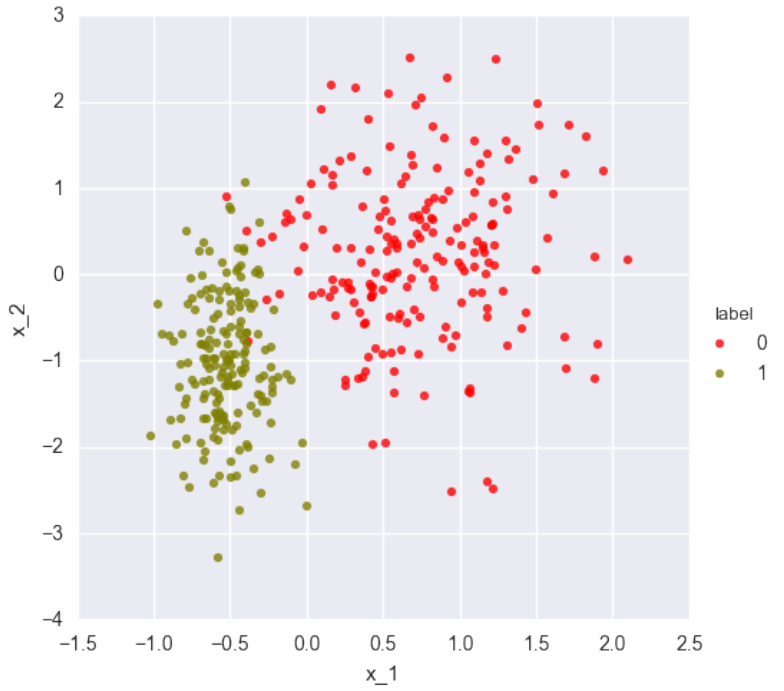
Out[3]:

	x_1	x_2	label
0	-0.234443	-1.075960	1
1	0.730359	-0.918093	0
2	1.432270	-0.439449	0
3	0.026733	1.050300	0
4	1.879650	0.207743	0

In [4]:
```
# Helper functions from Logistic Regression Lesson
def make_scatter_plot(df, x="x_1", y="x_2", hue="label",
                      palette={0: "red", 1: "olive"},
                      size=5,
                      centers=None):
    sns.lmplot(x=x, y=y, hue=hue, data=df, palette=palette,
               fit_reg=False)
    if centers is not None:
        plt.scatter(centers[:,0], centers[:,1],
                    marker=u'*', s=500,
                    c=[palette[0], palette[1]])

def mark_matches(a, b, exact=False):
    """
    Given two Numpy arrays of {0, 1} labels, returns a new boolean
    array indicating at which locations the input arrays have the
    same label (i.e., the corresponding entry is True).

    This function can consider "inexact" matches. That is, if `exact`
    is False, then the function will assume the {0, 1} labels may be
    regarded as the same up to a swapping of the labels. This feature
    allows

      a == [0, 0, 1, 1, 0, 1, 1]
      b == [1, 1, 0, 0, 1, 0, 0]

    to be regarded as equal. (That is, use `exact=False` when you
    only care about "relative" labeling.)
    """
    assert a.shape == b.shape
    a_int = a.astype(dtype=int)
    b_int = b.astype(dtype=int)
    all_axes = tuple(range(len(a.shape)))
    assert ((a_int == 0) | (a_int == 1)).all()
    assert ((b_int == 0) | (b_int == 1)).all()

    exact_matches = (a_int == b_int)
    if exact:
        return exact_matches
```

```
    assert exact == False
    num_exact_matches = np.sum(exact_matches)
    if (2*num_exact_matches) >= np.prod (a.shape):
        return exact_matches
    return exact_matches == False # Invert

def count_matches(a, b, exact=False):
    """
    Given two sets of {0, 1} labels, returns the number of mismatches.

    This function can consider "inexact" matches. That is, if `exact`
    is False, then the function will assume the {0, 1} labels may be
    regarded as similar up to a swapping of the labels. This feature
    allows

      a == [0, 0, 1, 1, 0, 1, 1]
      b == [1, 1, 0, 0, 1, 0, 0]

    to be regarded as equal. (That is, use `exact=False` when you
    only care about "relative" labeling.)
    """
    matches = mark_matches(a, b, exact=exact)
    return np.sum(matches)
```

In [5]:
```
make_scatter_plot(df)
```



Let's extract the data points as a data matrix, `points`, and the labels as a vector, `labels`. Note that the k-means algorithm you will implement should **not** reference `labels` -- that's the solution we will try to predict given only the point coordinates (`points`) and target number of clusters (k).

In [6]:
```
points = df.as_matrix(['x_1', 'x_2'])
labels = df['label'].as_matrix()
n, d = points.shape
k = 2
```

Note that the labels should *not* be used in the k-means algorithm. We use them here only as ground truth for later verification.

How to start? Initializing the k centers

To start the algorithm, you need an initial guess. Let's randomly choose k observations from the data.

Exercise 1 (2 points). Complete the following function, `init_centers(X, k)`, so that it randomly selects k of the given observations to serve as centers. It should return a Numpy array of size `k`-by-`d`, where `d` is the number of columns of `X`.

In [7]:

Student's answer (Top)

```
def init_centers(X, k):
    """
    Randomly samples k observations from X as centers.
    Returns these centers as a (k x d) numpy array.
    """
    ### BEGIN SOLUTION
    from numpy.random import choice
    samples = choice(len(X), size=k, replace=False)
    return X[samples, :]
    ### END SOLUTION
```

In [8]:

Grade cell: `init_centers_test` Score: 2.0 / 2.0 (Top)

```
# Test cell: `init_centers_test`

centers_initial = init_centers(points, k)
print("Initial centers:\n", centers_initial)

assert type(centers_initial) is np.ndarray, "Your function should return a Numpy array
instead of a {}".format(type(centers_initial))
assert centers_initial.shape == (k, d), "Returned centers do not have the right shape (
{} x {})".format(k, d)
assert (sum(centers_initial[0, :] == points) == [1, 1]).all(), "The centers must come f
rom the input."
assert (sum(centers_initial[1, :] == points) == [1, 1]).all(), "The centers must come f
rom the input."

print("\n(Passed!)")
```

```
Initial centers:
 [[ 0.727148  0.470508]
 [-0.610862 -1.35298 ]]

(Passed!)
```

Computing the distances

Exercise 2 (3 points). Implement a function that computes a distance matrix, $S = (s_{ij})$ such that $s_{ij} = d_{ij}^2$ is the *squared* distance from point $\hat{x_i}$ to center μ_j. It should return a Numpy matrix `S[:m, :k]`.

In [9]:

Student's answer (Top)

```
def compute_d2(X, centers):
    m = len(X)
    k = len(centers)

    S = np.empty((m, k))

    ### BEGIN SOLUTION
    for i in range(m):
        d_i = np.linalg.norm(X[i, :] - centers, ord=2, axis=1)
        S[i, :] = d_i**2
    ### END SOLUTION

    return S
```

In [10]:

Grade cell: `compute_d2_test` Score: 3.0 / 3.0 (Top)

```
# Test cell: `compute_d2_test`

centers_initial_testing = np.load("{}centers_initial_testing.npy".format(DATA_PATH))
compute_d2_soln = np.load("{}compute_d2_soln.npy".format(DATA_PATH))

S = compute_d2 (points, centers_initial_testing)
assert (np.linalg.norm (S - compute_d2_soln, axis=1) <= (10.0 * np.finfo(float).eps)).a
ll ()

print("\n(Passed!)")
```

```
(Passed!)
```

Exercise 3 (2 points). Write a function that uses the (squared) distance matrix to assign a "cluster label" to each point.

That is, consider the $m \times k$ squared distance matrix S. For each point i, if $s_{i,j}$ is the minimum squared distance for point i, then the index j is i's cluster label. In other words, your function should return a (column) vector y of length m such that

$$y_i = \underset{j \in \{0,\ldots,k-1\}}{\operatorname{argmin}} s_{ij}.$$

> Hint: Judicious use of Numpy's `argmin()` (https://docs.scipy.org/doc/numpy/reference/generated/numpy.argmin.html) makes for a nice one-line solution.

In [11]:

Student's answer (Top)

```
def assign_cluster_labels(S):
    ### BEGIN SOLUTION
    return np.argmin(S, axis=1)
    ### END SOLUTION

# Cluster labels:     0    1
S_test1 = np.array([[0.3, 0.2],  # --> cluster 1
                    [0.1, 0.5],  # --> cluster 0
                    [0.4, 0.2]]) # --> cluster 1
y_test1 = assign_cluster_labels(S_test1)
print("You found:", y_test1)

assert (y_test1 == np.array([1, 0, 1])).all()
```

```
You found: [1 0 1]
```

In [12]:

Grade cell: `assign_cluster_labels_test` Score: 2.0 / 2.0 (Top)

```
# Test cell: `assign_cluster_labels_test`

S_test2 = np.load("{}assign_cluster_labels_S.npy".format(DATA_PATH))
y_test2_soln = np.load("{}assign_cluster_labels_soln.npy".format(DATA_PATH))
y_test2 = assign_cluster_labels(S_test2)
assert (y_test2 == y_test2_soln).all()

print("\n(Passed!)")
```

```
(Passed!)
```

Exercise 4 (2 points). Given a clustering (i.e., a set of points and assignment of labels), compute the center of each cluster.

In [13]:

Student's answer (Top)

```
def update_centers(X, y):
    # X[:m, :d] == m points, each of dimension d
    # y[:m] == cluster labels
    m, d = X.shape
    k = max(y) + 1
    assert m == len(y)
```

```
    assert (min(y) >= 0)

    centers = np.empty((k, d))
    for j in range(k):
        # Compute the new center of cluster j,
        # i.e., centers[j, :d].
        ### BEGIN SOLUTION
        centers[j, :d] = np.mean(X[y == j, :], axis=0)
        ### END SOLUTION
    return centers
```

In [14]:

Grade cell: `update_centers_test` Score: 2.0 / 2.0 (Top)

```
# Test cell: `update_centers_test`

y_test3 = np.load("{}y_test3.npy".format(DATA_PATH))
centers_test3_soln = np.load("{}centers_test3_soln.npy".format(DATA_PATH))
centers_test3 = update_centers(points, y_test3)

delta_test3 = np.abs(centers_test3 - centers_test3_soln)
assert (delta_test3 <= 2.0*len(centers_test3_soln)*np.finfo(float).eps).all()

print("\n(Passed!)")
```

```
(Passed!)
```

Exercise 5 (2 points). Given the squared distances, return the within-cluster sum of squares.

In particular, your function should have the signature,

```
def WCSS(S):
        ...
```

where `S` is an array of distances as might be computed from Exercise 2.

For example, suppose `S` is defined as follows:

```
S = np.array([[0.3, 0.2],
              [0.1, 0.5],
              [0.4, 0.2]])
```

Then `WCSS(S) == 0.2 + 0.1 + 0.2 == 0.5`.

> *Hint*: See numpy.amin (https://docs.scipy.org/doc/numpy/reference/generated/numpy.amin.html#numpy.amin).

In [15]:

Student's answer (Top)

```
def WCSS(S):
    ### BEGIN SOLUTION
    return np.sum(np.amin(S, axis=1))
    ### END SOLUTION

# Quick test:
print("S ==\n", S_test1)
WCSS_test1 = WCSS(S_test1)
print("\nWCSS(S) ==", WCSS(S_test1))
```

```
S ==
 [[ 0.3  0.2]
 [ 0.1  0.5]
 [ 0.4  0.2]]

WCSS(S) == 0.5
```

In [16]:

Grade cell: `wcss_test` Score: 2.0 / 2.0 (Top)

```
# Test cell: `WCSS_test`

assert np.abs(WCSS_test1 - 0.5) <= 3.0*np.finfo(float).eps, "WCSS(S_test1) should be cl
ose to 0.5, not {}".format(WCSS_test1)
print("\n(Passed!)")
```

```
(Passed!)
```

Lastly, here is a function to check whether the centers have "moved," given two instances of the center values. It accounts for the fact that the order of centers may have changed.

In [17]:
```
def has_converged(old_centers, centers):
    return set([tuple(x) for x in old_centers]) == set([tuple(x) for x in centers])
```

Exercise 6 (3 points). Put all of the preceding building blocks together to implement Lloyd's k-means algorithm.

In [18]:

Student's answer (Top)

```
def kmeans(X, k,
           starting_centers=None,
           max_steps=np.inf):
    if starting_centers is None:
        centers = init_centers(X, k)
    else:
        centers = starting_centers

    converged = False
    labels = np.zeros(len(X))
    i = 1
    while (not converged) and (i <= max_steps):
        old_centers = centers
        ### BEGIN SOLUTION
        S = compute_d2(X, centers)
        labels = assign_cluster_labels(S)
        centers = update_centers(X, labels)
        converged = has_converged(old_centers, centers)
        ### END SOLUTION
        print ("iteration", i, "WCSS = ", WCSS (S))
        i += 1
    return labels

clustering = kmeans(points, k, starting_centers=points[[0, 187], :])
```

```
iteration 1 WCSS =  549.917553549
iteration 2 WCSS =  339.800663303
iteration 3 WCSS =  300.330112922
iteration 4 WCSS =  289.807007773
iteration 5 WCSS =  286.074559106
iteration 6 WCSS =  284.190770558
iteration 7 WCSS =  283.227322499
iteration 8 WCSS =  282.456491303
iteration 9 WCSS =  281.848382253
iteration 10 WCSS =  281.572420827
iteration 11 WCSS =  281.531562799
```

Let's visualize the results.

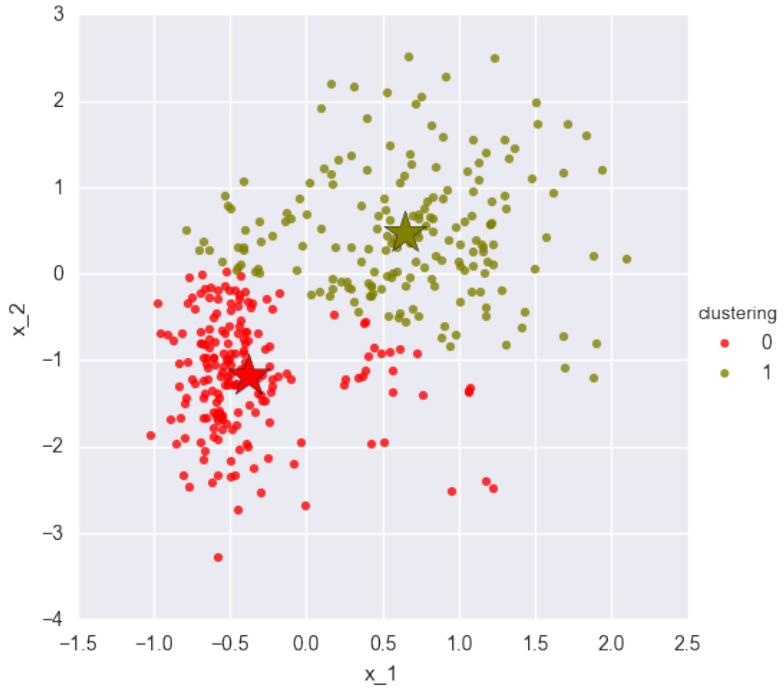
In [19]:

Grade cell: `kmeans_test` Score: 3.0 / 3.0 (Top)

```
# Test cell: `kmeans_test`

df['clustering'] = clustering
centers = update_centers(points, clustering)
make_scatter_plot(df, hue='clustering', centers=centers)
```

```
n_matches = count_matches(df['label'], df['clustering'])
print(n_matches,
      "matches out of",
      len(df), "possible",
      "(~ {:.1f}%)".format(100.0 * n_matches / len(df)))

assert n_matches >= 320
```

```
329 matches out of 375 possible (~ 87.7%)
```



Built-in k-means

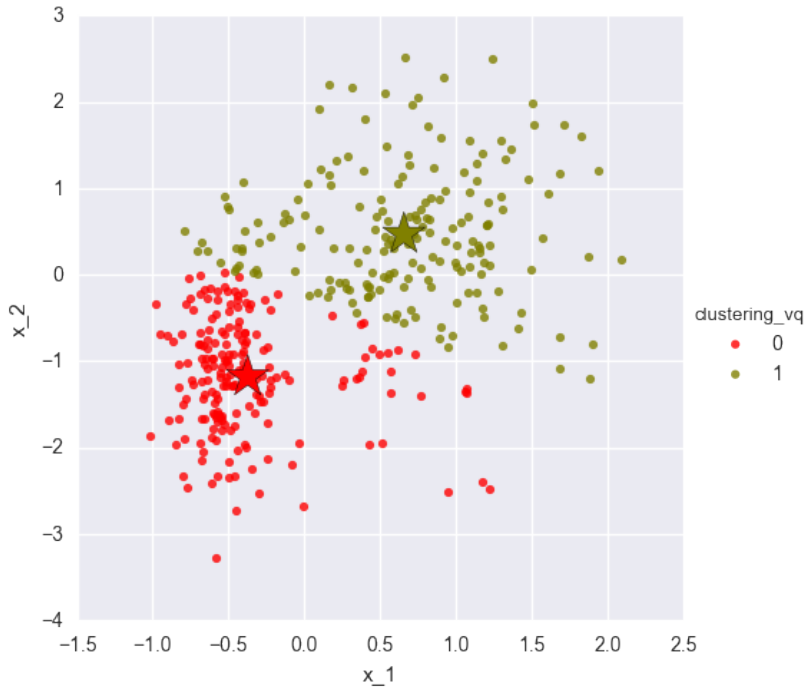
The preceding exercises walked you through how to implement k-means, but as you might have imagined, there are existing implementations as well! The following shows you how to use Scipy's implementation, which should yield similar results. If you are asked to use k-means in a future lab (or exam!), you can use this one.

In [20]:
```
from scipy.cluster import vq
```

In [21]:
```
# `distortion` below is the similar to WCSS.
# It is called distortion in the Scipy documentation
# since clustering can be used in compression.
centers_vq, distortion_vq = vq.kmeans(points, k)

# vq return the clustering (assignment of group for each point)
# based on the centers obtained by the kmeans function.
# _ here means ignore the second return value
clustering_vq, _ = vq.vq(points, centers_vq)

print("Centers:\n", centers_vq)
print("\nCompare with your method:\n", centers, "\n")
print("Distortion (WCSS):", distortion_vq)

df['clustering_vq'] = clustering_vq
make_scatter_plot(df, hue='clustering_vq', centers=centers_vq)

n_matches_vq = count_matches(df['label'], df['clustering_vq'])
print(n_matches_vq,
      "matches out of",
      len(df), "possible",
```

```
    "(~ {:.1f}%)".format(100.0 * n_matches_vq / len(df)))
```

```
Centers:
 [[-0.3742504  -1.17922941]
 [ 0.65580448  0.4690796 ]]

Compare with your method:
 [[-0.37382602 -1.18565619]
 [ 0.64980076  0.4667703 ]]

Distortion (WCSS): 0.750376271319

329 matches out of 375 possible (~ 87.7%)
```



Fin! That marks the end of this notebook. Don't forget to submit it!