Lecture 12
Data Processing (2)

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Last Time

- Data Processing 1
  - Statistical/Monte Carlo Simulation
  - Simulate the solution of real with less samples
  - How to write the corresponding code

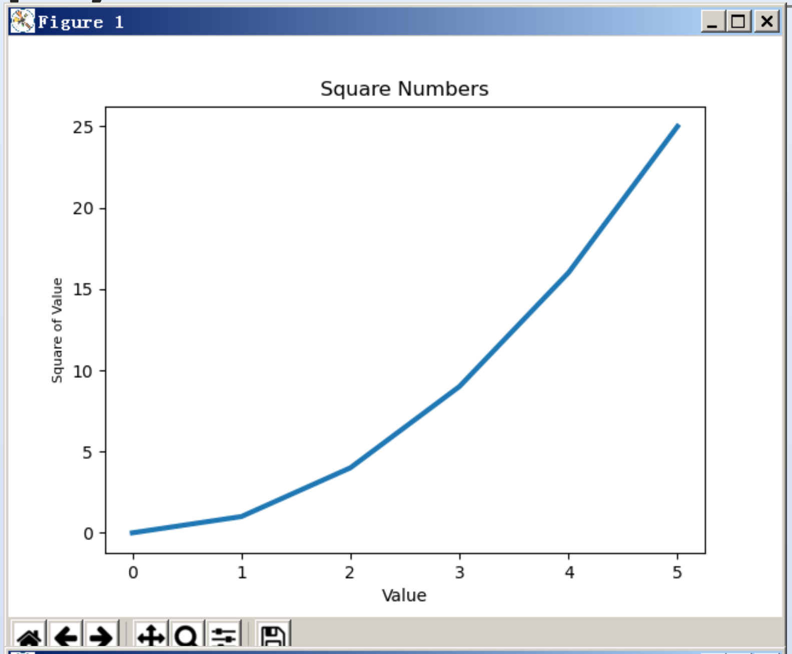
Today

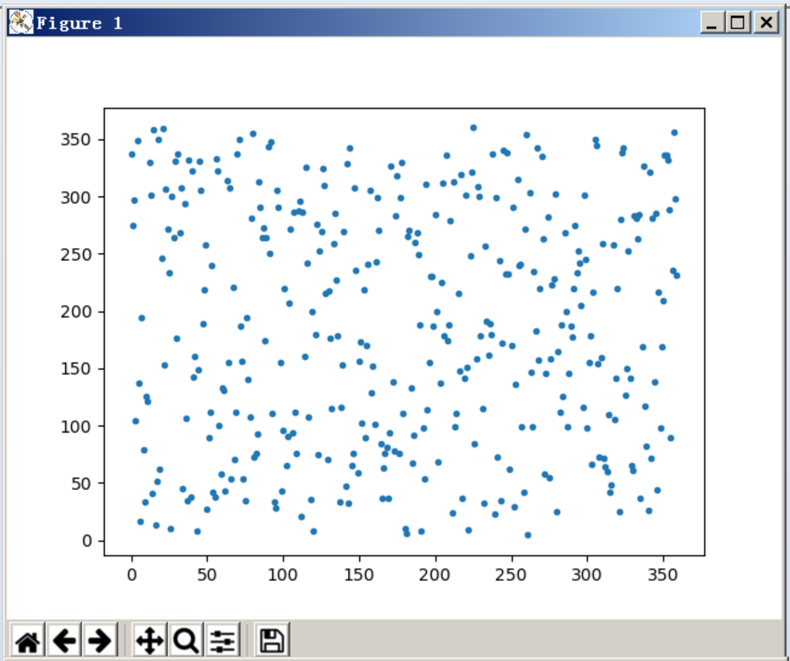
- Data Processing (Part 2)
  - Data visualization
  - Clustering
  - Classification

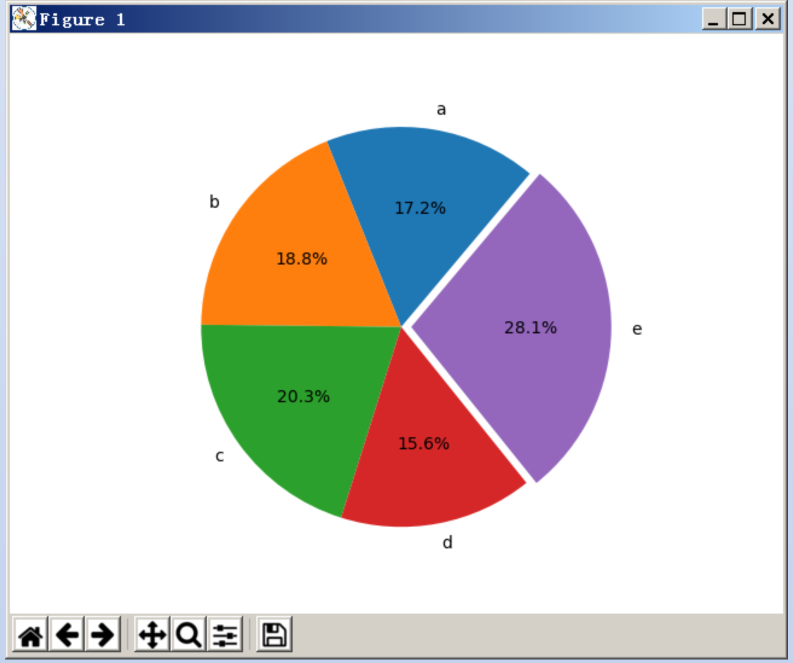
Part 1: Data visualization

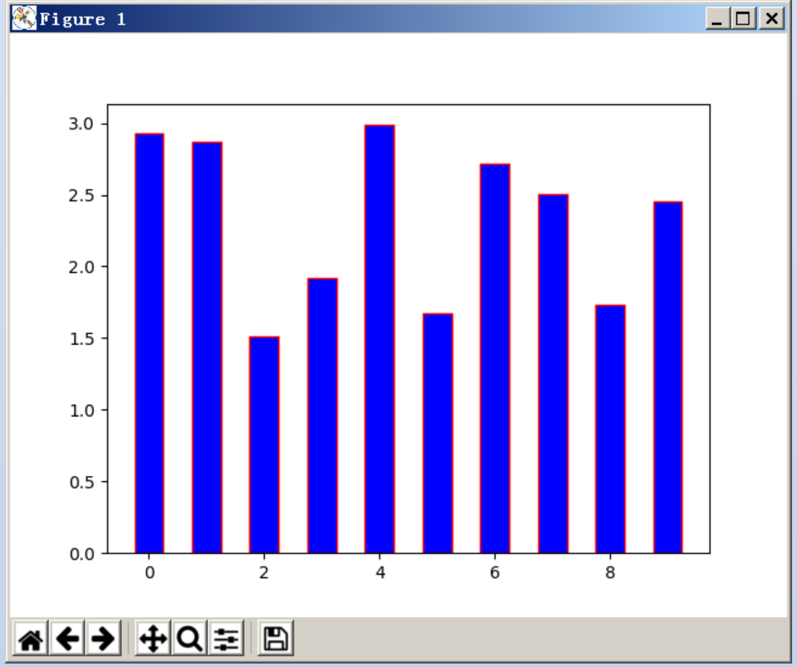
- The data is represented as a graphical image
- Python pylab:
  - Draw the data into various 2D graphs (histogram, scatter chart, bar-chart, etc.).
  - This course requires the use of graphics in Project
  - **self-learning pylab**
- Install matplotlib from official website
  - pylab is its submodule
- Import pylab into your program
  - import pylab
  - Import pylab as pl   # pl is the alias of pylab

pylab Demo: demopylab-line









About Dada Processing

- The Computer way
  1. Data processing Method (Need to find)
  2. Design Algorithm
     - procedural
  3. Implement in a programming language
     - paradigm

Part 2 Clustering

$$variability(c) = \sum_{e \in c} distance(mean(c), e)^2$$

$$dissimilarity(C) = \sum_{c \in C} variability(c)$$

- ◆ Why not divide variability by size of cluster?
  - Big and bad worse than small and bad
- ◆ Is optimization problem finding a C that minimizes dissimilarity(C)?
  - No, otherwise could put each example in its own cluster
- **Clustering Is an Optimization Problem**

Clustering

- One of the dada Processing methods
- Called:
  - Cluster analysis
  - Cluster method
- A “Cluster" is a set of similar data
  - **The data to be analyzed is divided into Clusters(簇)**
- **Question is**
  - **How to division?**
  - How to computerize
- **…….**

Machine Learning Paradigm

- Observe set of examples: training data
- Infer something about process that generated that data
- Use inference to make predictions about previously unseen data: test data
- Supervised: given a set of feature/label pairs, find a rule that predicts the label associated with a previously unseen input
- *Unsupervised*: given a set of feature vectors (without labels) group them into “natural clusters”

Clustering Is an Optimization Problem

- Need a constraint, e.g.,
  - Minimum distance between clusters
  - Number of clusters

- Two Popular Methods
  - Hierarchical clustering
  - K-means clustering

Hiearchical Clustering

1. Start by assigning each item to a cluster, so that if you have N items, you now have N clusters, each containing just one item.

2. Find the closest (most similar) pair of clusters and merge them into a single cluster, so that now you have one fewer cluster.

3. Continue the process until all items are clustered into a single cluster of size N.

What does distance mean?

Linkage Metrics

- *Single-linkage:* consider the distance between one cluster and another cluster to be equal to the <u>shortest</u> distance from any member of one cluster to any member of the other cluster
- *Complete-linkage*: consider the distance between one cluster and another cluster to be equal to the <u>greatest</u> distance from any member of one cluster to any member of the other cluster
- *Average-linkage:* consider the distance between one cluster and another cluster to be equal to the <u>average</u> distance from any member of one cluster to any member of the other cluster

Example of Hierarchical Clustering

	BOS	**NY**	**CHI**	**DEN**	**SF**	**SEA**
BOS	0	206	963	1949	3095	2979
NY		0	802	1771	2934	2815
CHI			0	966	2142	2013
DEN				0	1235	1307
SF					0	808
SEA						0

{BOS} {NY} {CHI} {DEN} {SF} {SEA}

{BOS, NY} {CHI} {DEN} {SF} {SEA}

{BOS, NY, CHI} {DEN} {SF} {SEA}

{BOS, NY, CHI} {DEN} {SF, SEA}

{BOS, NY, CHI, DEN} {SF, SEA} Single linkage

or

{BOS, NY, CHI} {DEN, SF, SEA} Complete linkage

Clustering Algorithms

- Hierarchical clustering
  - Can select number of clusters using dendogram
  - Deterministic
  - Flexible with respect to linkage criteria
  - Slow
    - Naïve algorithm n^3
    - n^2 algorithms exist for some linkage criteria
- K-means a much faster greedy algorithm
  - Most useful when you know how many clusters you want

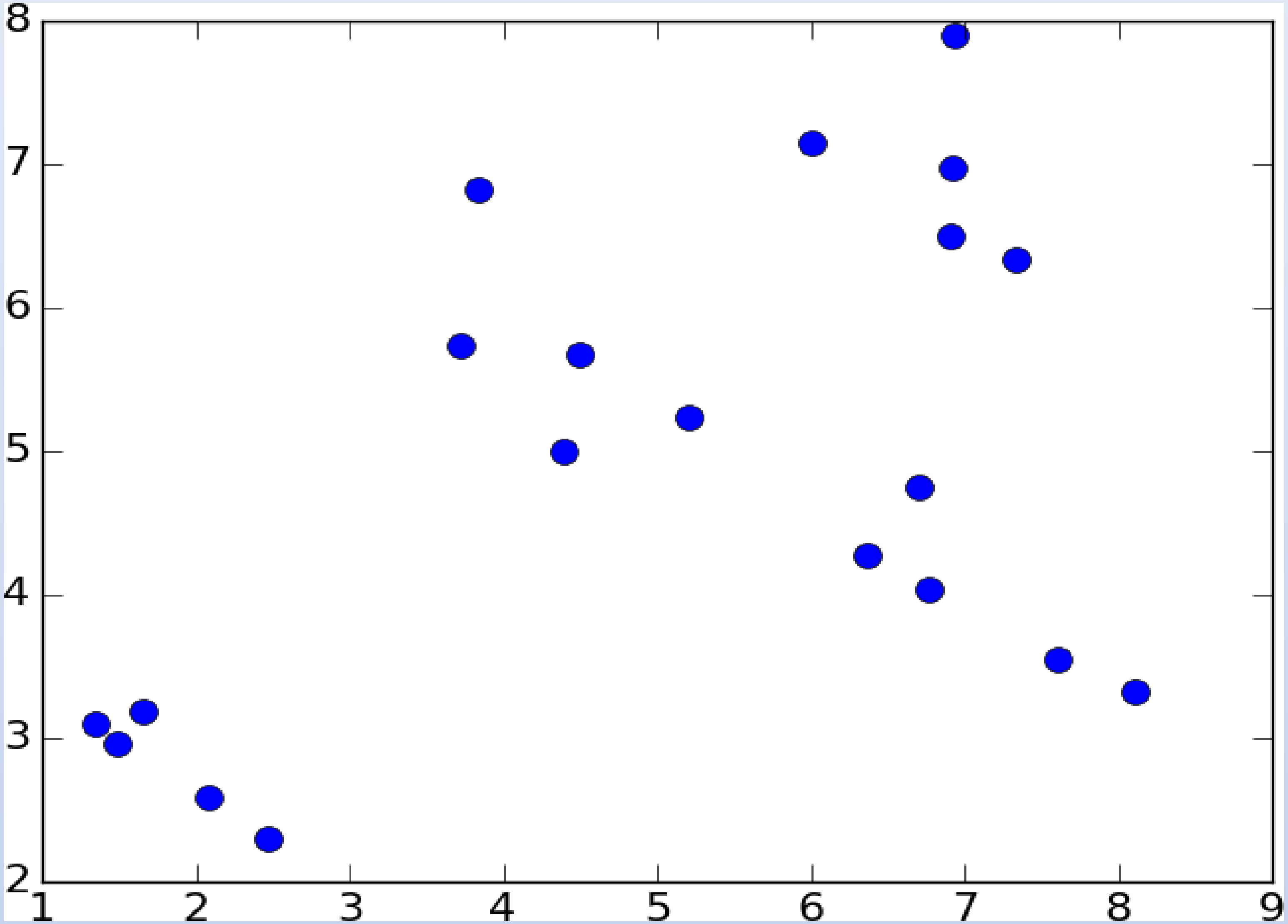
K-means Algorithm

```
randomly chose k examples as initial centroids

while true:
    create k clusters by assigning each
        example to closest centroid
    compute k new centroids by averaging
        examples in each cluster
    if centroids don't change:
        break
```

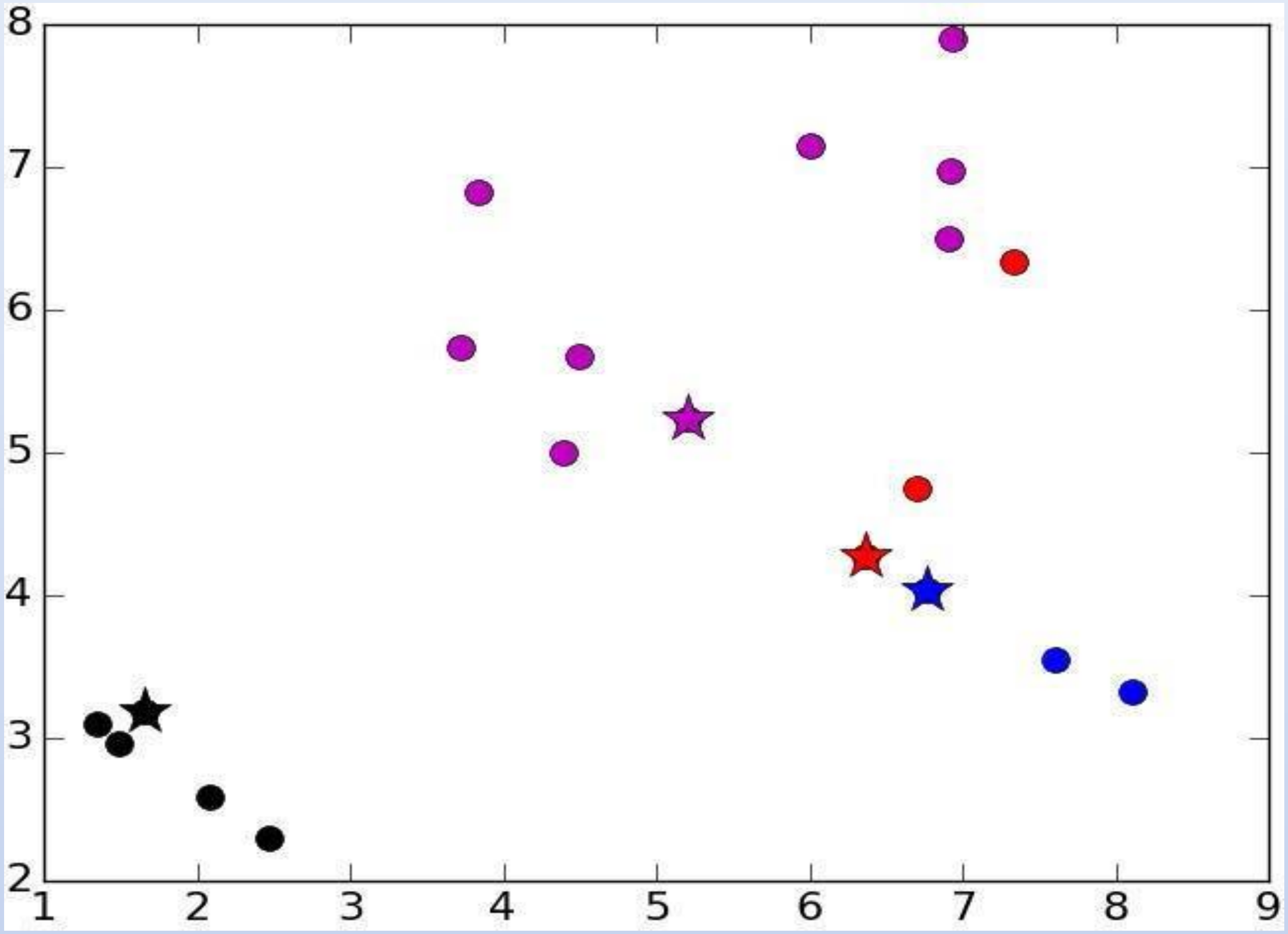
What is complexity of one iteration?

k*n*d, where n is number of points and d time required to compute the distance between a pair of points

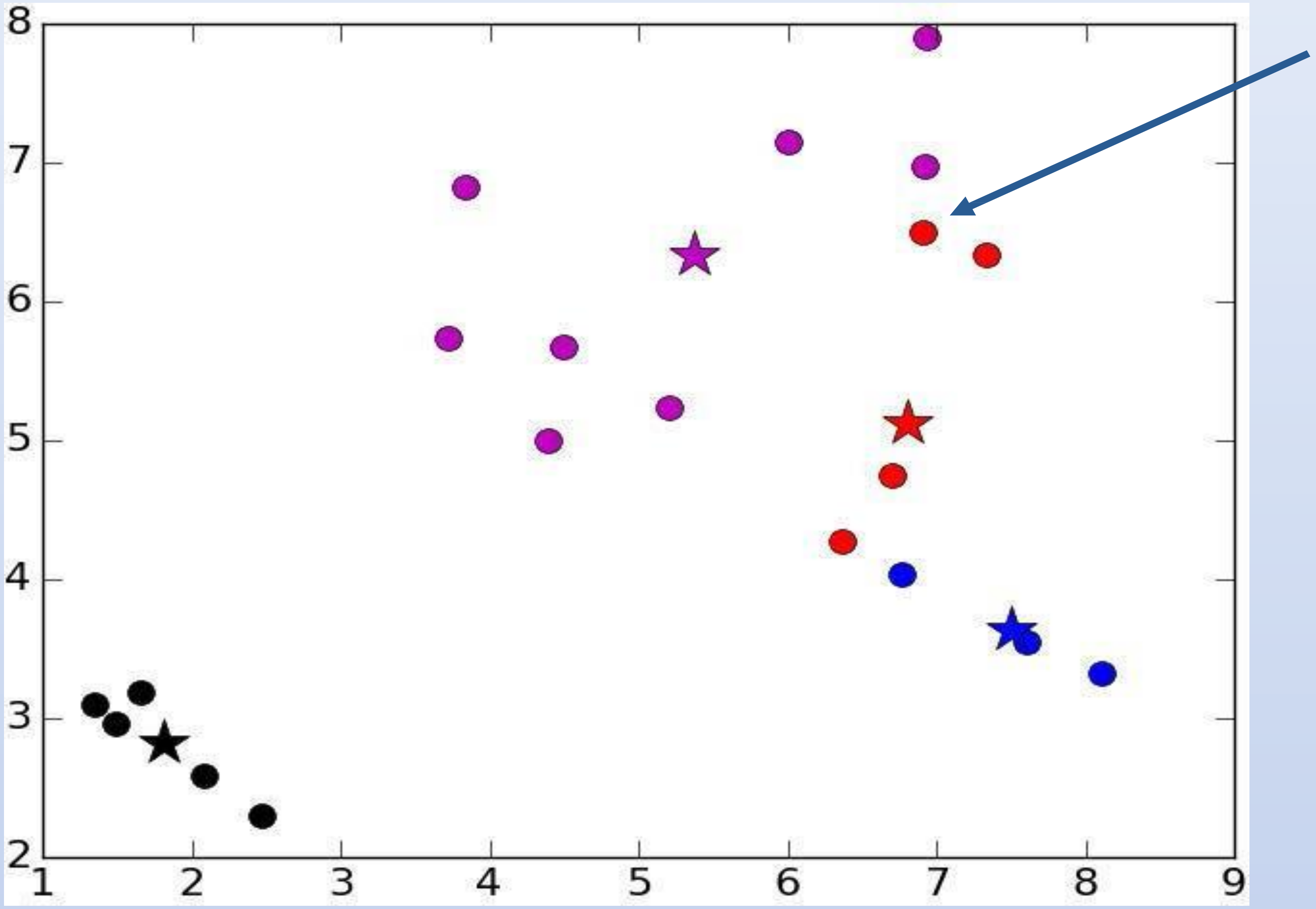
An Example



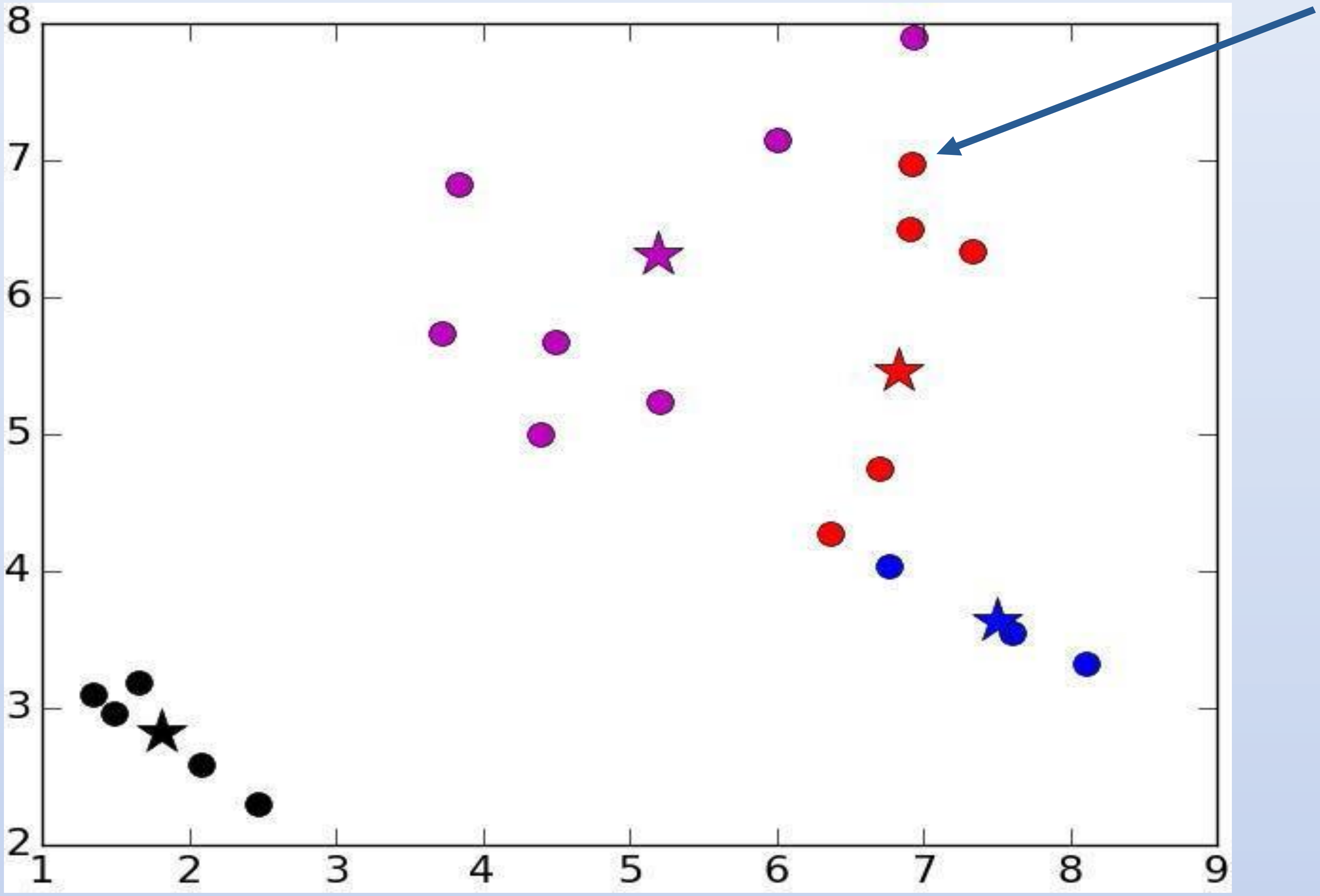
K = 4, Initial Centroids



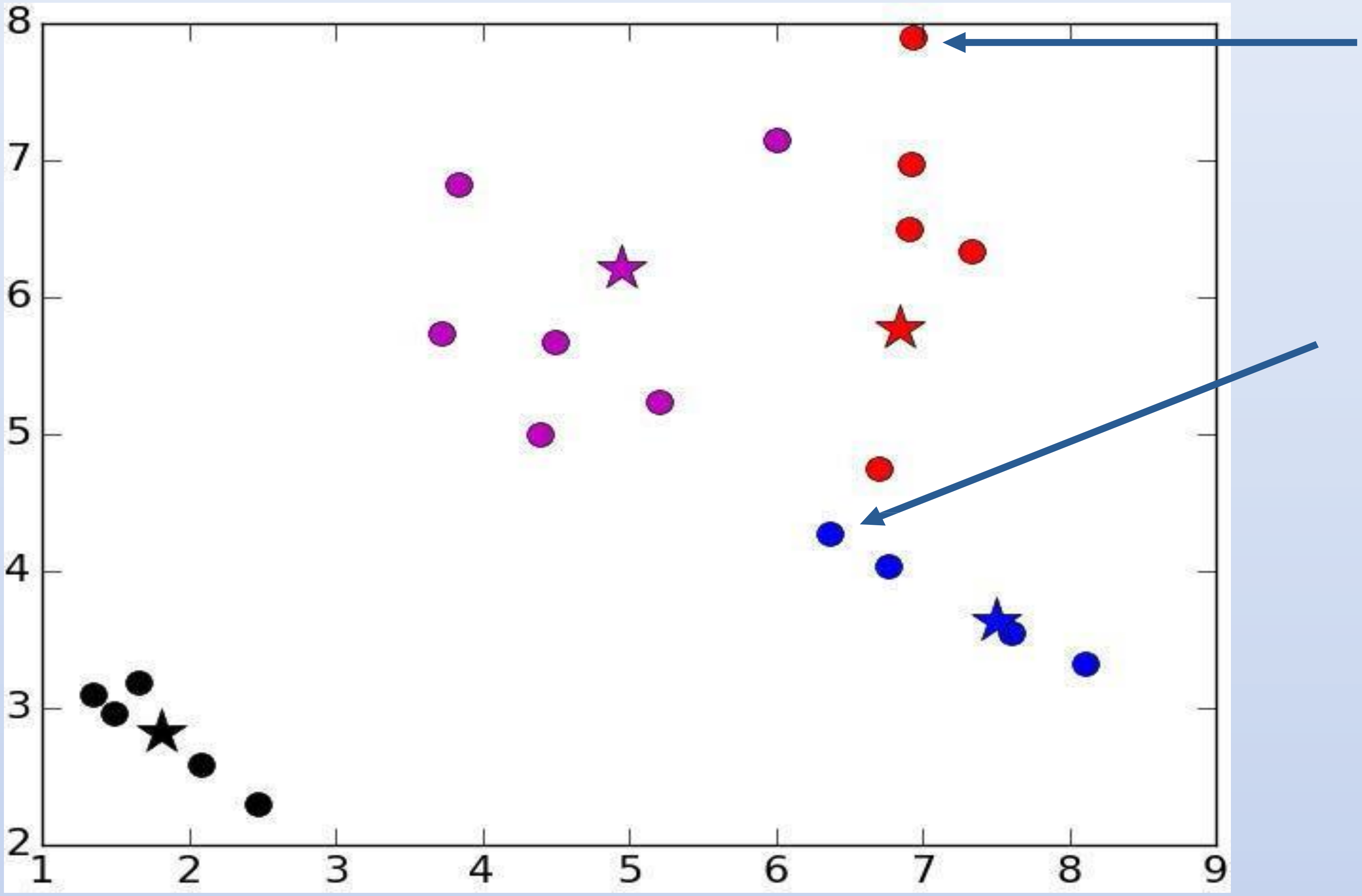
Iteration 1



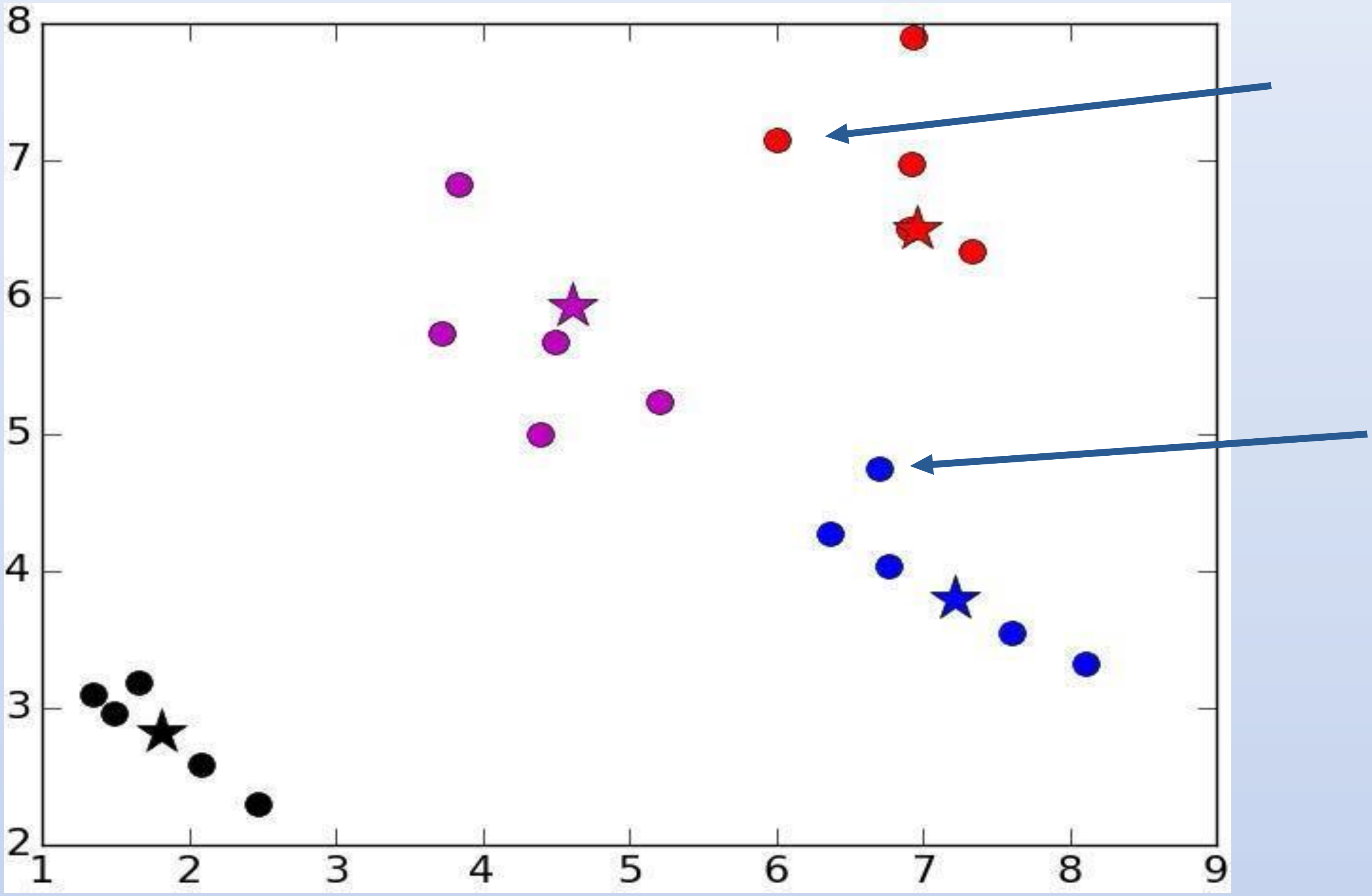
Iteration 2



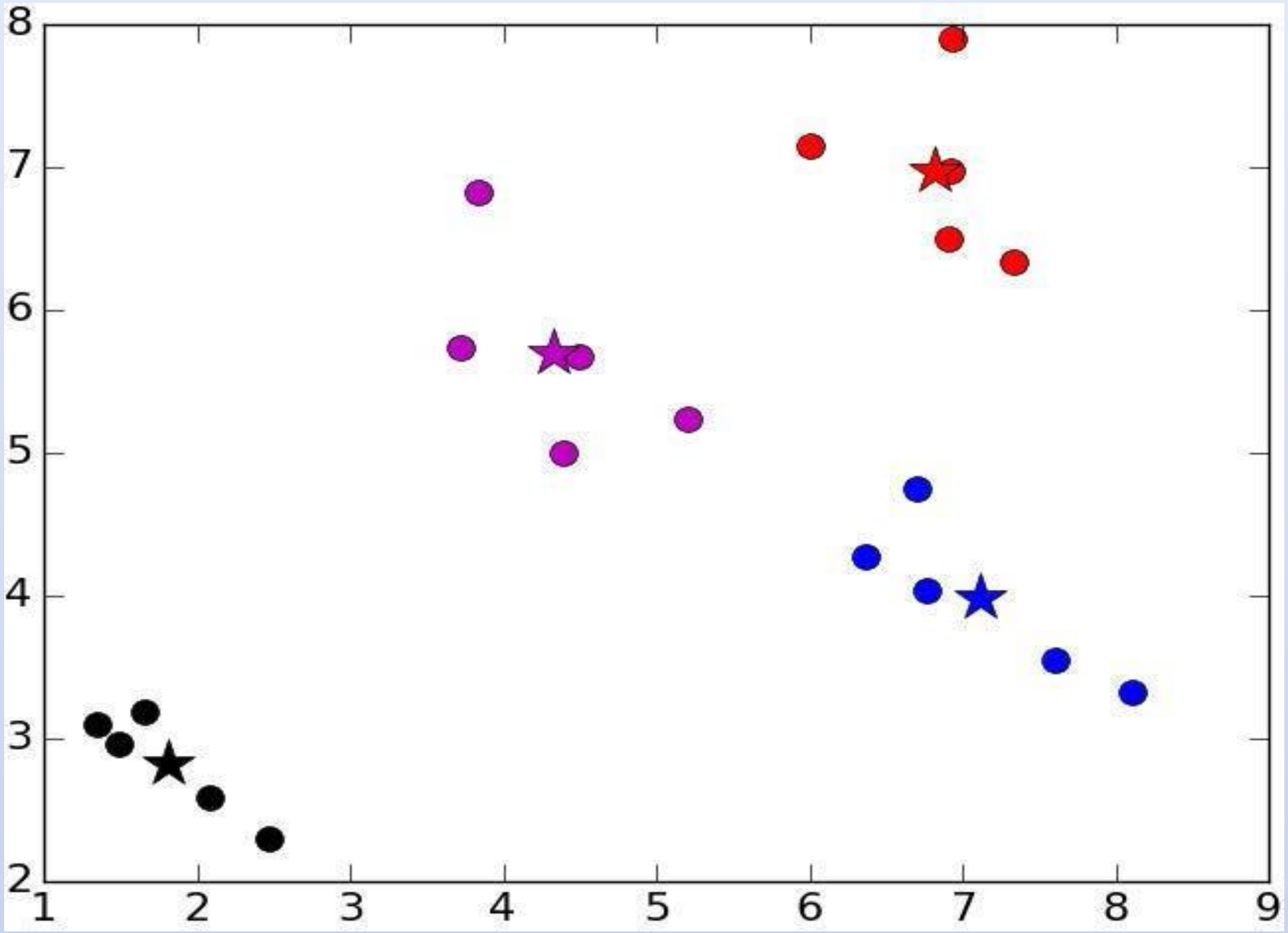
Iteration 3



Iteration 4

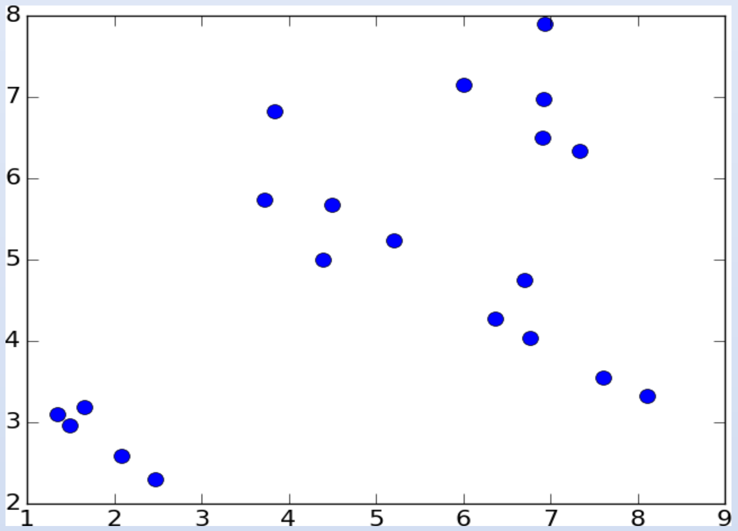


Iteration 5



Issues with k-means

- Choosing the “wrong” k can lead to strange results
  - Consider k = 3

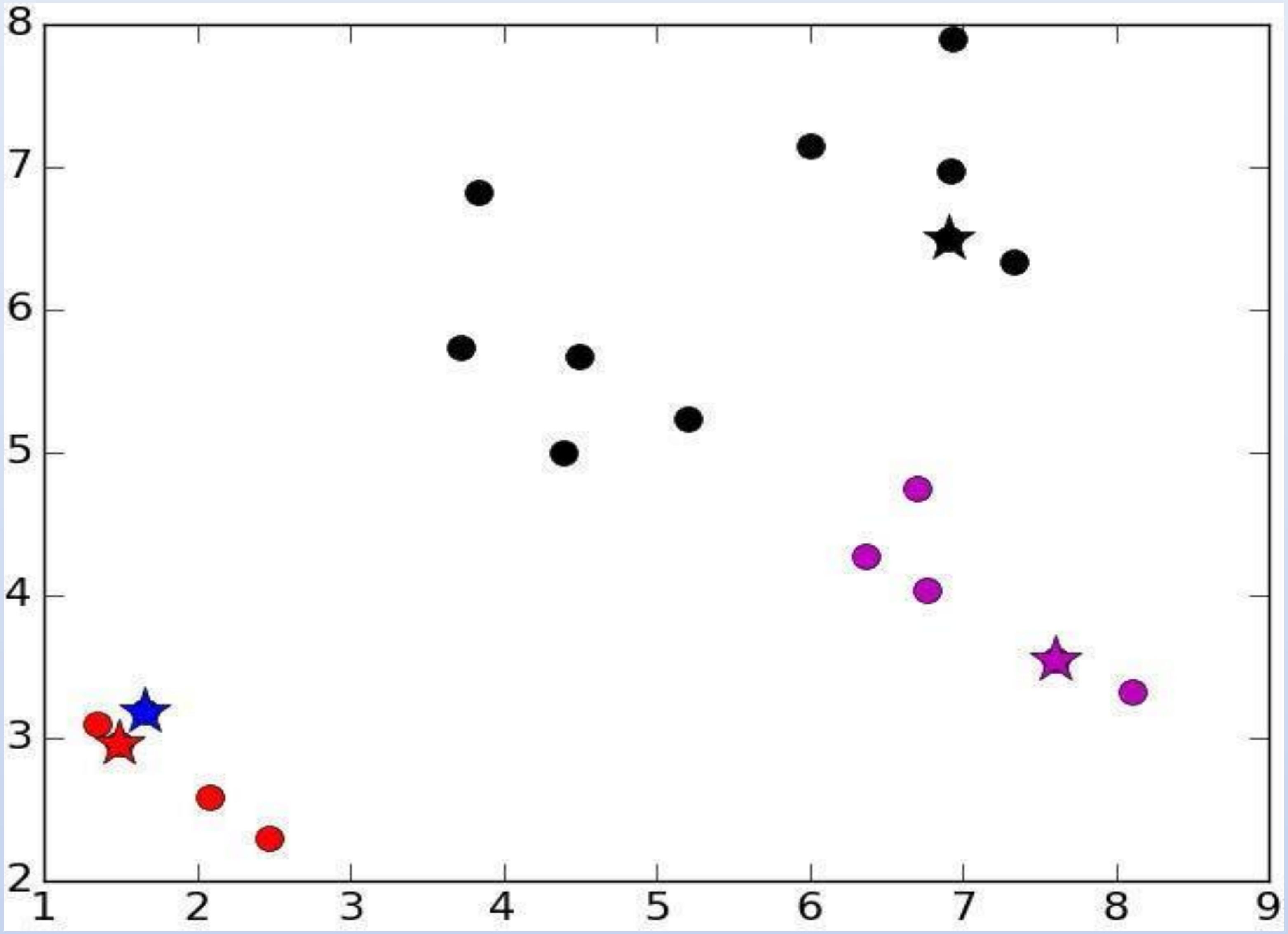


- Result can depend upon initial centroids
  - Number of iterations
  - Even final result
    - Greedy algorithm can find different local optimas

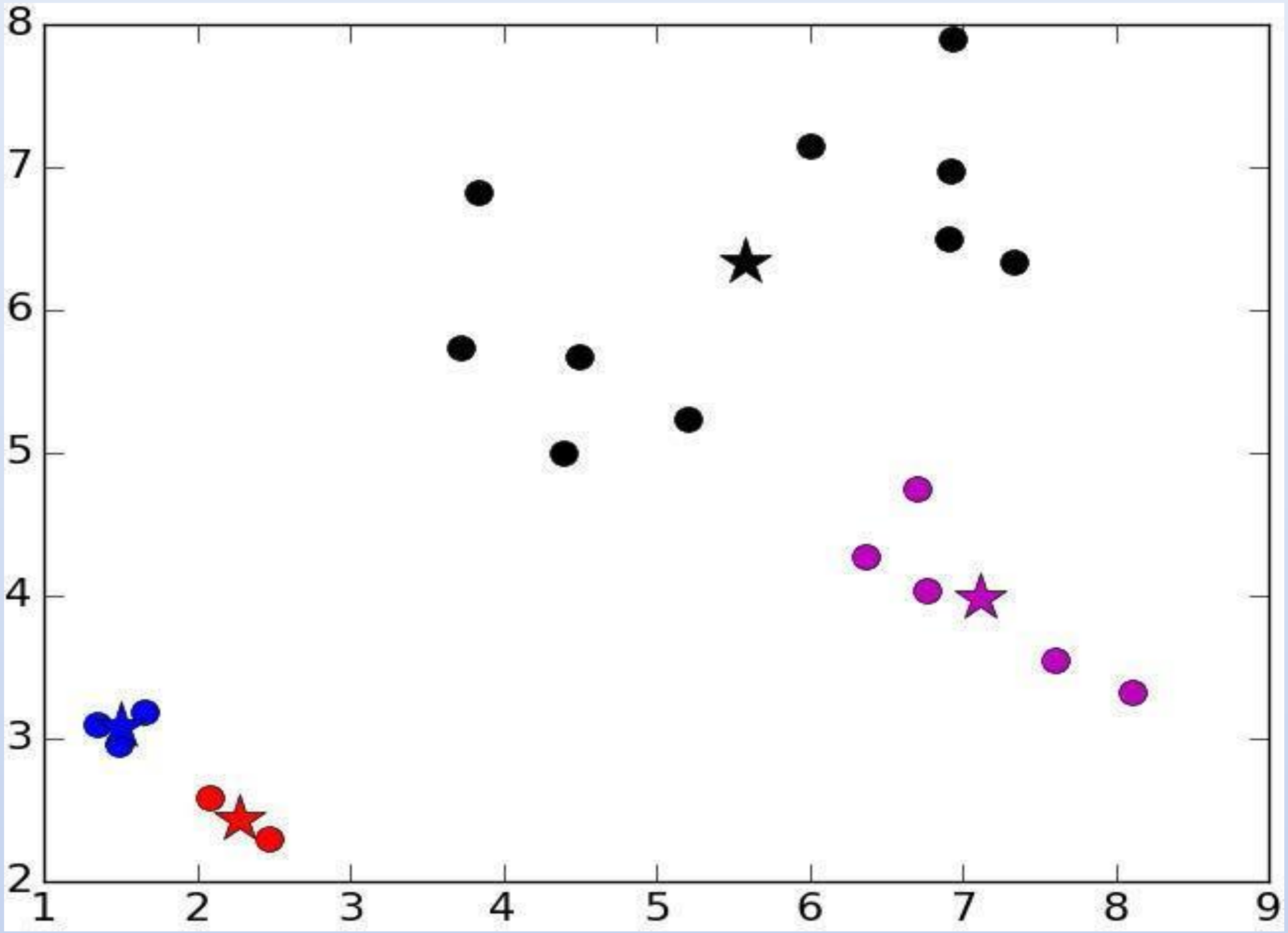
How to Choose K

- *A priori* knowledge about application domain
  - There are two kinds of people in the world: k = 2
  - There are five different types of bacteria: k = 5
- Search for a good k
  - Try different values of k and evaluate quality of results
  - Run hierarchical clustering on subset of data

Unlucky Initial Centroids



Converges On



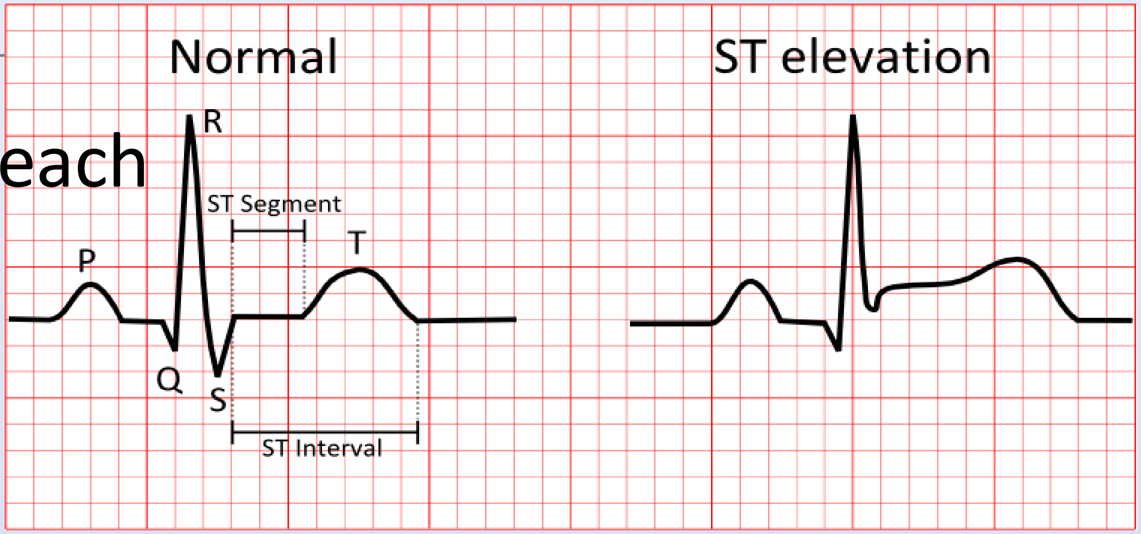
Mitigating Dependence on Initial Centroids

Try multiple sets of randomly chosen initial centroids

Select “best” result

```
best = kMeans(points)
for t in range(numTrials):
    C = kMeans(points)
    if dissimilarity(C) < dissimilarity(best):
        best = C
return best
```

An Example

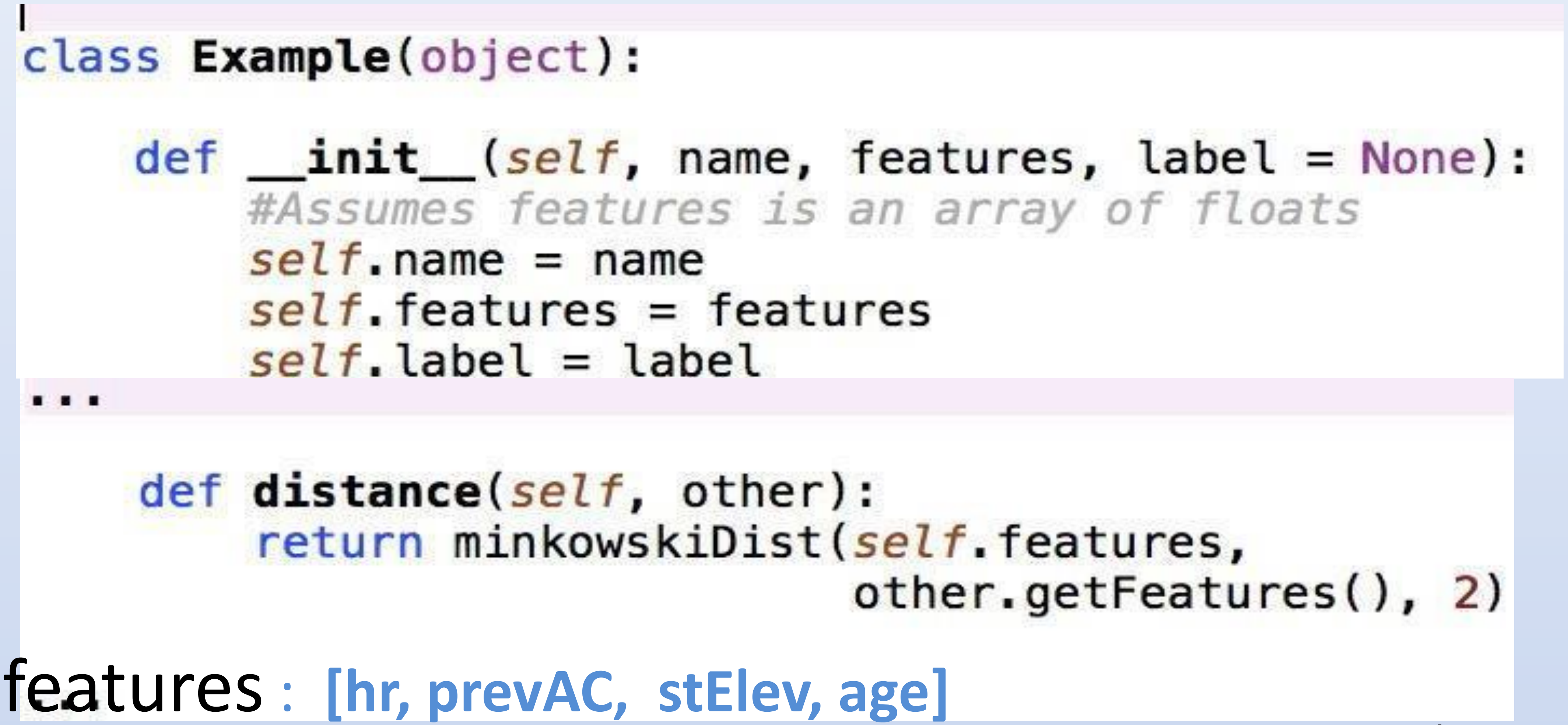


- Many patients with 4 features each
  - Heart rate in beats per minute
  - Number of past heart attacks
  - Age
  - ST elevation (binary)
- Outcome (death) based on features
  - Probabilistic, not deterministic
  - E.g., older people with multiple heart attacks at higher risk
- Cluster, and examine purity of clusters relative to outcomes

Data Sample

```
                HR      Att     STE     Age     Outcome

P000: [ 89.       1.      0.     66.]   :   1
P001: [ 59.       0.      0.     72.]   :   0
P002: [ 73.       0.      0.     73.]   :   0
P003: [ 56.       1.      0.     65.]   :   0
P004: [ 75.       1.      1.     68.]   :   1
P005: [ 68.       1.      0.     56.]   :   0
P006: [ 73.       1.      0.     75.]   :   1
P007: [ 72.       0.      0.     65.]   :   0
P008: [ 73.       1.      0.     64.]   :   1
P009: [ 73.       0.      0.     58.]   :   0
P010: [ 100.      0.      0.     75.]   :   0
P011: [ 79.       0.      0.     31.]   :   0
P012: [ 81.       0.      0.     58.]   :   0
P013: [ 89.       1.      0.     50.]   :   1
P014: [ 81.       0.      0.     70.]   :   0
```

Class Example



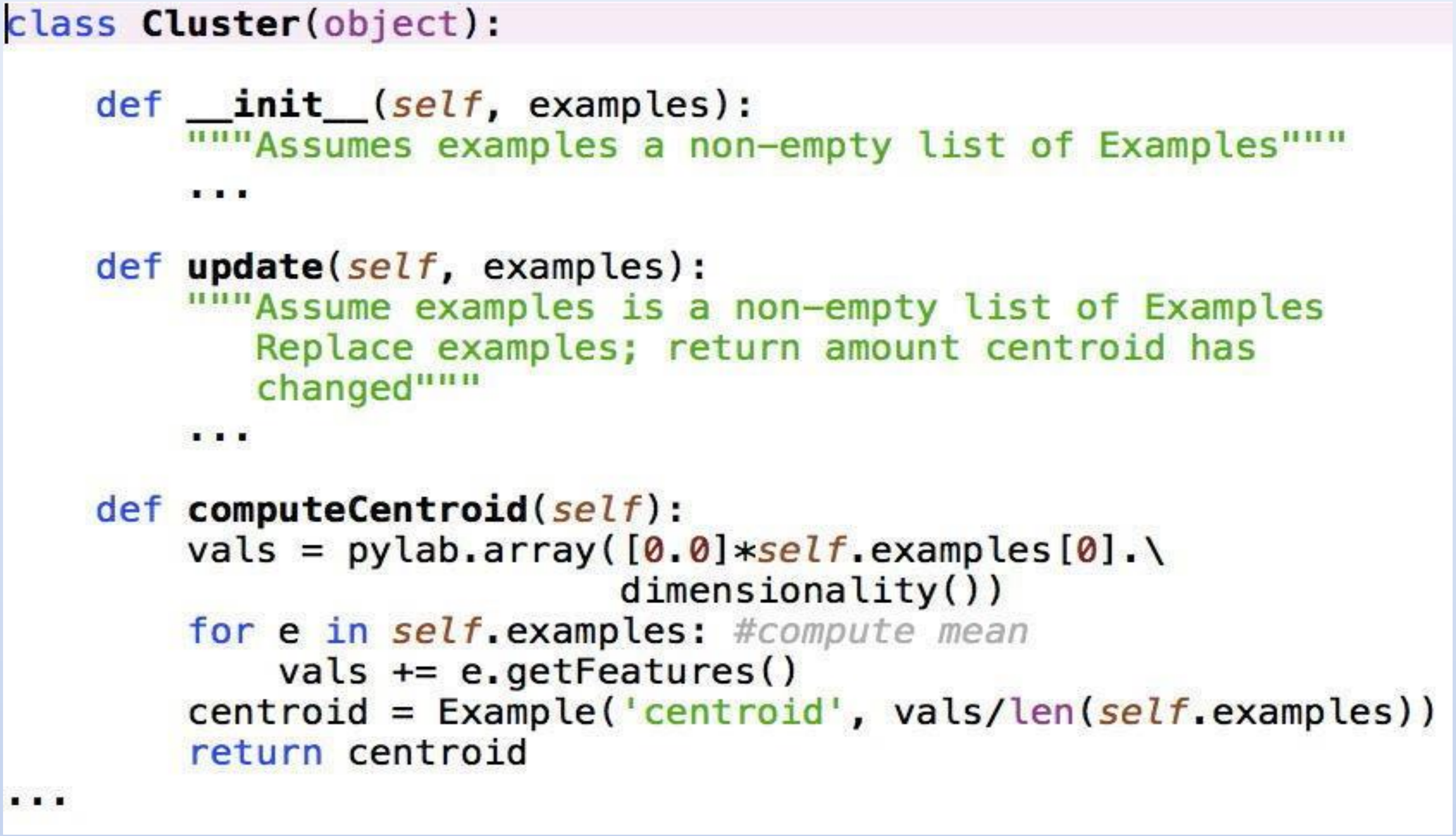
```
class Example(object):

    def __init__(self, name, features, label = None):
        #Assumes features is an array of floats
        self.name = name
        self.features = features
        self.label = label
...

    def distance(self, other):
        return minkowskiDist(self.features,
                             other.getFeatures(), 2)
```

features : **[hr, prevAC, stElev, age]**

Minkowski Distance:

$$Distance(x,y) = \left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p}$$

class Cluster



```
class Cluster(object):

    def __init__(self, examples):
        """Assumes examples a non-empty list of Examples"""
        ...

    def update(self, examples):
        """Assume examples is a non-empty list of Examples
           Replace examples; return amount centroid has
           changed"""
        ...

    def computeCentroid(self):
        vals = pylab.array([0.0]*self.examples[0].\
                           dimensionality())
        for e in self.examples: #compute mean
            vals += e.getFeatures()
        centroid = Example('centroid', vals/len(self.examples))
        return centroid
...
```

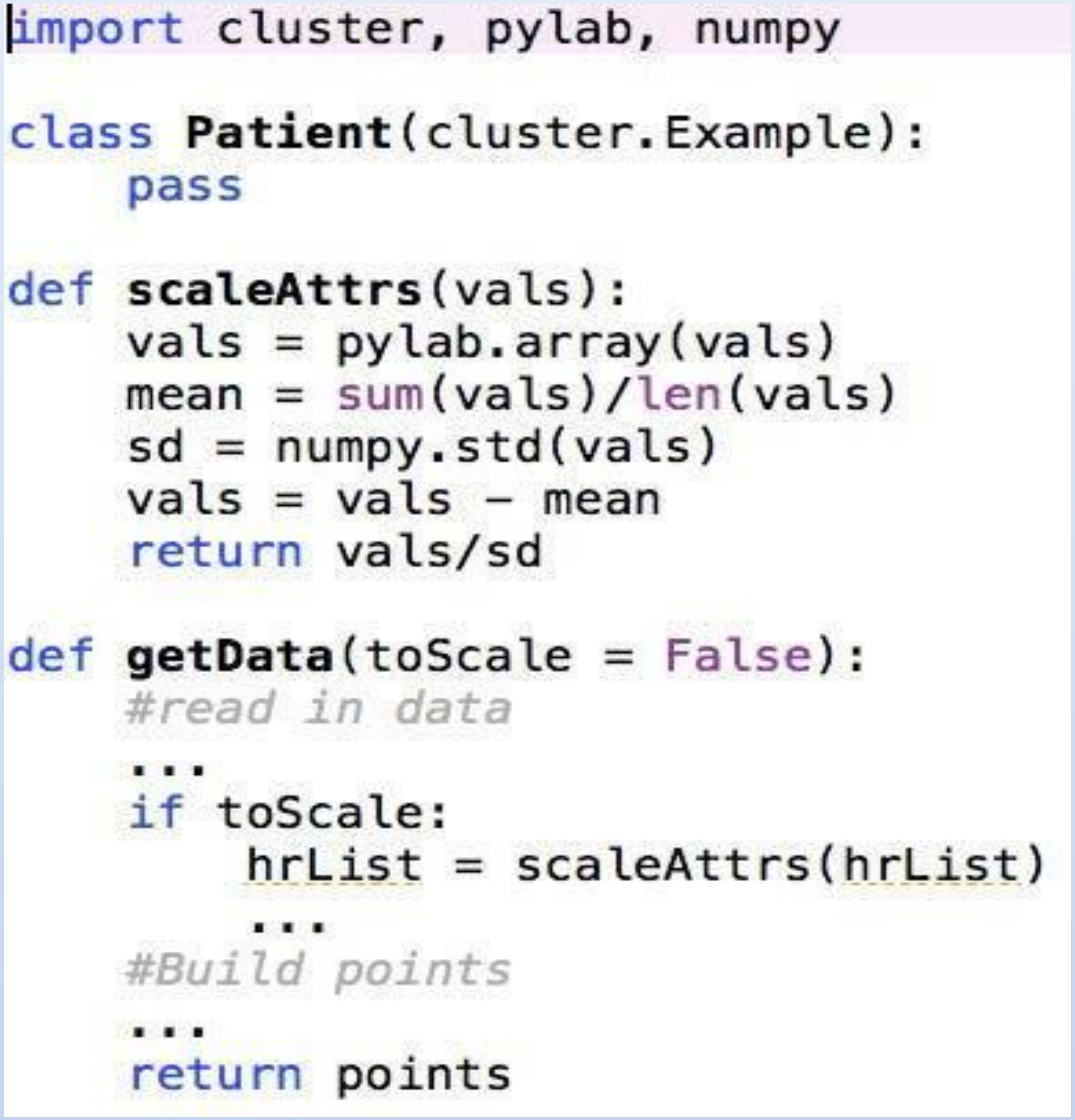
Class Cluster, cont.

```
    def variability(self):
        totDist = 0
        for e in self.examples:
            totDist += (e.distance(self.centroid))**2
        return totDist

    def members(self):
        for e in self.examples:
            yield e
...
```

Evaluating a Clustering

```python
def dissimilarity(clusters):
    """Assumes clusters a list of clusters
       Returns a measure of the total dissimilarity of the
       clusters in the list"""
    totDist = 0
    for c in clusters:
        totDist += c.variability()
    return totDist
```

Patients



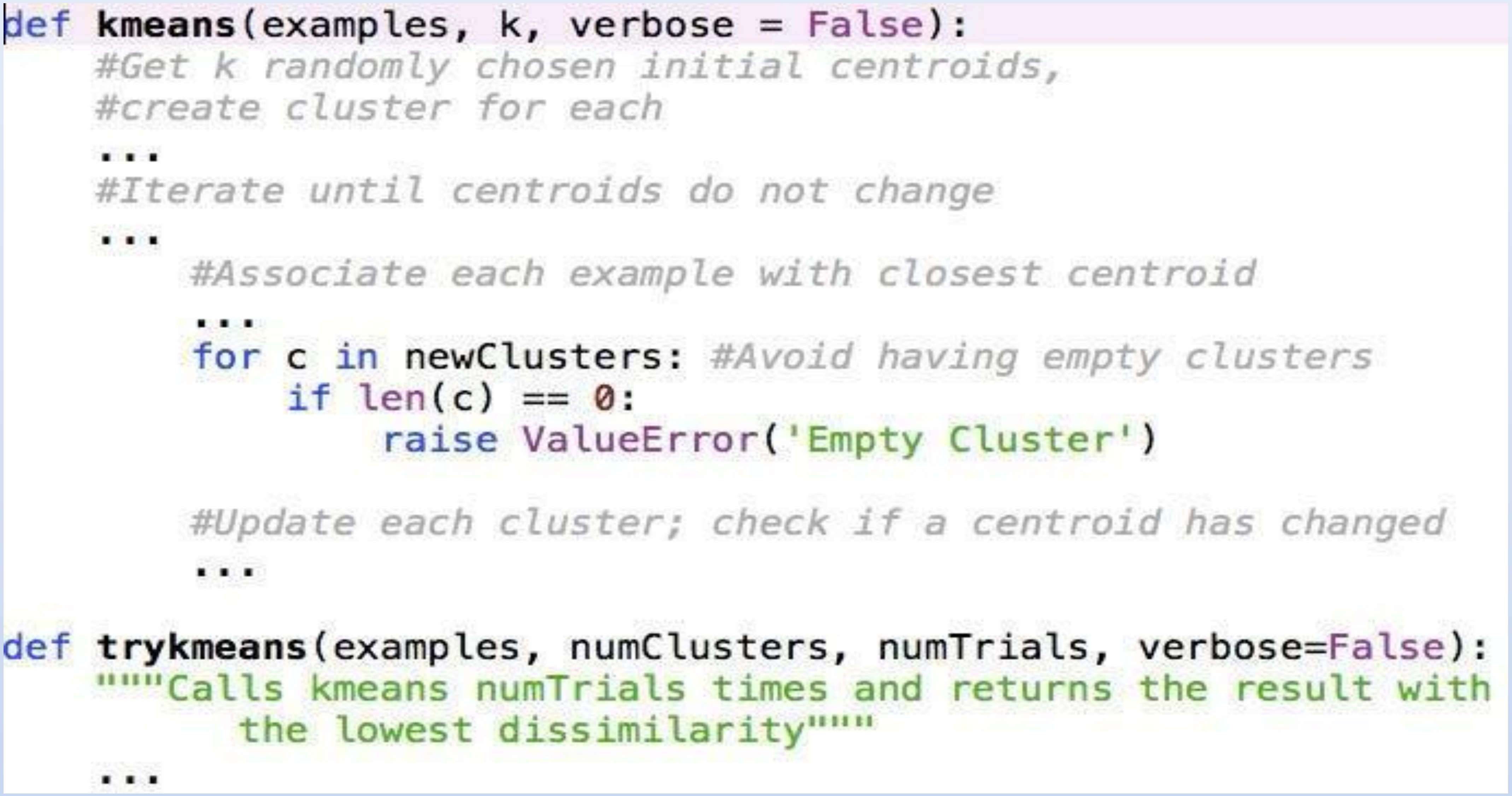
```
import cluster, pylab, numpy

class Patient(cluster.Example):
    pass

def scaleAttrs(vals):
    vals = pylab.array(vals)
    mean = sum(vals)/len(vals)
    sd = numpy.std(vals)
    vals = vals - mean
    return vals/sd

def getData(toScale = False):
    #read in data
    ...
    if toScale:
        hrList = scaleAttrs(hrList)
        ...
    #Build points
    ...
    return points
```

<u>Z-Scaling</u>

Mean = ?

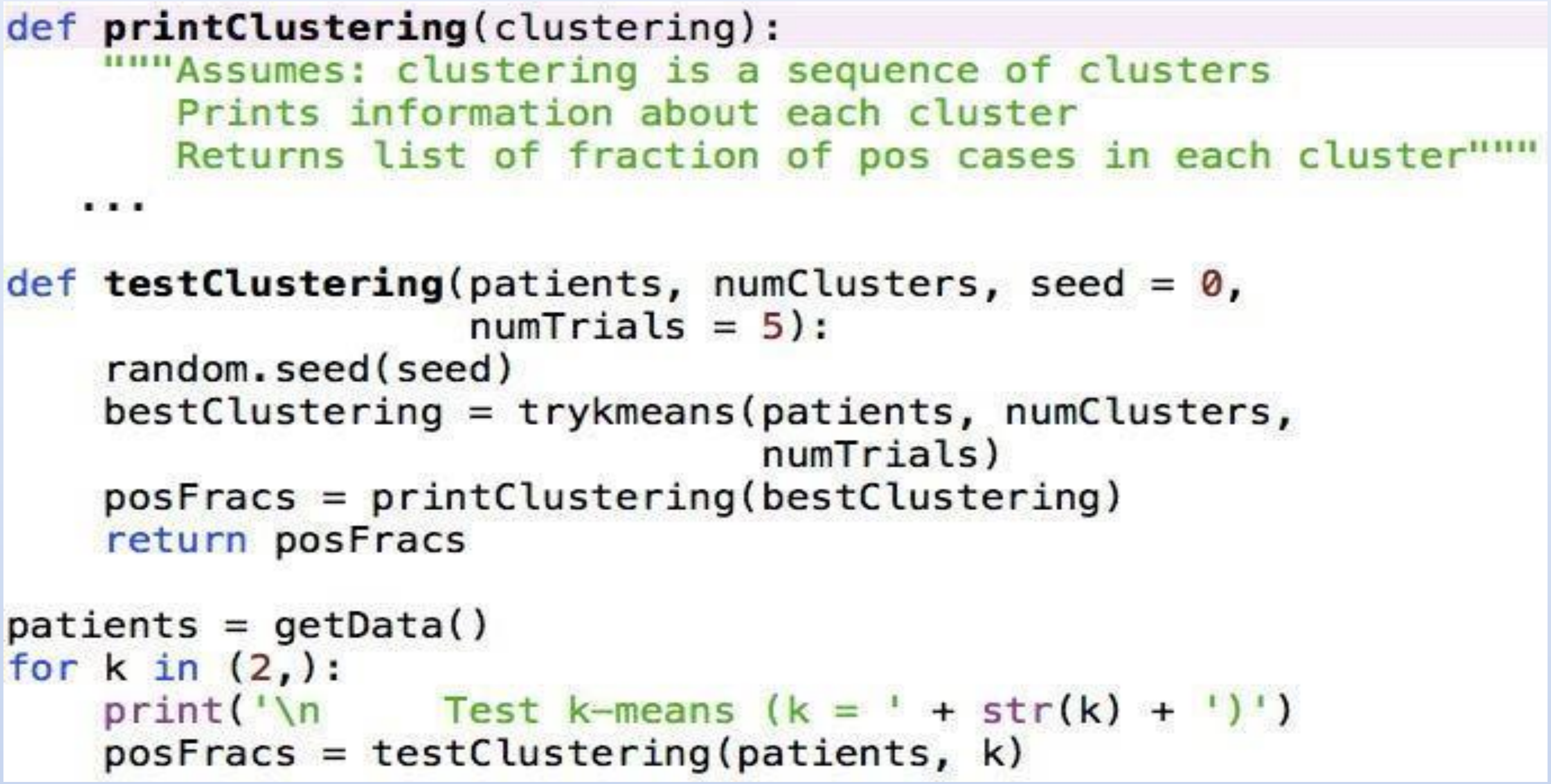
Std = ?

kmeans



```
def kmeans(examples, k, verbose = False):
    #Get k randomly chosen initial centroids,
    #create cluster for each
    ...
    #Iterate until centroids do not change
    ...
        #Associate each example with closest centroid
        ...
        for c in newClusters: #Avoid having empty clusters
            if len(c) == 0:
                raise ValueError('Empty Cluster')

        #Update each cluster; check if a centroid has changed
        ...

def trykmeans(examples, numClusters, numTrials, verbose=False):
    """Calls kmeans numTrials times and returns the result with
         the lowest dissimilarity"""
    ...
```

Examining Results



```
def printClustering(clustering):
    """Assumes: clustering is a sequence of clusters
       Prints information about each cluster
       Returns list of fraction of pos cases in each cluster"""
  ...

def testClustering(patients, numClusters, seed = 0,
                   numTrials = 5):
    random.seed(seed)
    bestClustering = trykmeans(patients, numClusters,
                               numTrials)
    posFracs = printClustering(bestClustering)
    return posFracs

patients = getData()
for k in (2,):
    print('\n     Test k-means (k = ' + str(k) + ')')
    posFracs = testClustering(patients, k)
```

Result of Running It

- ✓ Try patients = getData( )

```
Test k-means (k = 2)
Cluster of size 118 with fraction of positives = 0.3305
Cluster of size 132 with fraction of positives = 0.3333
```

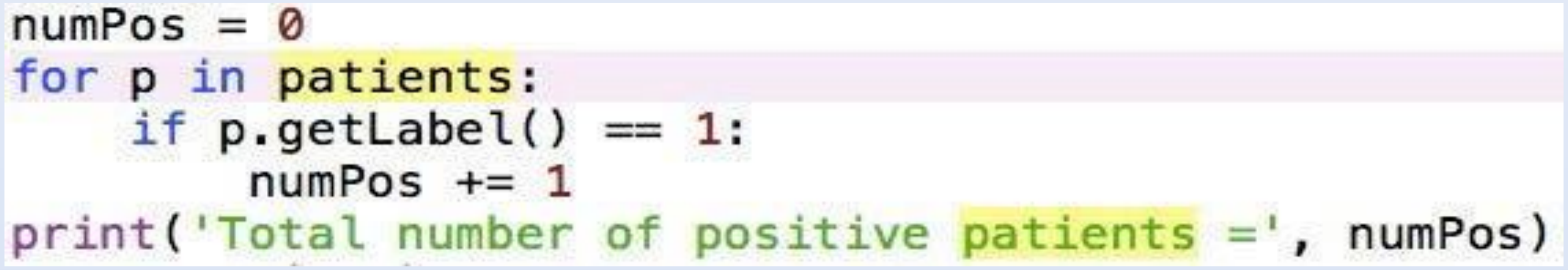
Like it?

- ✓ Try patients = getData(True)

```
Test k-means (k = 2)
Cluster of size 224 with fraction of positives = 0.2902
Cluster of size 26 with fraction of positives = 0.6923
```

Happy with sensitivity?

How Many Positives Are There?



```python
numPos = 0
for p in patients:
    if p.getLabel() == 1:
        numPos += 1
print('Total number of positive patients =', numPos)
```

Total number of positive patients = 83

Test k-means (k = 2)

Cluster of size 224 with fraction of positives = 0.2902

(Positive , 0.2902*224=65)

Cluster of size 26 with fraction of positives = 0.6923

(Positive, 0.6923*26=18)

A Hypothesis

- Different subgroups of positive patients have different characteristics
- How might we test this?
- Try some other values of k

True

```
patients = getData()
for k in (2,4,6):
    print('\n     Test k-means (k = ' + str(k) + ')')
    posFracs = testClustering(patients, k, 2)
```

Testing Multiple Values of k

```
 Test k-means (k = 2)
Cluster of size 224 with fraction of positives = 0.2902
Cluster of size 26 with fraction of positives = 0.6923
     Test k-means (k = 4)
Cluster of size 26 with fraction of positives = 0.6923
Cluster of size 86 with fraction of positives = 0.0814
Cluster of size 76 with fraction of positives = 0.7105
Cluster of size 62 with fraction of positives = 0.0645
     Test k-means (k = 6)
Cluster of size 49 with fraction of positives = 0.0204
Cluster of size 26 with fraction of positives = 0.6923
Cluster of size 45 with fraction of positives = 0.0889
Cluster of size 54 with fraction of positives = 0.0926
Cluster of size 36 with fraction of positives = 0.7778
Cluster of size 40 with fraction of positives = 0.675
```

Pick a k, Which?

Homework, DIY

1. Self-learning pylab, numpy

   Demo_Pylab.py

2. Read the lect12.py and cluster.py

   comment the main code

   Prepare for the project

Project will be assigned next week

Next week's test: lect11, 12