Lecture 11: Clustering

(download slides and .py files from Stellar to follow along)

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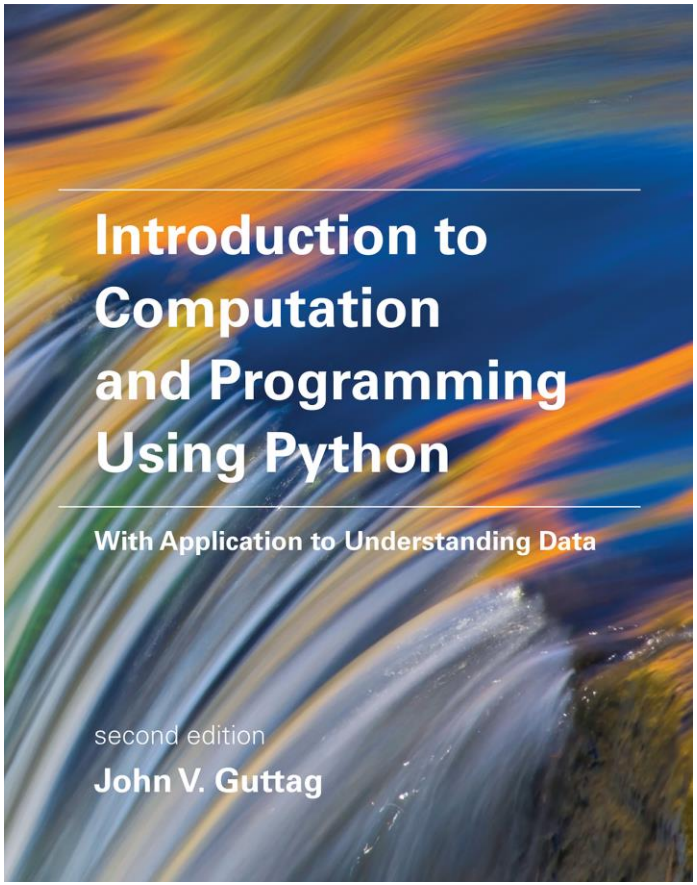
Relevant Reading

- Chapter 23



Subject Evaluations Now Open

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Both MIT and cross-registered students should be able to supply evaluations

Machine Learning Paradigm (review)

- 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

- Minimize dissimilarity of a set of clusters, e.g.,

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

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

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

Two Popular Methods

- Hierarchical clustering
- K-means clustering

Agglomerative Hierarchical 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.

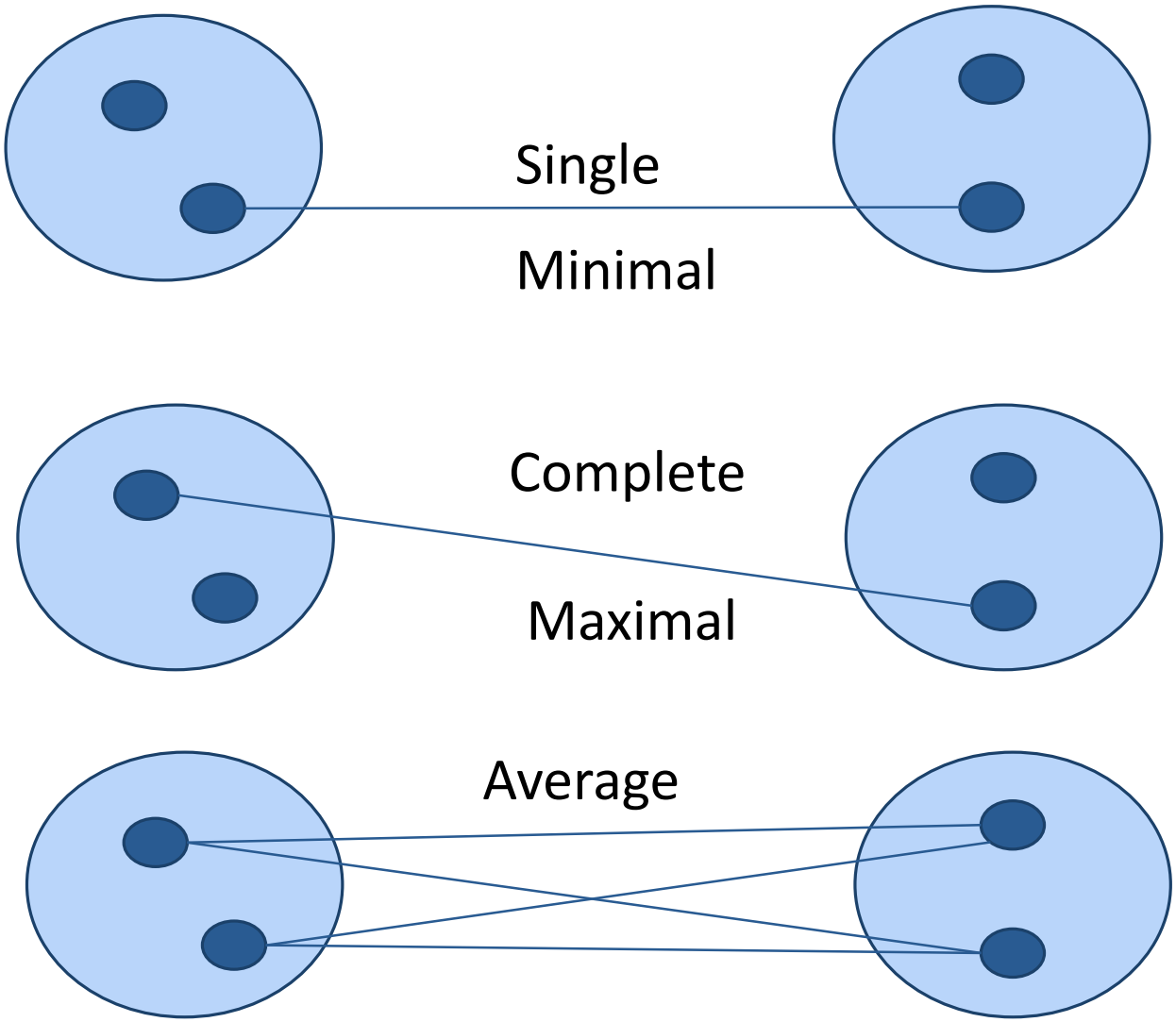
3. Continue the process until all items are clustered into a single cluster of size N.

What does distance mean?

Linkage Metrics

- S*ingle-linkage:* consider the distance between one cluster and another cluster to be equal to the shortest distance from any member of one cluster to any member of the other cluster
- C*omplete-linkage*: consider the distance between one cluster and another cluster to be equal to the greatest distance from any member of one cluster to any member of the other cluster
- A*verage-linkage:* consider the distance between one cluster and another cluster to be equal to the average distance from any member of one cluster to any member of the other cluster

Linkage Criteria



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

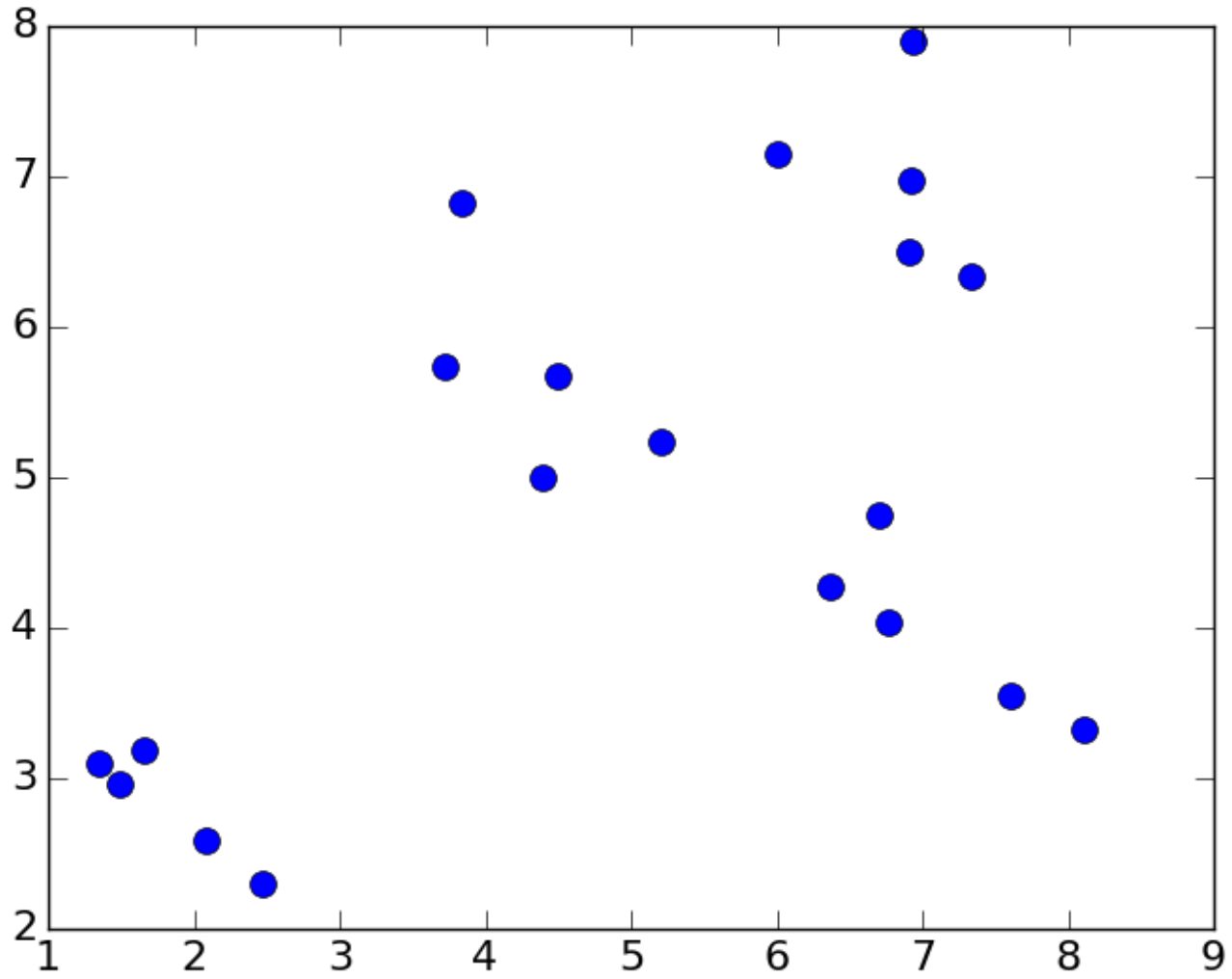
K-means Algorithm

```
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
```

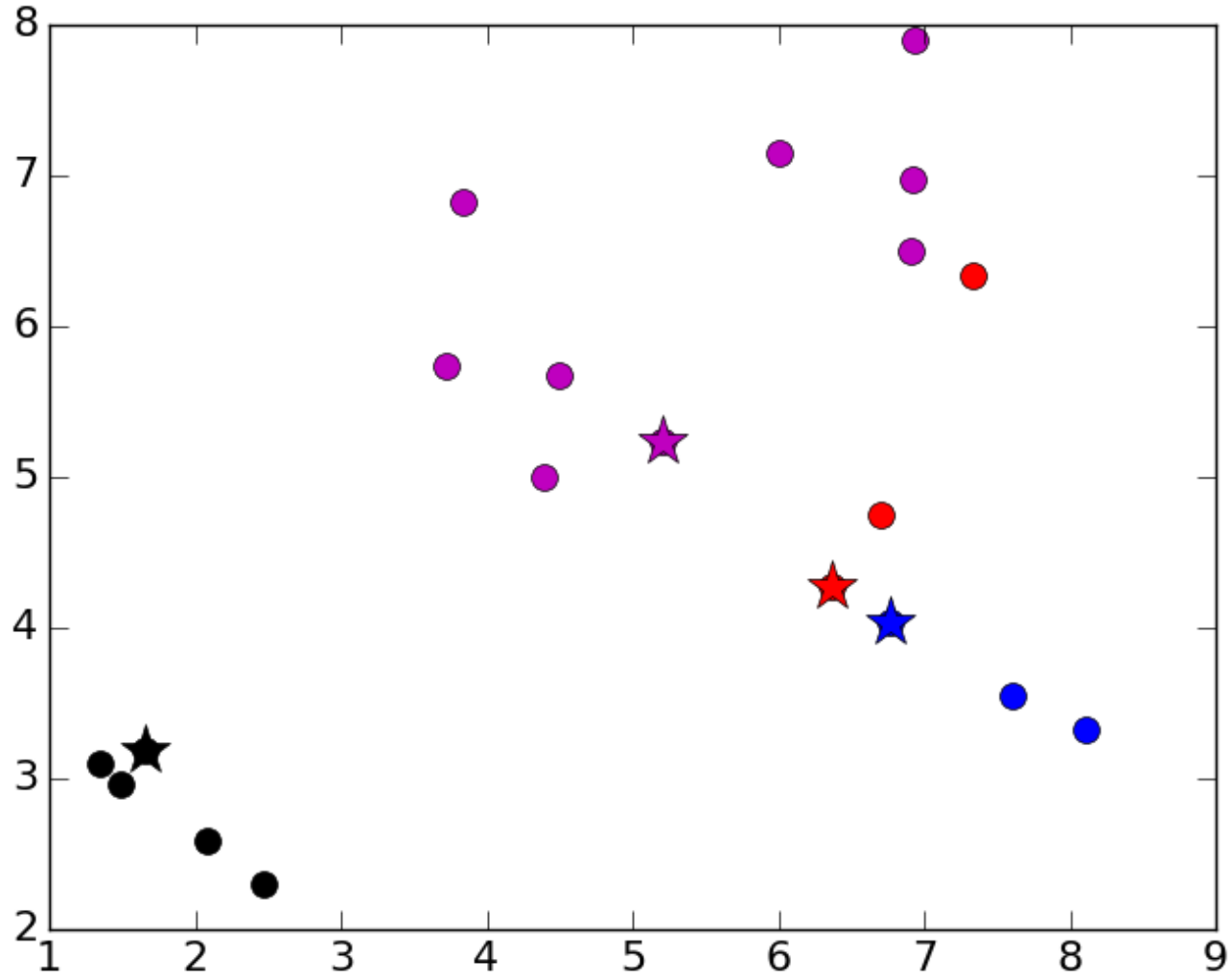
What is complexity of one iteration?

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

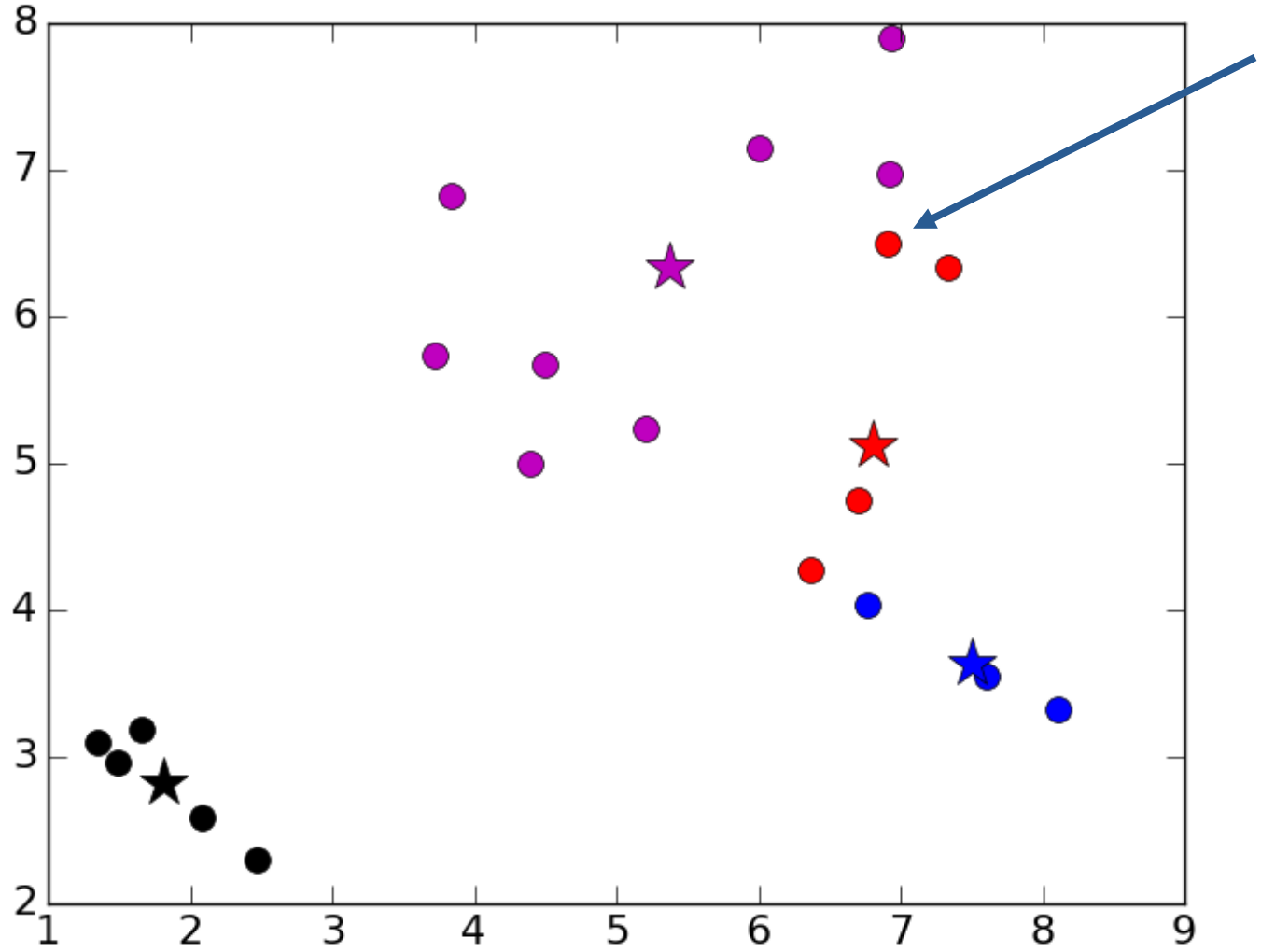
An Example



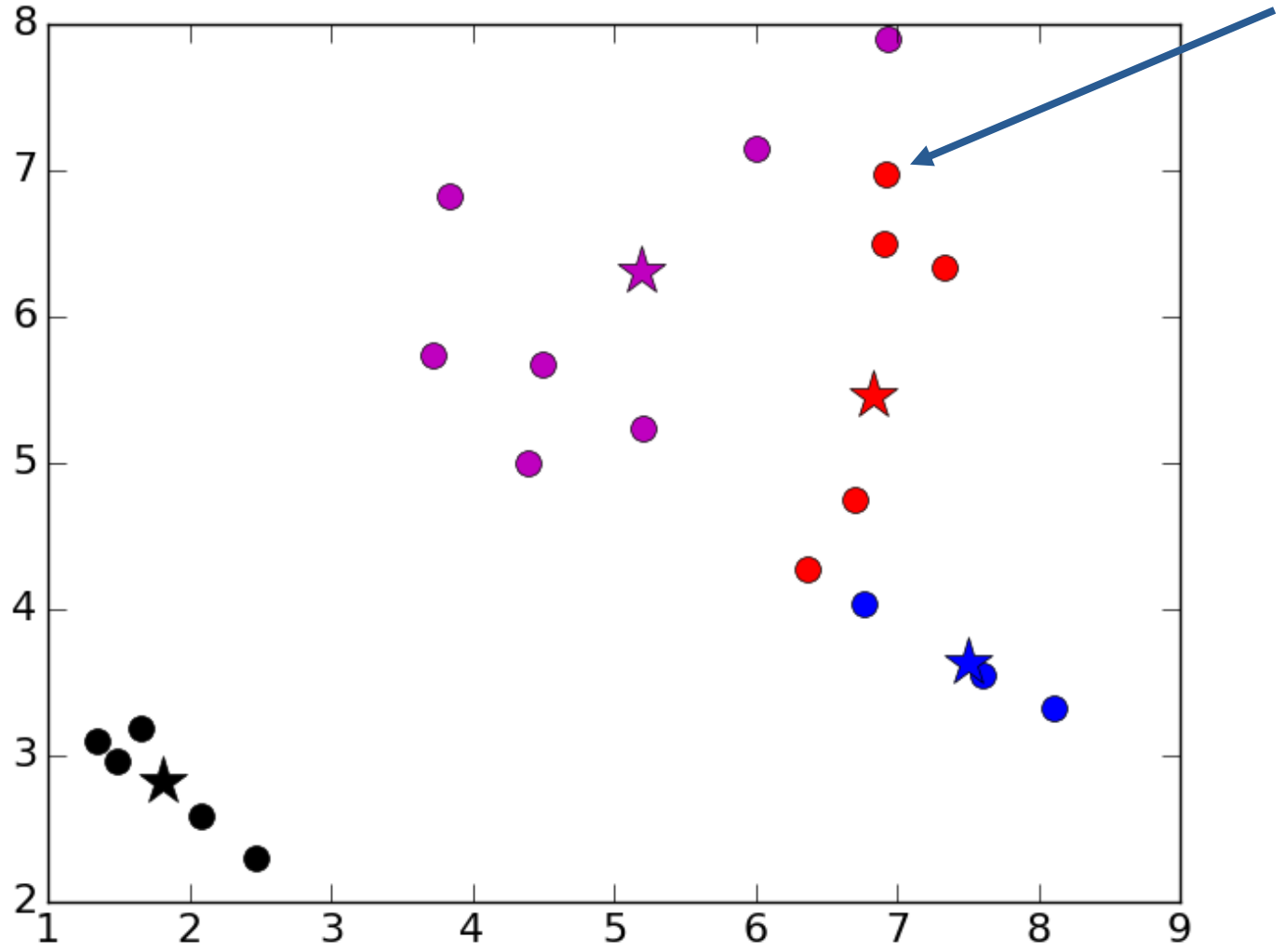
K = 4, Initial Centroids



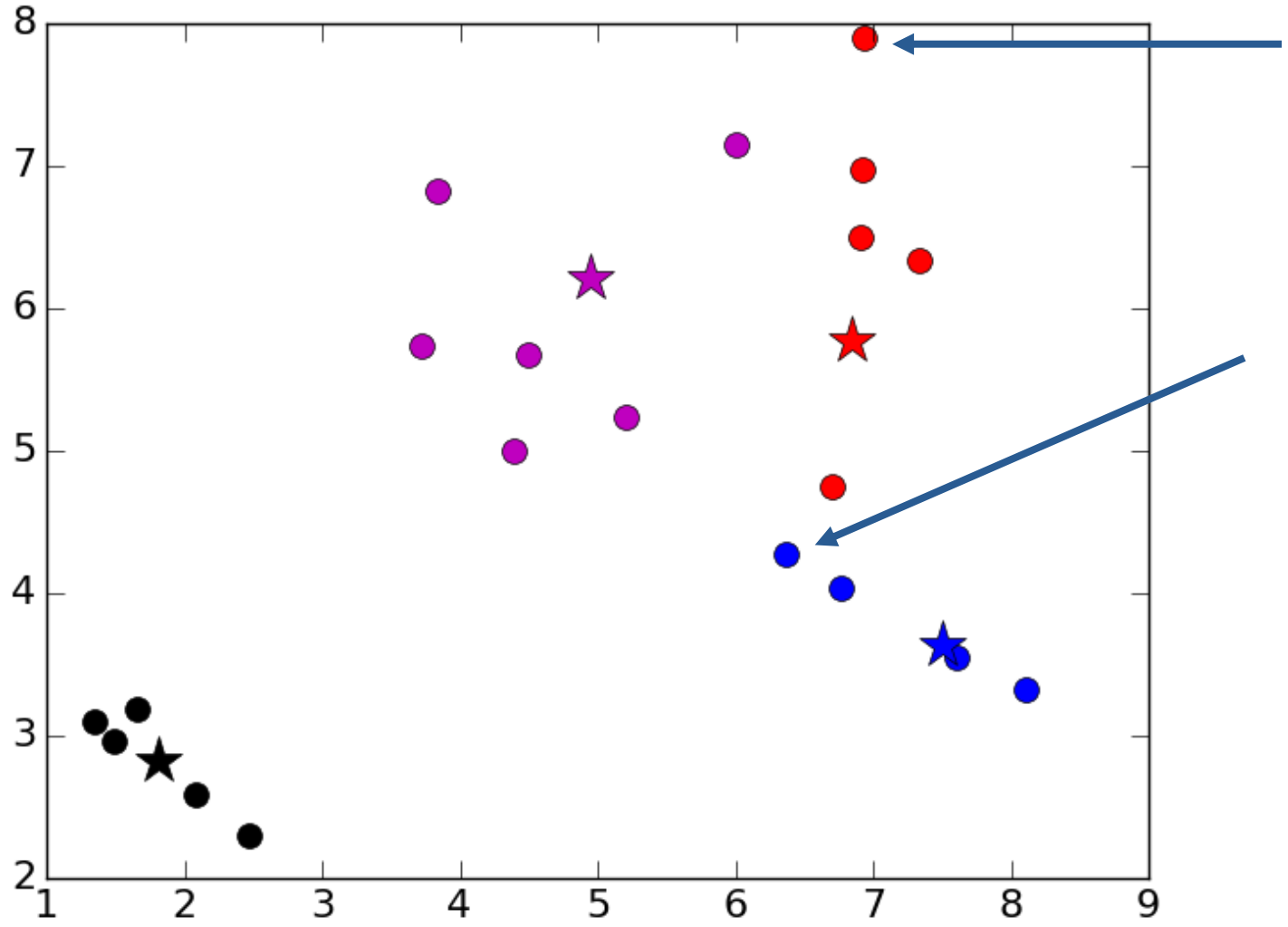
Iteration 1



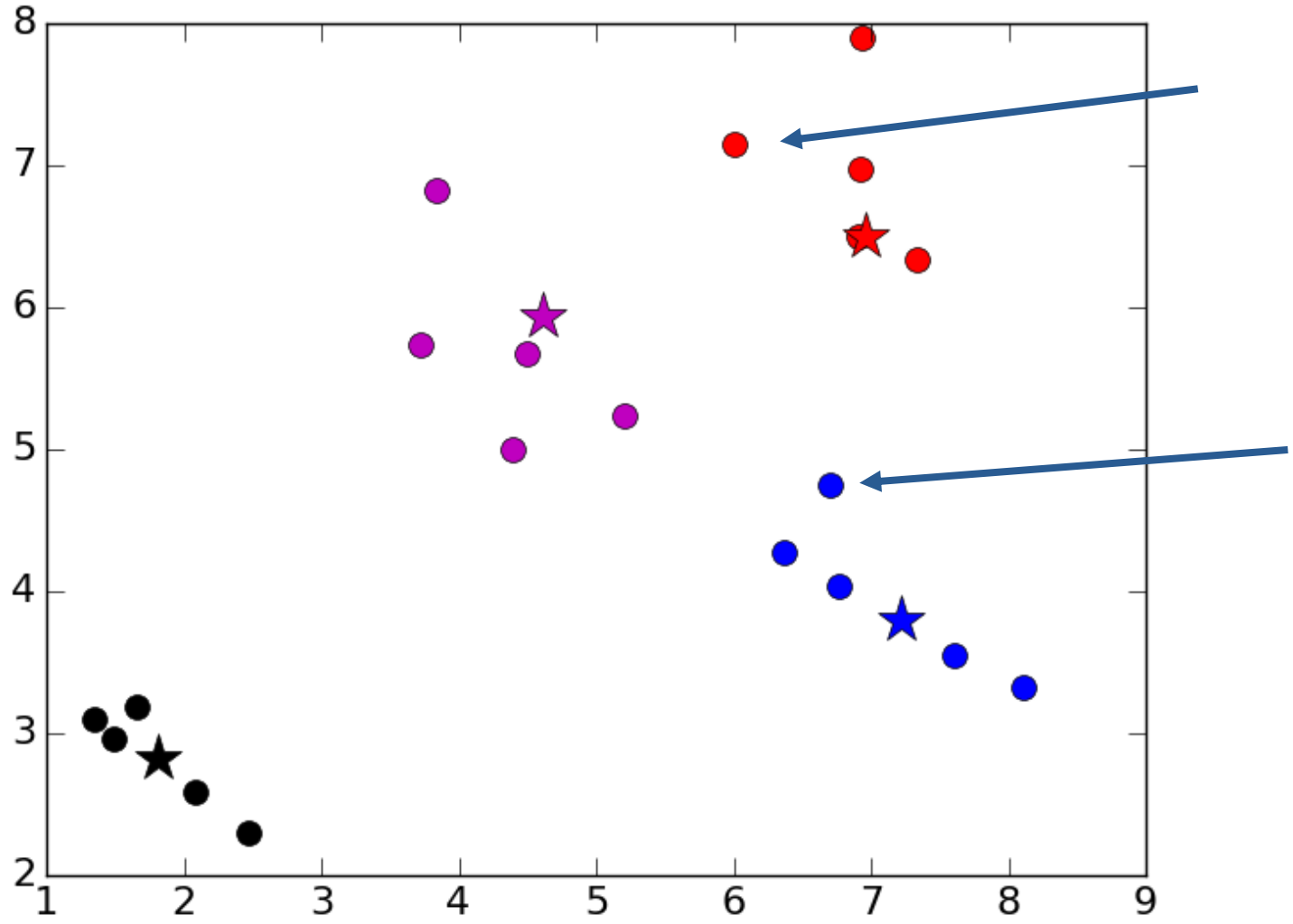
Iteration 2



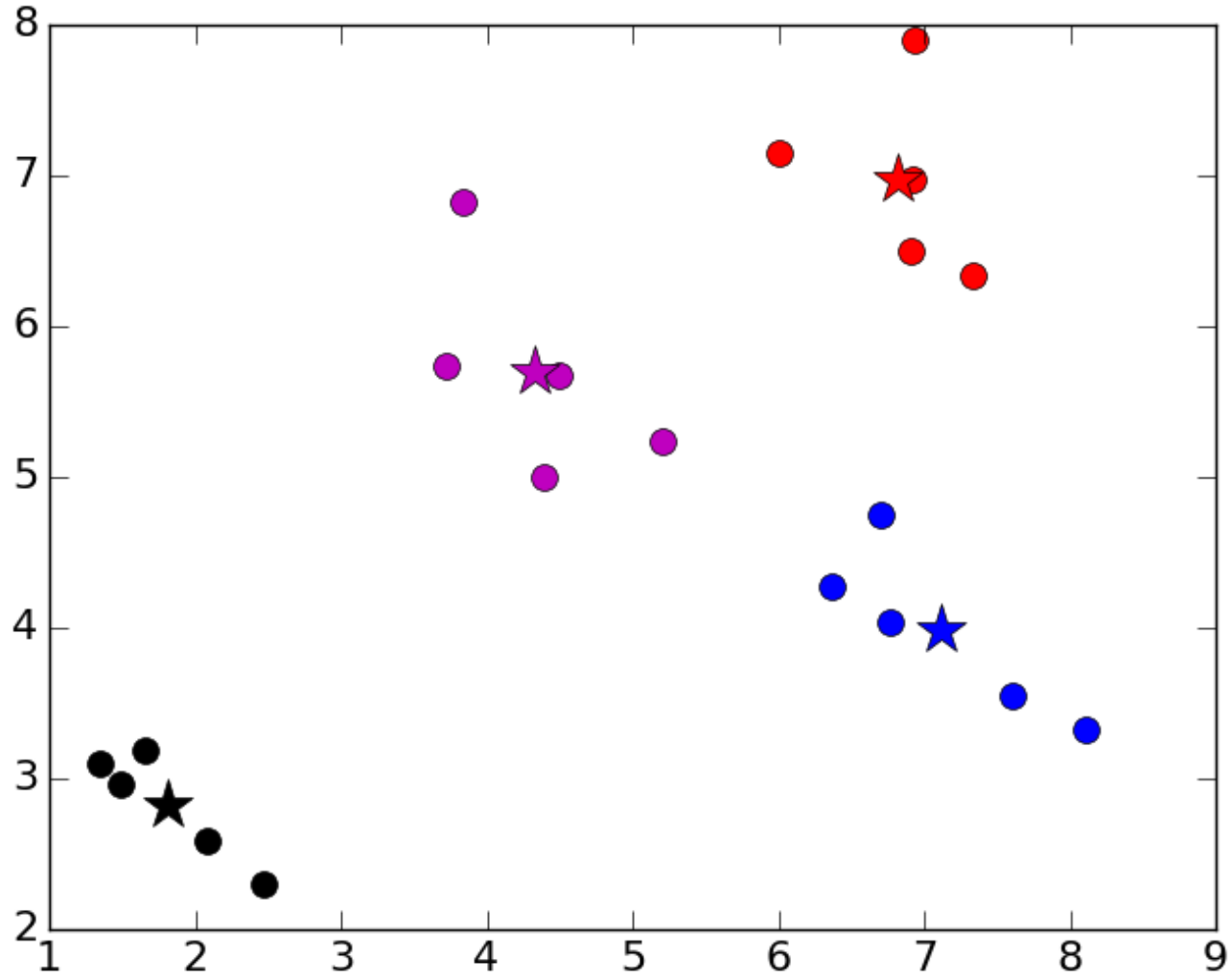
Iteration 3



Iteration 4

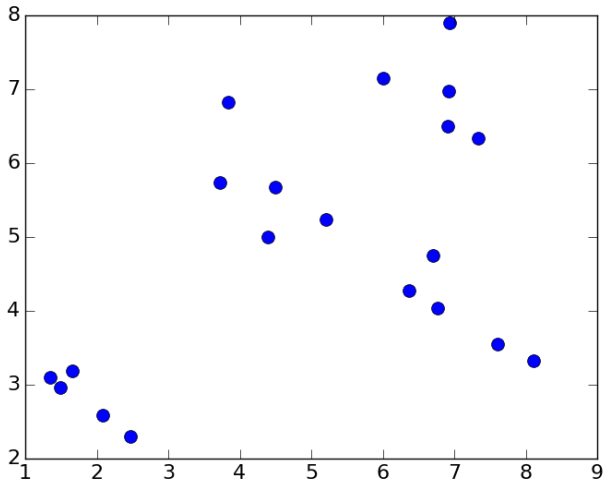


Iteration 5



Issues with k-means

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

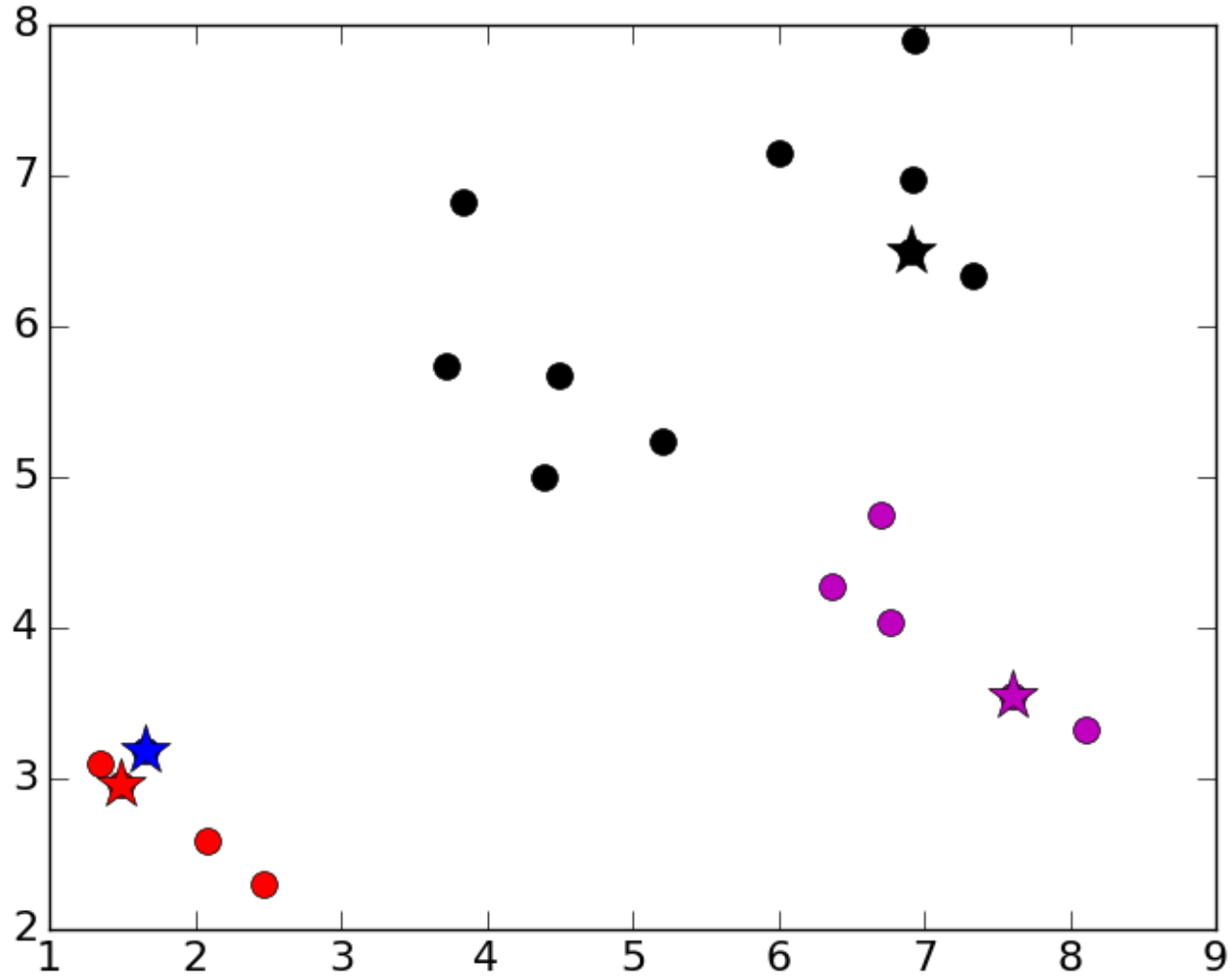


- Result can depend upon initial centroids
  - Number of iterations
  - Even final result

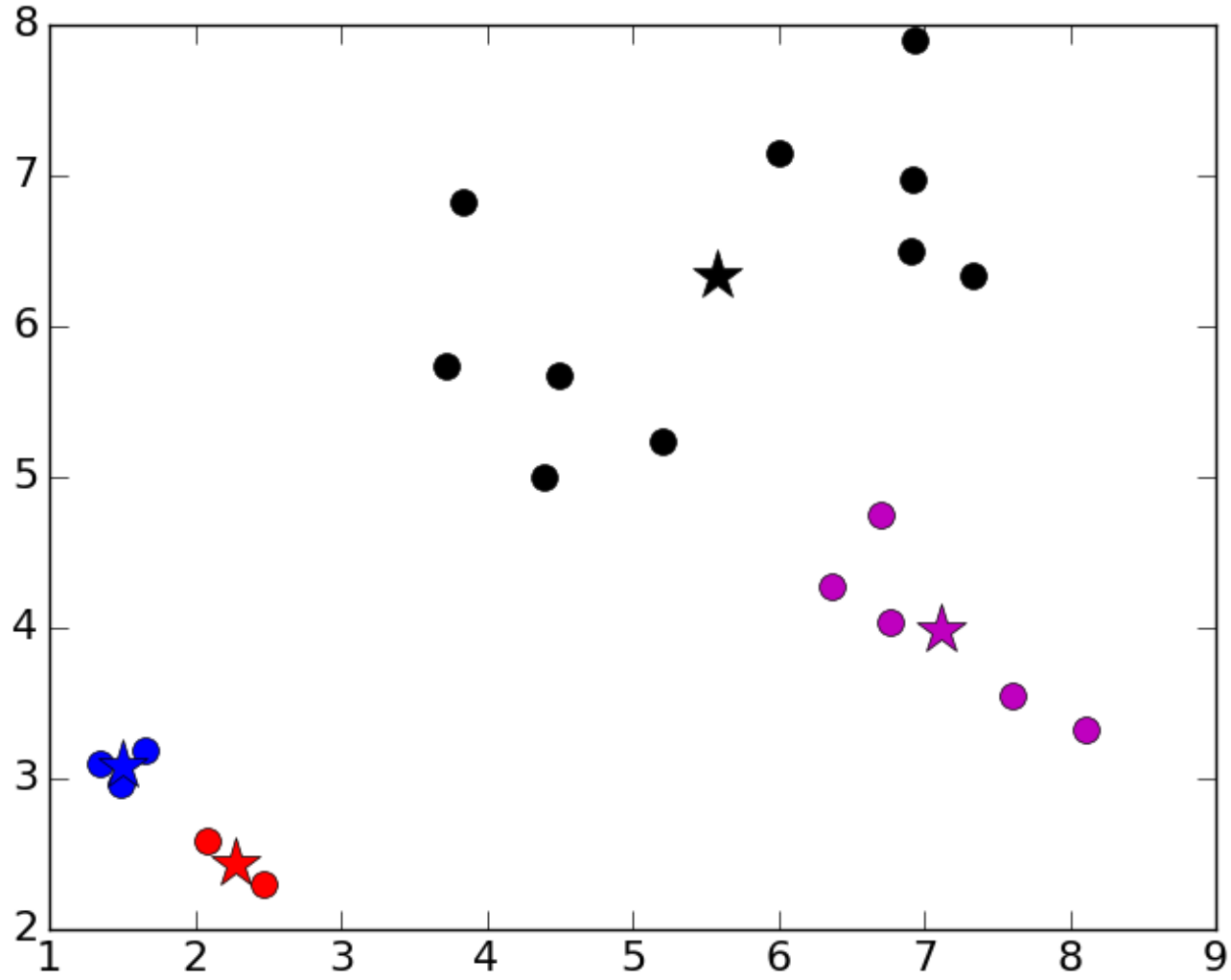
Why?

- **Greedy algorithm can find different local optima**

Different Initial Centroids



Converges On



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

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
```

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)

    ...
```

Class Cluster

```
class Cluster(object):

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

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

    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
```

Generator
8.3.1 in text

Evaluating a Clustering

```
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
```

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, posLabel, printMembers = True,
                    printStats = False):
    """Assumes: clustering is a sequence of clusters
       Prints information about each cluster
       Returns list of fraction of pos cases in each cluster"""

def testClustering(points, numClusters, numTrials = 5, posLabel = 1,
                   printMembers = True, printStats = False):
    bestClustering = trykmeans(points, numClusters, numTrials)
    posFracs = printClustering(bestClustering, posLabel, printMembers,
                               printStats)
    return posFracs
```

Example: Football Players

```
edelman = ['edelman', 70, 200]
hogan = ['hogan', 73, 210]
gronkowski = ['gronkowski', 78, 26
gordon = ['gordon', 75, 225]
hollister = ['hollister', 76, 245]
dorsett = ['dorsett', 70, 192]
allen = ['allen', 75, 265]
cannon = ['cannon', 77, 335]
brown = ['brown', 80, 380]
mason = ['mason', 73, 310]
thuney = ['thuney', 77, 305]
guy = ['guy', 76, 315]
shelton = ['shelton', 74, 345]
karras = ['karras', 76, 305]
mason = ['mason', 73, 310]
michel = ['michel', 71, 215]
white = ['white', 70, 205]
patterson = ['patterson', 74, 228]
develin = ['develin', 75, 255]
brady = ['brady', 76, 225]
```

```
pats = []
for p in receivers:
    pats.append((p, 'receiver'))
for p in dLine:
    pats.append((p, 'Dline'))
for p in oLine:
    pats.append((p, 'Oline'))
for p in tights:
    pats.append((p, 'tight end'))
for p in backs:
    pats.append((p, 'back'))
```

```
receivers = [edelman, hogan, gordon, dorsett]
dLine = [guy, shelton]
oLine = [brown, cannon, mason, karras, thuney]
tights = [gronkowski, hollister, allen]
backs = [michel, white, patterson, develin, brady]
```

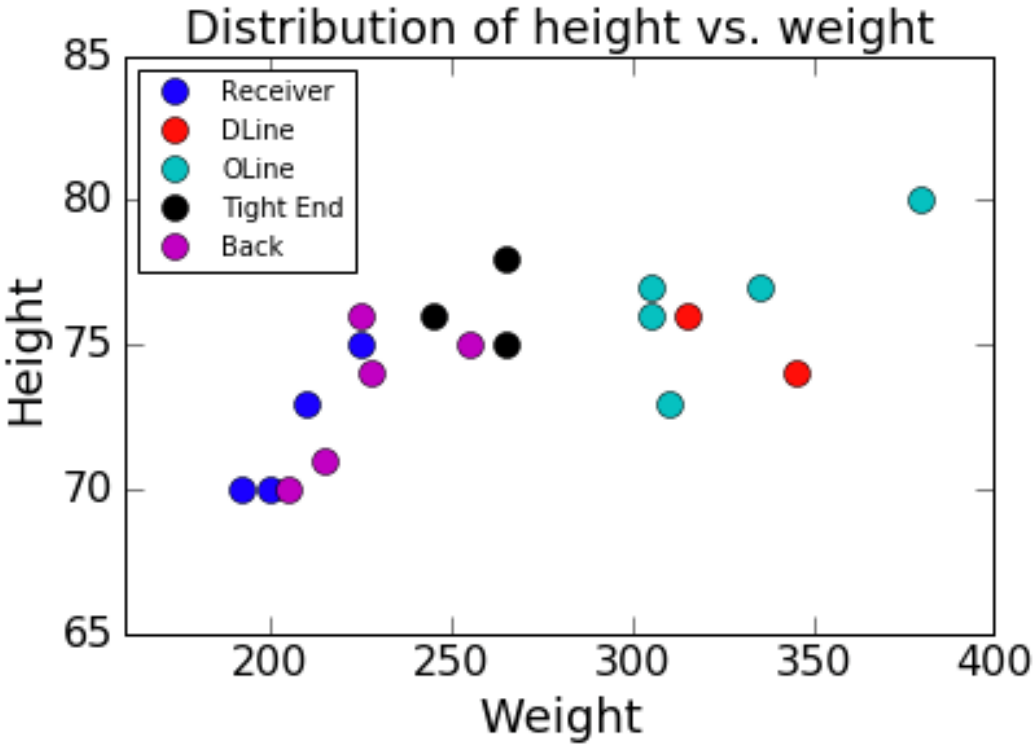
Build Set of Examples

```
class Player(Example):
    pass

def buildPatriotsData(players, toScale = False):
    heightList, weightList = [],[]
    for p in players:
        heightList.append(p[0][1])
        weightList.append(p[0][2])
    if toScale:
        heightList = scaleAttrs(heightList)
        weightList = scaleAttrs(weightList)
    #Build points
    points = []
    for i in range(len(players)):
        features = np.array([heightList[i], weightList[i]])
        features = np.array([heightList[i], weightList[i]])
        points.append(Player(players[i][0][0], features, players[i][1]))
    return points

players = buildPatriotsData(pats, False)
```

Plot the Data



Trent Brown and Sony Michel

Let's Try It Twice

```
k = 3
for seed in (0, 1):
    random.seed(seed)
    print('\n     Test k-means (k = ' + str(k) + ')')
    testClustering(players, k, 1)
```

```
Cluster of size 7
   gordon:[ 75 225]:receiver
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   patterson:[ 74 228]:back
   develin:[ 75 255]:back
   brady:[ 76 225]:back
Cluster of size 7
   guy:[ 76 315]:Dline
   shelton:[ 74 345]:Dline
   brown:[ 80 380]:Oline
   cannon:[ 77 335]:Oline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
Cluster of size 5
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   dorsett:[ 70 192]:receiver
   michel:[ 71 215]:back
   white:[ 70 205]:back
```

```
Cluster of size 3
   shelton:[ 74 345]:Dline
   brown:[ 80 380]:Oline
   cannon:[ 77 335]:Oline
Cluster of size 12
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   gordon:[ 75 225]:receiver
   dorsett:[ 70 192]:receiver
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   michel:[ 71 215]:back
   white:[ 70 205]:back
   patterson:[ 74 228]:back
   develin:[ 75 255]:back
   brady:[ 76 225]:back
Cluster of size 4
   guy:[ 76 315]:Dline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
```

Choose Best of 20

```
Cluster of size 4
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   develin:[ 75 255]:back
Cluster of size 8
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   gordon:[ 75 225]:receiver
   dorsett:[ 70 192]:receiver
   michel:[ 71 215]:back
   white:[ 70 205]:back
   patterson:[ 74 228]:back
   brady:[ 76 225]:back
Cluster of size 7
   guy:[ 76 315]:Dline
   shelton:[ 74 345]:Dline
   brown:[ 80 380]:Oline
   cannon:[ 77 335]:Oline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
```

```
Cluster of size 8
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   gordon:[ 75 225]:receiver
   dorsett:[ 70 192]:receiver
   michel:[ 71 215]:back
   white:[ 70 205]:back
   patterson:[ 74 228]:back
   brady:[ 76 225]:back
Cluster of size 4
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   develin:[ 75 255]:back
Cluster of size 7
   guy:[ 76 315]:Dline
   shelton:[ 74 345]:Dline
   brown:[ 80 380]:Oline
   cannon:[ 77 335]:Oline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
```

Try Different Values of k

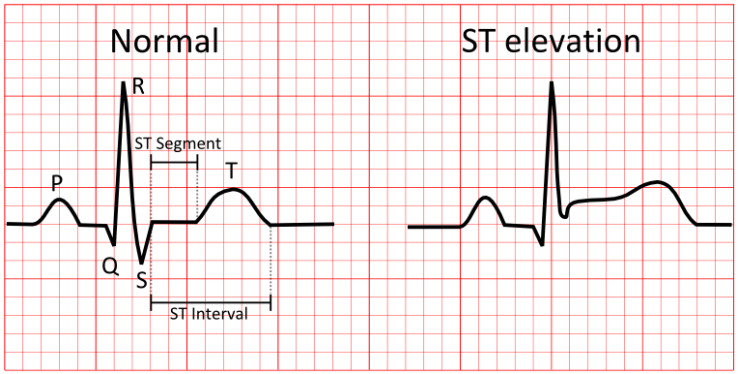
```
     Test k-means (k = 3)
Cluster of size 4
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   develin:[ 75 255]:back
Cluster of size 8
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   gordon:[ 75 225]:receiver
   dorsett:[ 70 192]:receiver
   michel:[ 71 215]:back
   white:[ 70 205]:back
   patterson:[ 74 228]:back
   brady:[ 76 225]:back
Cluster of size 7
   guy:[ 76 315]:Dline
   shelton:[ 74 345]:Dline
   brown:[ 80 380]:Oline
   cannon:[ 77 335]:Oline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
```

```
     Test k-means (k = 5)
Cluster of size 1
   brown:[ 80 380]:Oline
Cluster of size 2
   shelton:[ 74 345]:Dline
   cannon:[ 77 335]:Oline
Cluster of size 8
   edelman:[ 70 200]:receiver
   hogan:[ 73 210]:receiver
   gordon:[ 75 225]:receiver
   dorsett:[ 70 192]:receiver
   michel:[ 71 215]:back
   white:[ 70 205]:back
   patterson:[ 74 228]:back
   brady:[ 76 225]:back
Cluster of size 4
   gronkowski:[ 78 265]:tight end
   hollister:[ 76 245]:tight end
   allen:[ 75 265]:tight end
   develin:[ 75 255]:back
Cluster of size 4
   guy:[ 76 315]:Dline
   mason:[ 73 310]:Oline
   karras:[ 76 305]:Oline
   thuney:[ 77 305]:Oline
```

Time for a Short Break

Example: Cardiovascular Death

- 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

Patients

```
class Patient(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
```

Result of Running It

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?

Certainly doesn't seem to have clustered patients based upon survival

What's going on?

Try It With Scaling

```
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 Now?

One Way to Think About Question

$$sensitivity = \frac{true\ positive}{true\ positive + false\ negative}$$

$$specificity = \frac{true\ negative}{true\ negative + false\ positive}$$

Percentage correctly found
Percentage correctly rejected

Cluster of size 224 with fraction of positives = 0.2902
Cluster of size 26 with fraction of positives = 0.6923

If we use cluster membership to classify, sensitivity is about 0.22

Missing most of the positives

A Hypothesis

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

```
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

Sensitivity

0.22

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

0.87

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

0.88

Which k

	Sensitivity	Specificity
Cluster of size 26 with fraction of positives = 0.6923		
Cluster of size 86 with fraction of positives = 0.0814	0.87	0.82
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	0.88	0.79
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		

Don't forget specificity

Don't forget Occam's razor

Coming Up

- Classification