A Quick Introduction to Machine Learning (K-means Clustering)

Lecturer: John Guttag

K-means Clustering

Given a set of points *X*, and a positive integer *k*, partition *X* into *k* clusters such that it approximately minimizes the objective function

$$\sum_{c=1}^{k} \sum_{x \in c} \|x - m_c\|^2$$

clusters

points

distance from point to centroid of cluster

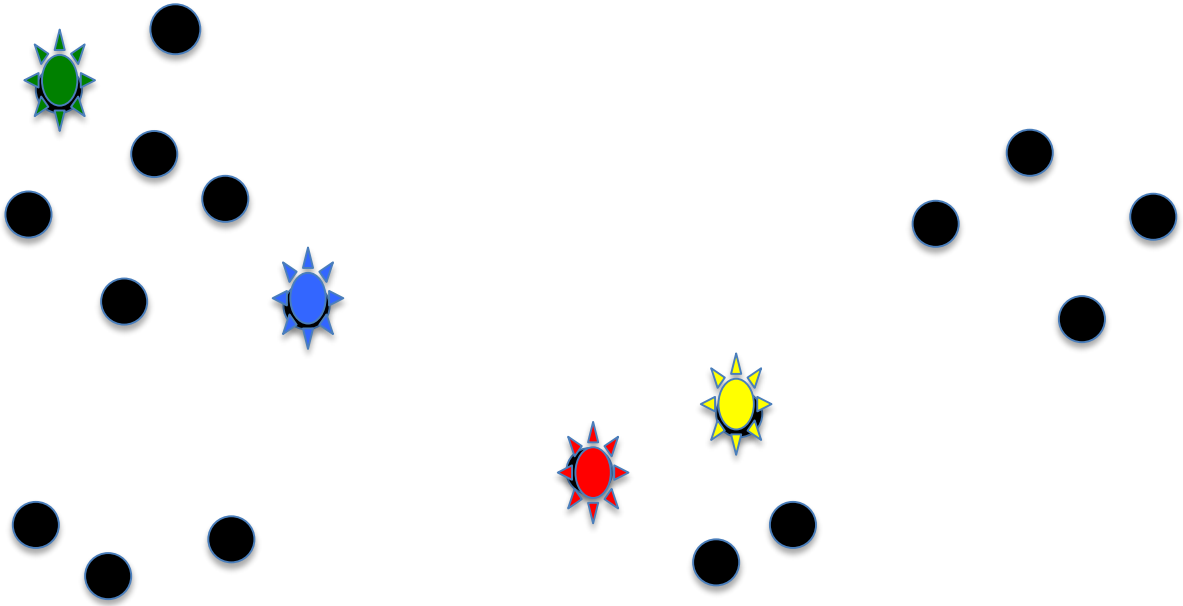
Minimizing the sum of the mean square differences

K-means Algorithm

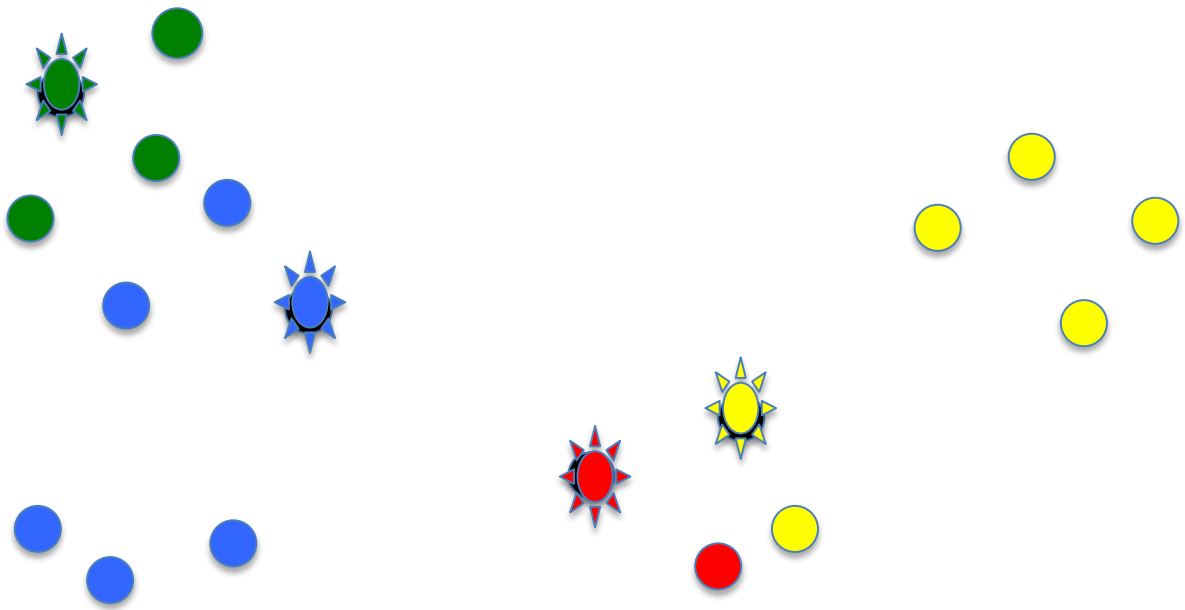
```
randomly choose k examples as centroids
while true:
   create k clusters by assigning each
       example to closest centroid
   compute k new centroids by averaging
       examples in each cluster
   if centroids don’t change:
       break
```

Example

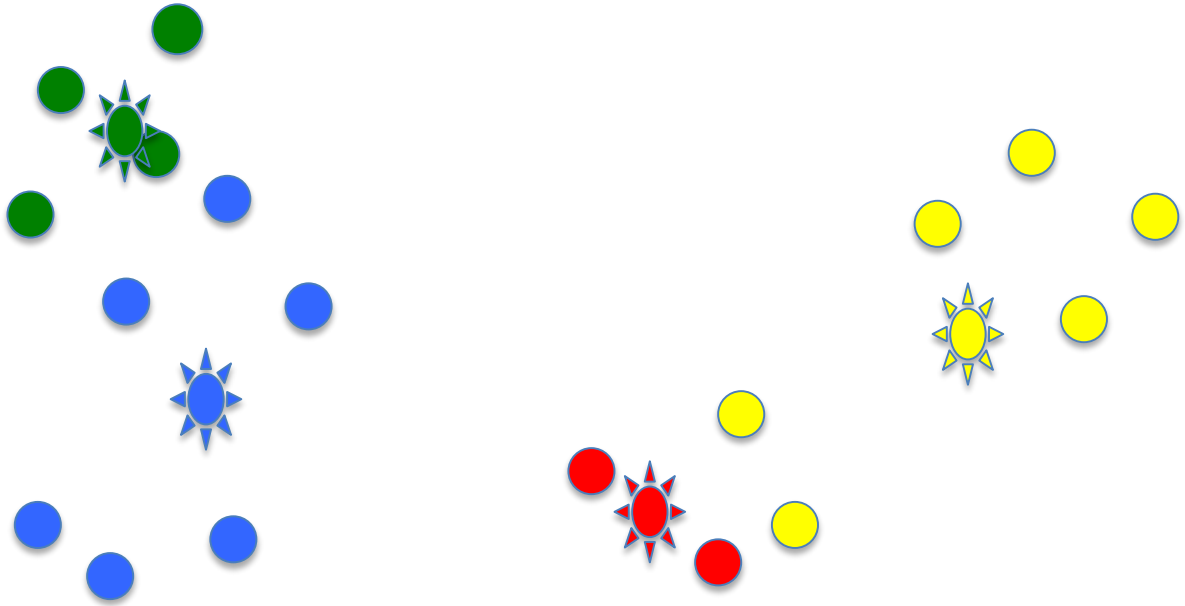
Choose Initial Centroids (k = 4)



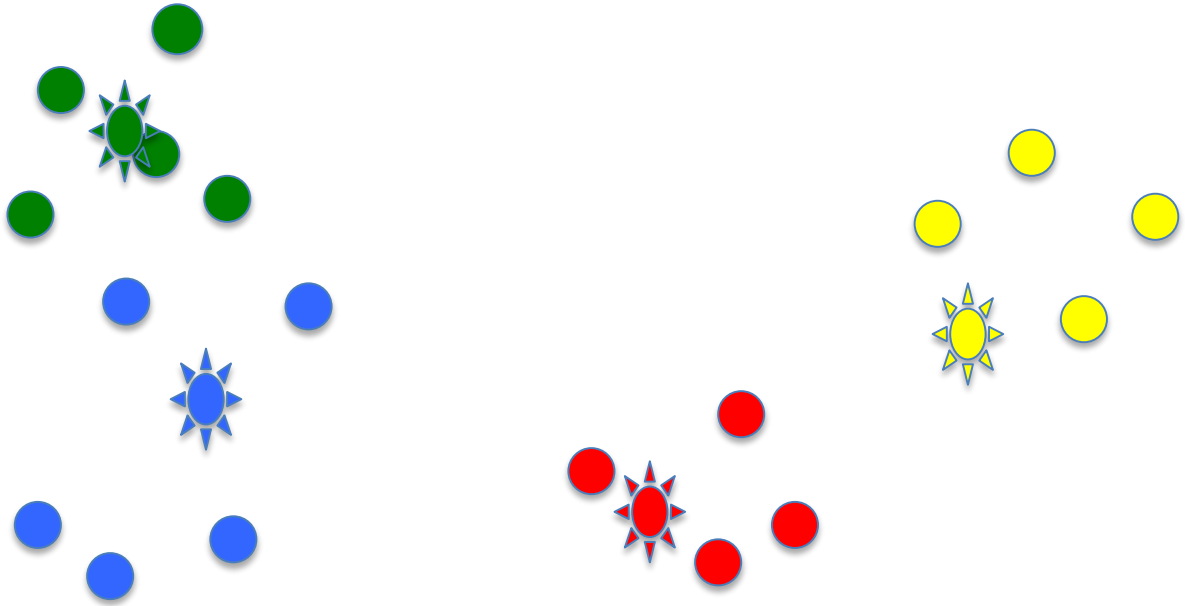
Assign Points to Clusters



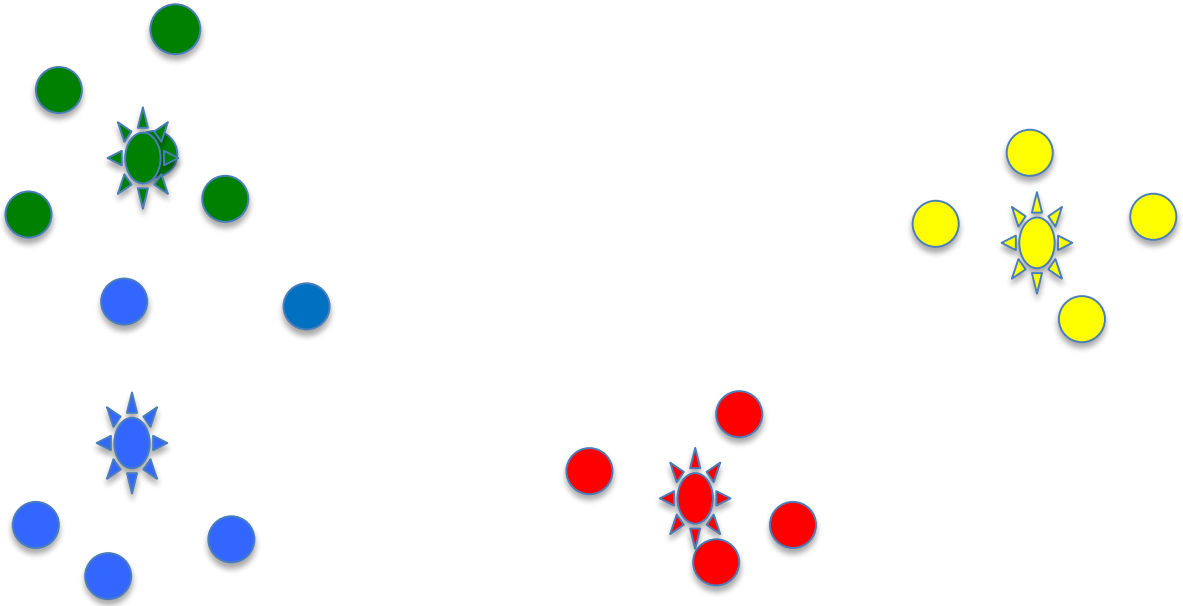
Compute New Centroids



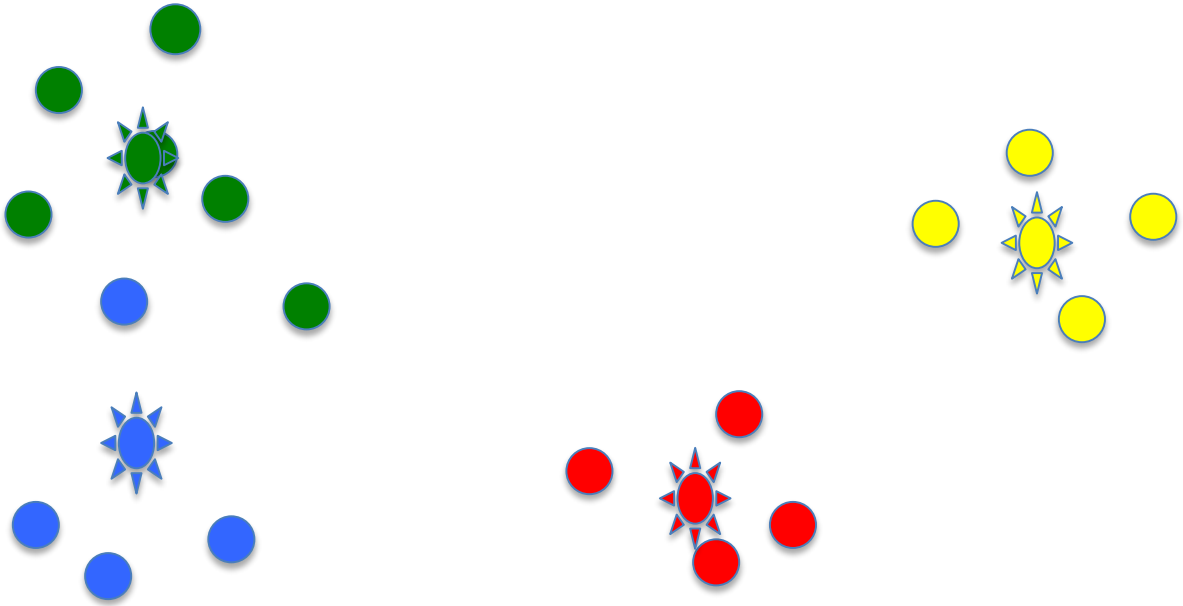
Reassign Points to Clusters



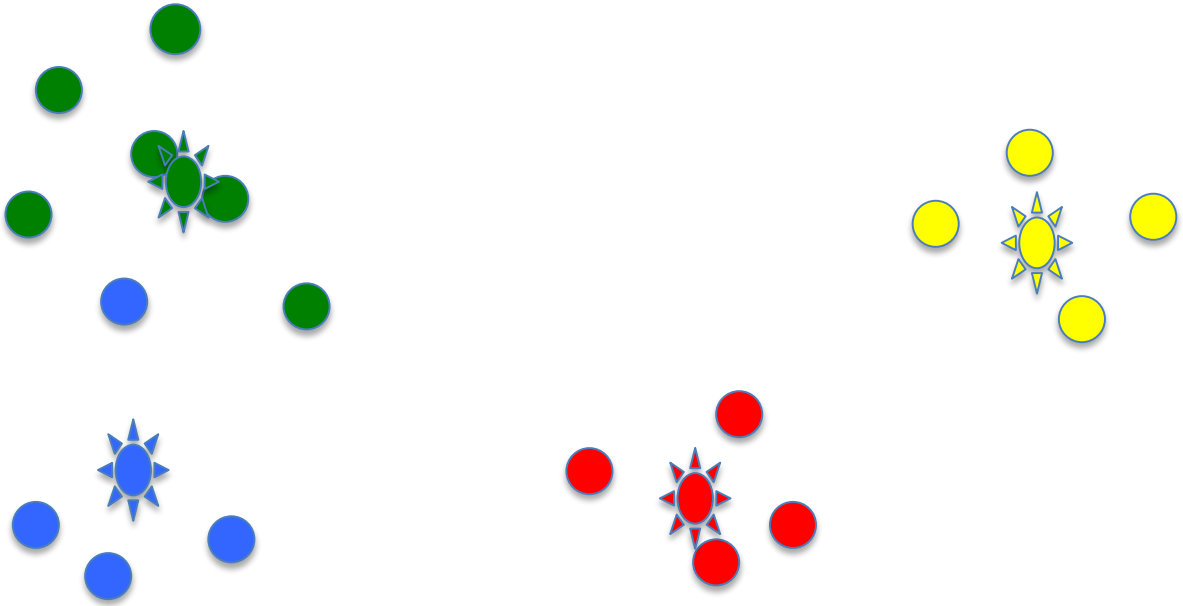
Compute New Centroids



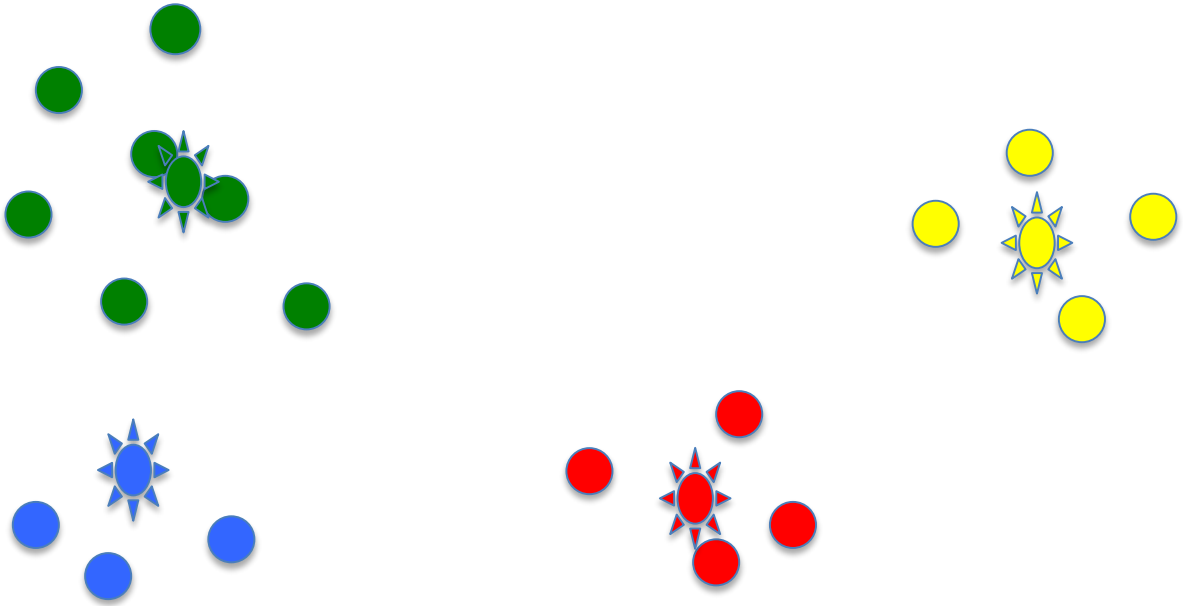
Reassign Points



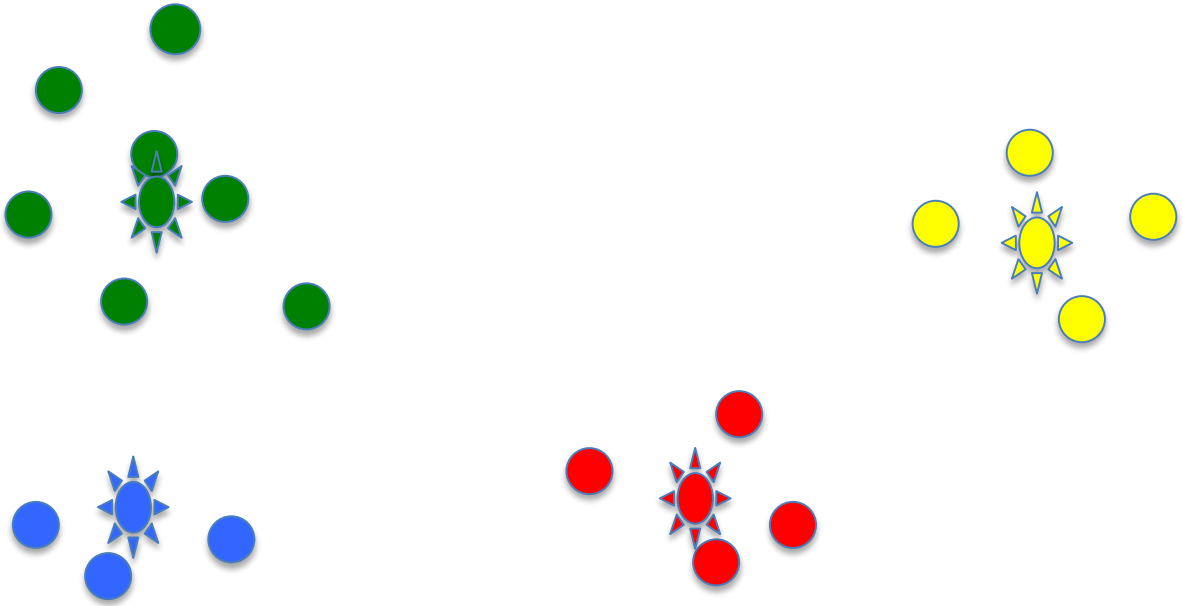
Compute New Centroids



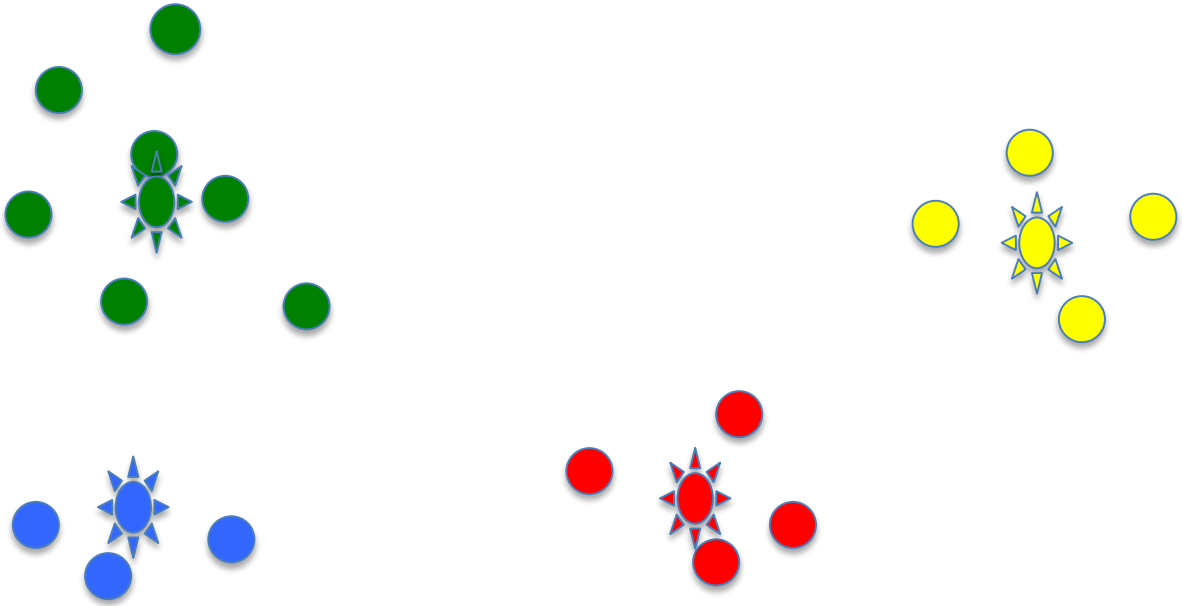
Reassign Points



Compute New Centroids



No Points Move

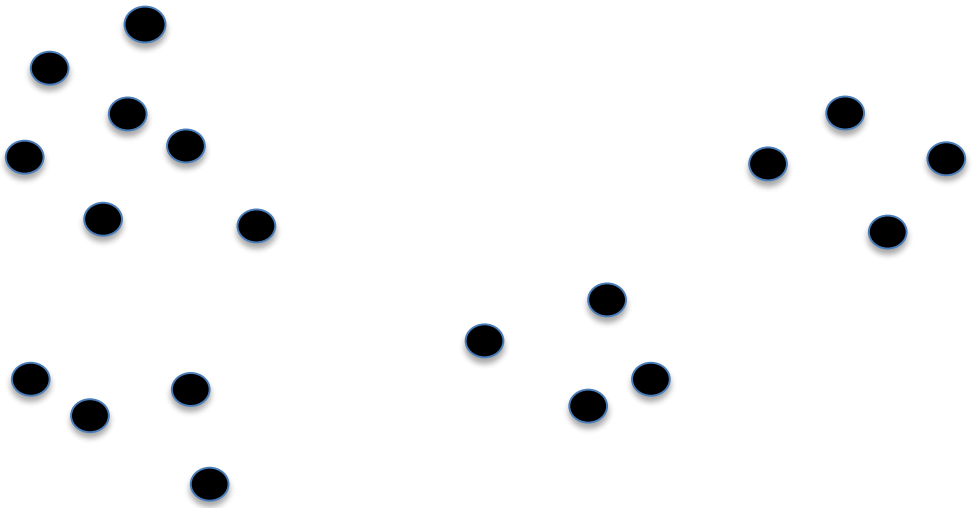


Issues with K-means

Final result can depend upon initial centroids

Greedy algorithm can find different local optima

Choosing the "wrong" k can lead to nonsense



Choosing K

A priori knowledge about application domain

There are five different kinds of bacteria: k = 5

There are two kinds of people in the world: k = 2

Search for a good k

Try different values of k, and evaluate quality of results

Choosing Centroids

Try multiple random choices and choose best

Finding the "Best" Solution

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

$$V(c) = \sum_{x \in c} (mean(c) - x)^2 \qquad badness(C) = \sum_{c \in C} V(c)$$

Hierarchical vs. K-means

Hierarchical looks at different numbers of clusters
From 1 to n

K-means looks at many ways of creating k clusters

Hierarchical is slow

K-means is fast

Hierarchical is deterministic

K-means is non-deterministic

A Quick Introduction to Machine Learning (Scaling)

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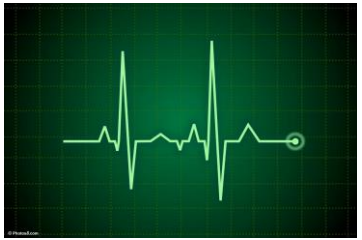
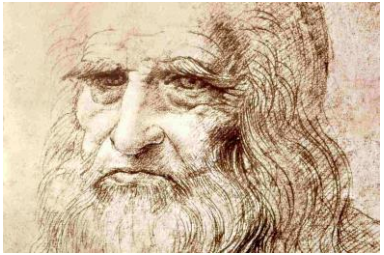
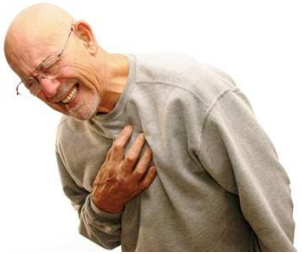
An Example

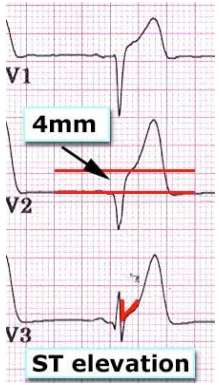


1000 patients with 4 features each

- Heart rate in beats per minute
- Number of past heart attacks
- ST segment elevation (binary)
- Age







Binary outcome based on features

- Probabilistic, not deterministic
- Roughly 31% positive

A Sampling of Examples

```
P0755:[ 48.   1.   0.  62.]:1
P0383:[ 103.  1.   1.  99.]:1
P0849:[ 42.   1.   1.  92.]:1
P0188:[ 71.   2.   0.  58.]:0
P0061:[ 87.   1.   0.  79.]:0
P0196:[ 52.   0.   0.  85.]:0
P0280:[ 78.   0.   0.  81.]:0
P0178:[ 50.   1.   0.  59.]:1
P0497:[ 80.   0.   0.  58.]:0
P0742:[ 78.   2.   0.  72.]:1
P0527:[ 78.   1.   0.  60.]:0
P0915:[ 60.   2.   0.  57.]:1
```

Fraction of positives in total population of 1000 was 0.312

Cluster Using K-means (k = 3)

Fraction of positives in population = 0.312

Ran k-means 100 times and chose best clustering

Cluster of size 354 with fraction of positives = 0.338 (1.08x)
Cluster of size 322 with fraction of positives = 0.315 (1.01x)
Cluster of size 324 with fraction of positives = 0.281 (0.90x)

What Happened?

Features have very different means and variance

Heart rate in beats per minute ($\mu = 70$, $\sigma = 15$)
Number of past heart attacks ($\mu = 0.25$, $\sigma = 1.0$)
ST segment elevation (binary)
Age ($\mu = 65$, $\sigma = 15$)

HR and age have higher means & greater dynamic range

Euclidean distance will be biased towards them

Does this seem like a good idea?

“No, No, a Thousand Times No”

Rescale Features

Each variable has same mean and variance

$$x' = \frac{x - \mu_x}{\sigma_x}$$

```
def scaleFeatures(vals):
    vals = pylab.array(vals)
    mean = sum(vals)/float(len(vals))
    sd = stdDev(vals)
    vals = vals - mean
    return vals/sd
```

What is the new mean?
What is the new standard deviation?

Testing Scaling

```
def testScaling(n, mean, std):
    vals = []
    for i in range(n):
        vals.append(int(random.gauss(mean, std)))
    print 'original values', vals
    sVals = scaleAttrs(vals)
    print '\n', 'scaled values', sVals
    print '\n', 'new mean =', sum(sVals/len(vals))
    print '\n', 'new sd =', stdDev(sVals)

testScaling(10, 25, 3)
```

Testing Scaling

```
original values [22, 24, 21, 26, 18, 26, 22, 26,
27, 21]

scaled values [-0.46517657  0.25047969 -0.82300471
0.96613596 -1.89648911  0.96613596
 -0.46517657  0.96613596  1.32396409 -0.82300471]

new mean = -2.22044604925e-16

new sd = 1.0
```

The Real Test

Fraction of positives = 0.312

Clustering with unscaled features

Cluster of size 354 with fraction of positives = 0.338 (1.08x)
Cluster of size 322 with fraction of positives = 0.315 (1.01x)
Cluster of size 324 with fraction of positives = 0.281 (0.90x)

Clustering with scaled features

Cluster of size 324 with fraction of positives = 0.055 (0.18x)
Cluster of size 108 with fraction of positives = 0.335 (1.07x)
Cluster of size 568 with fraction of positives = 0.454 (1.45x)