CPSC 340: Machine Learning and Data Mining

K-Means Clustering

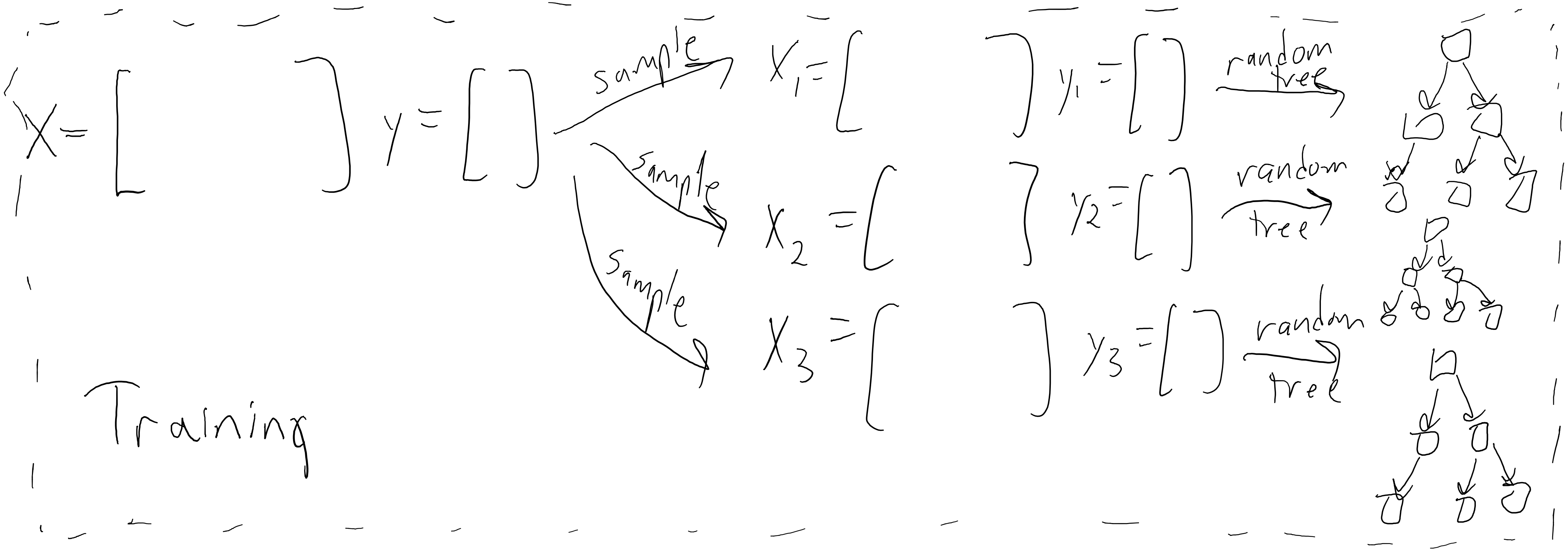
Fall 2015

Admin

- Assignment 1 solutions posted after class.
  - Tutorials for Assignment 2 on Monday.

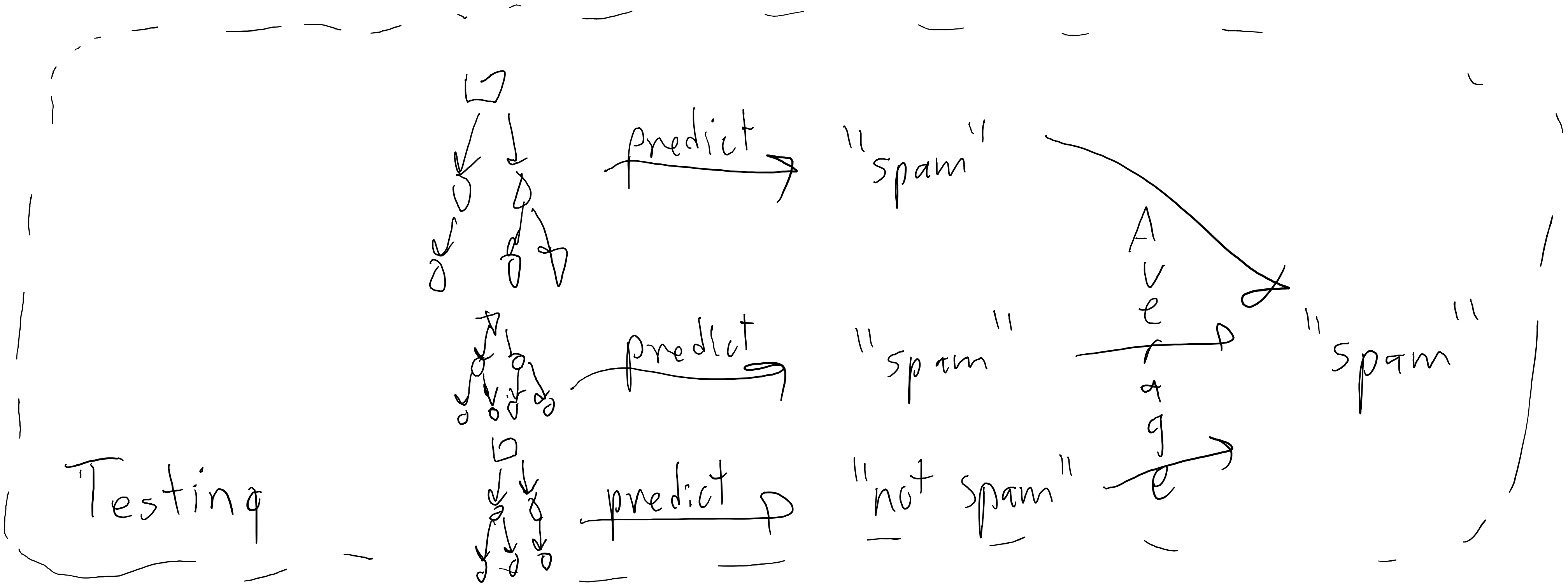
Random Forests

- Random forests are one of the best ‘out of the box’ classifiers.
- Fit deep decision trees to random bootstrap samples of data, base splits on random subsets of the features, and classify using mode.



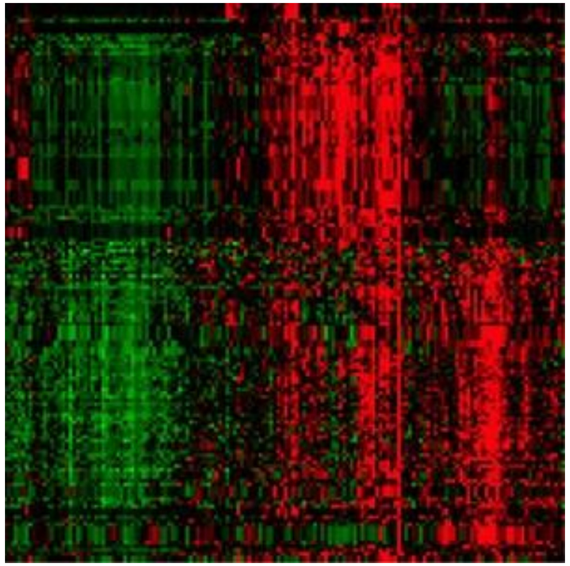
Random Forests

- Random forests are one of the best 'out of the box' classifiers.
- Fit deep decision trees to random bootstrap samples of data, base splits on random subsets of the features, and classify using mode.



Classifying Cancer Types

- "I collected gene expression data for 1000 different types of cancer cells, can you tell me the different classes of cancer?"

X = 

- We are not given the class labels y, but want meaningful labels.
- An example of unsupervised learning.

https://corelifesciences.com/human-long-non-coding-rna-expression-microarray-service.html

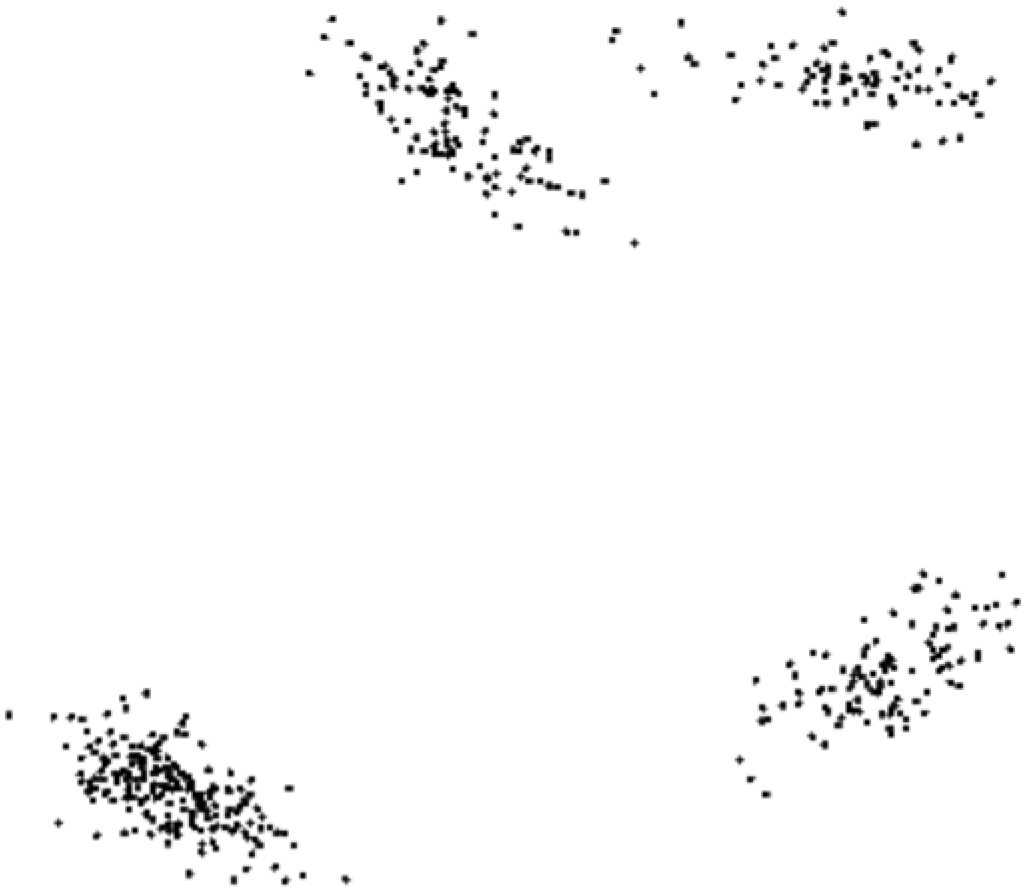
Unsupervised Learning

- Supervised learning:
  - We have features x_i and class labels y_i.
  - Write a program that produces y_i from x_i.
- Unsupervised learning:
  - We only have x_i values, but no explicit target labels.
  - You want to do 'something' with them.
- Some unsupervised learning tasks:
  - Outlier detection: Is this a 'normal' x_i?
  - Data visualization: What does the high-dimensional X look like?
  - Association rules: Which x_{ij} occur together?
  - Latent-factors: What 'parts' are the x_i made from?
  - Ranking: Which are the most important x_i?
  - Clustering: What types of x_i are there?

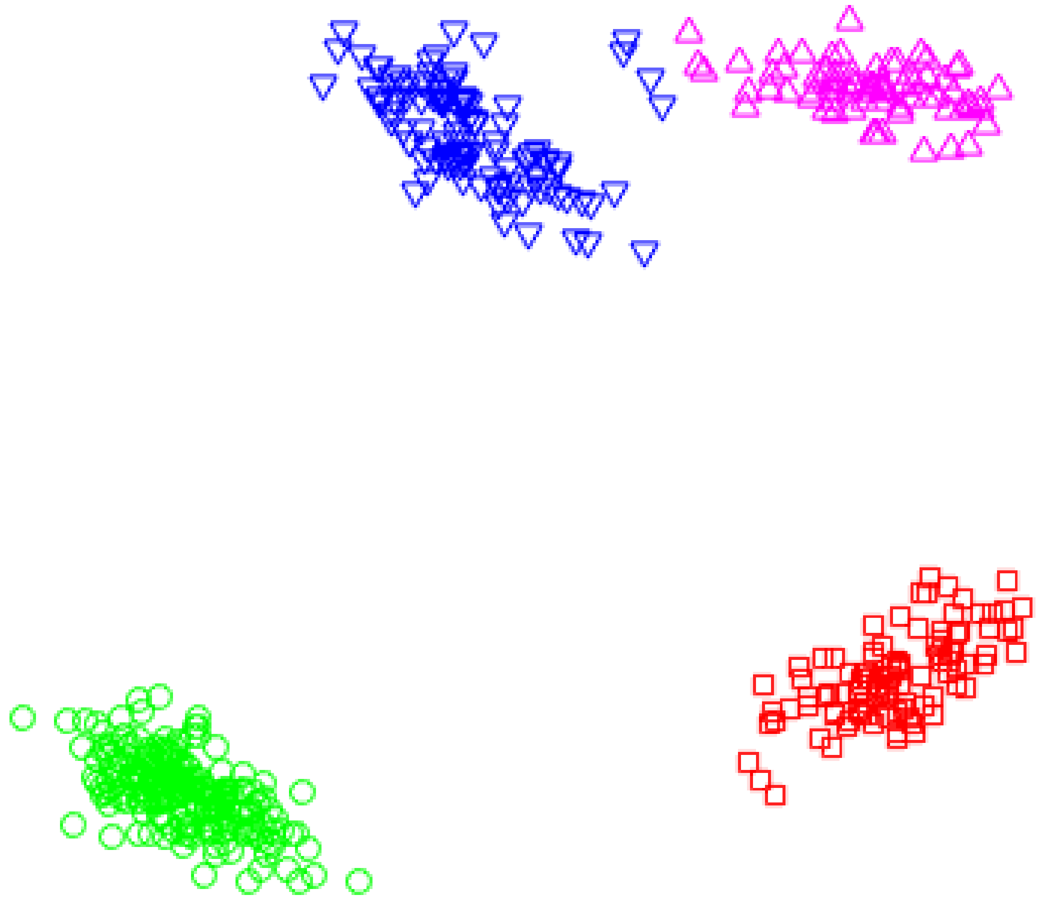
Clustering

- Clustering:
  - Input: set of objects described by features x_i.
  - Output: an assignment of objects to ‘groups’.
- Unlike classification, we are not given the ‘groups’.
  - Algorithm must discover groups.
- Example of groups we might discover in e-mail spam:
  - ‘Lucky winner’ group.
  - ‘Weight loss’ group.
  - ‘Nigerian prince’ group.

Clustering Example



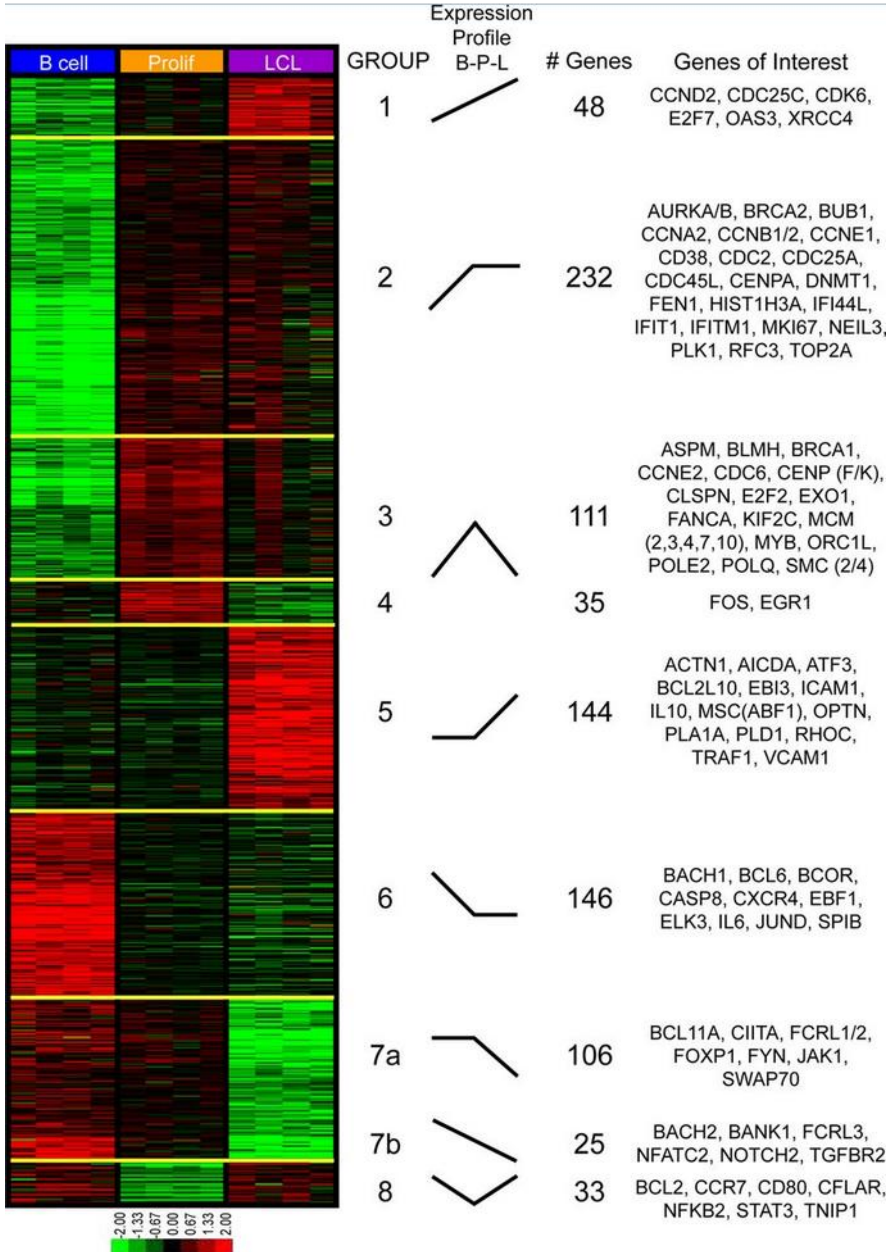
Clustering Example



Data Clustering

- General goal of clustering algorithms:
  - Objects in the same group should be ‘similar’.
  - Objects in different groups should be ‘different’.
- But the ‘best’ clustering is hard to define:
  - We don’t have a test error.
  - Generally, there is no ‘best’ method in unsupervised learning.
  - Means there are lots of methods: we’ll focus on important/representative ones.
- Why cluster?
  - You could want to know what the groups are.
  - You could want a ‘prototype’ example for each group.
  - You could want to find the group for a new example x.
  - You could want to find objects related to a new example x.

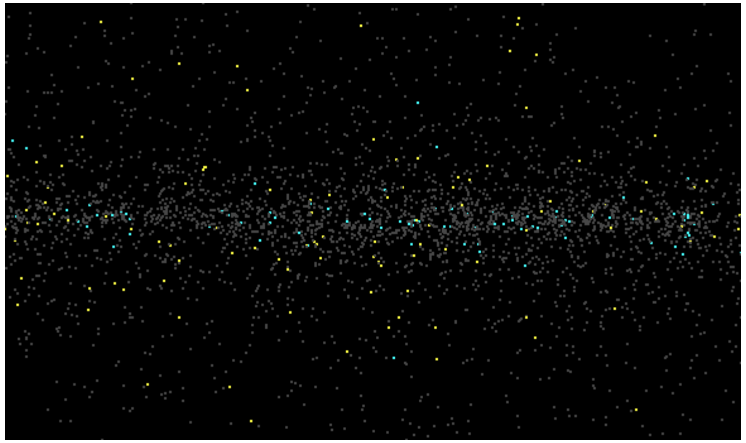
Clustering of Epstein-Barr Virus

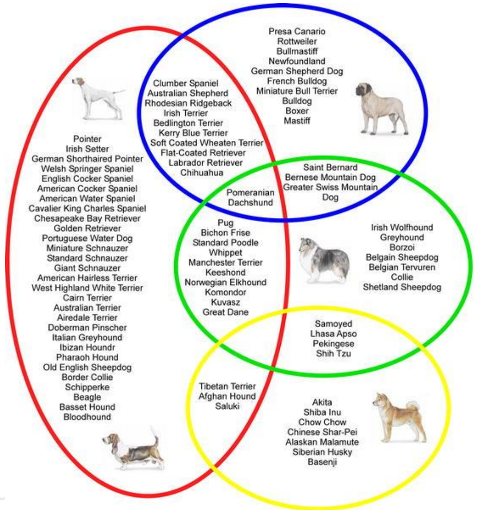


http://jvi.asm.org/content/86/20/11096.abstract

Other Clustering Applications

- NASA: what types of stars are there?
- Biology: are there sub-species?
- Documents: what kinds of documents are on my HD?
- Commercial: what kinds of customers do I have?
- Clothing: what sizes of clothing should I make?



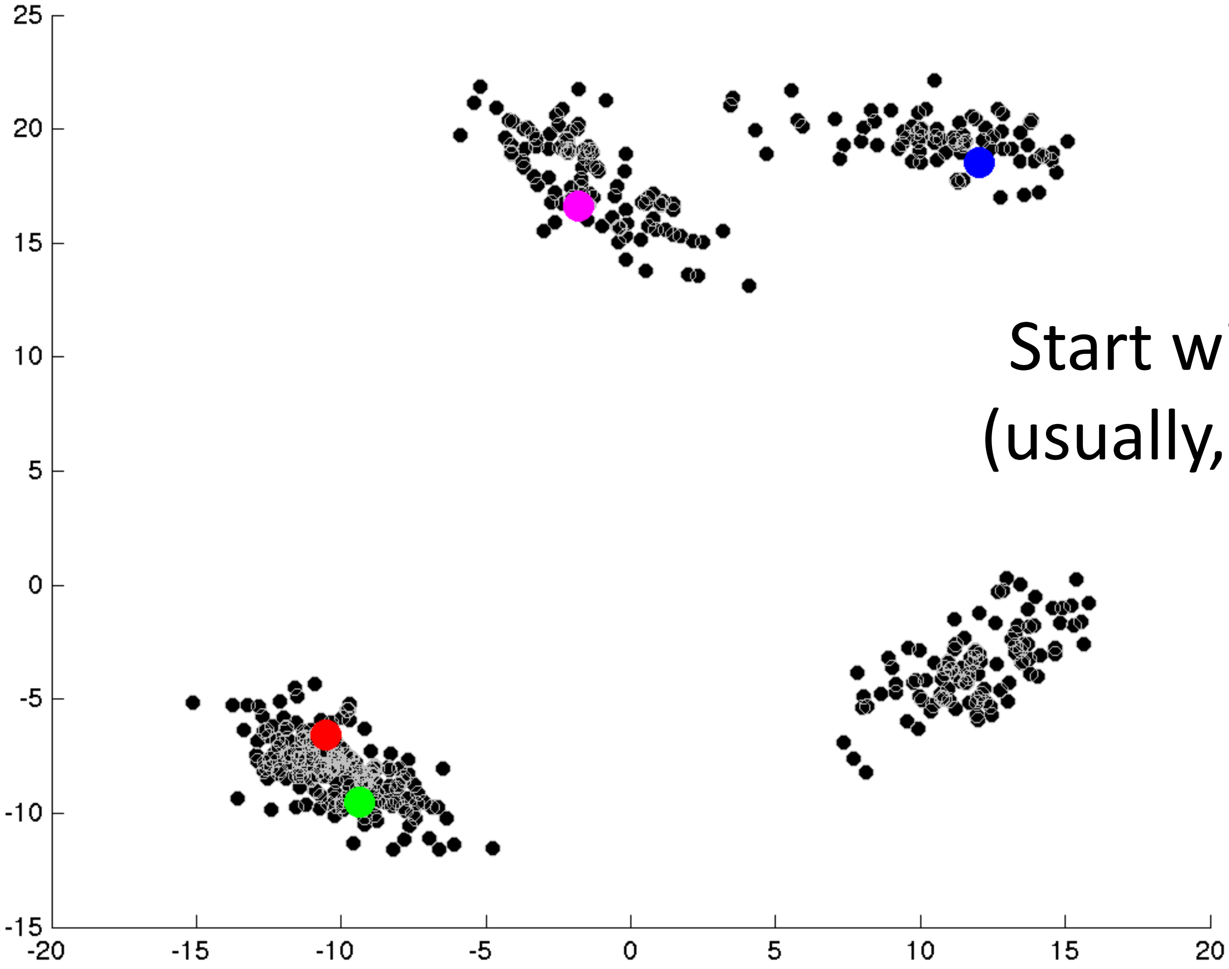


http://www.eecs.wsu.edu/~cook/dm/lectures/l9/index.html
http://www.biology-online.org/articles/canine_genomics_genetics_ru
http://wannabite.com/wp-content/uploads/2014/10/ragu-pasta-sauce-printable-coupon.jpg

K-Means

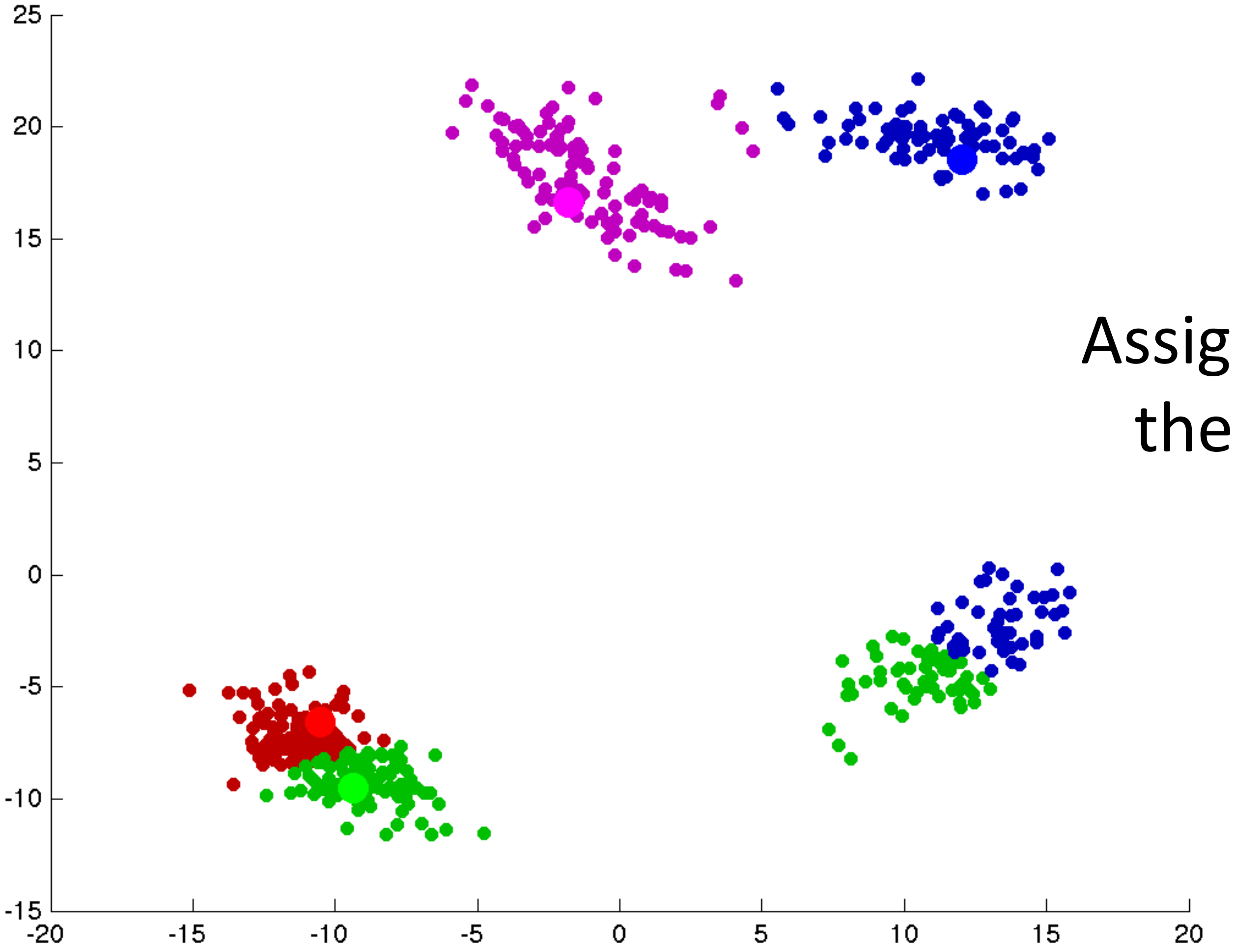
- Most popular clustering method is k-means.
- Input:
  - The number of clusters ‘k’.
  - Initial guesses of the ‘mean’ of each cluster.
- Algorithm:
  - Assign each x_i to its closest mean.
  - Update the means based on the assignment.
  - Repeat until convergence.

K-Means Example



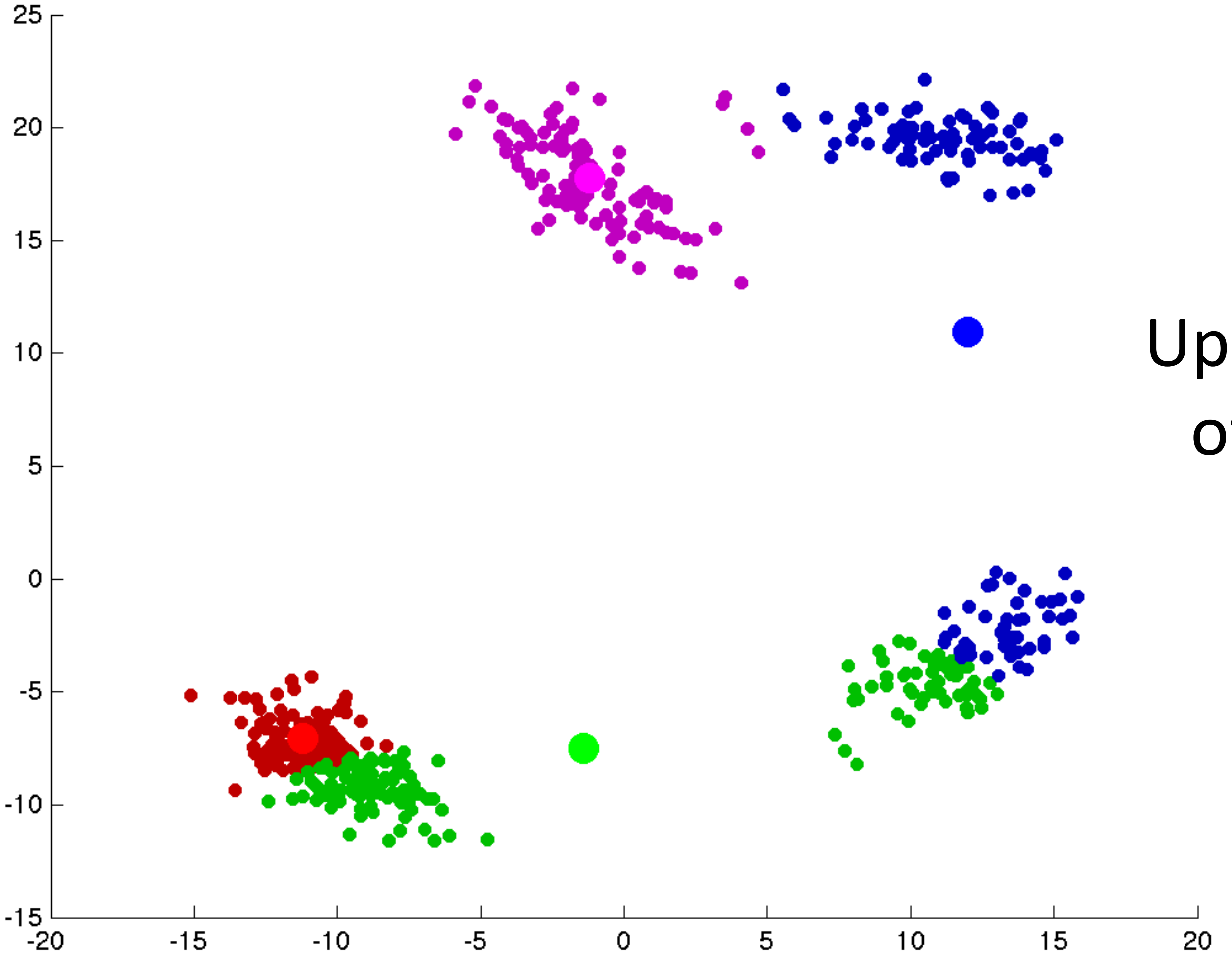
Start with ‘k’ initial ‘means’
(usually, random data points)

K-Means Example



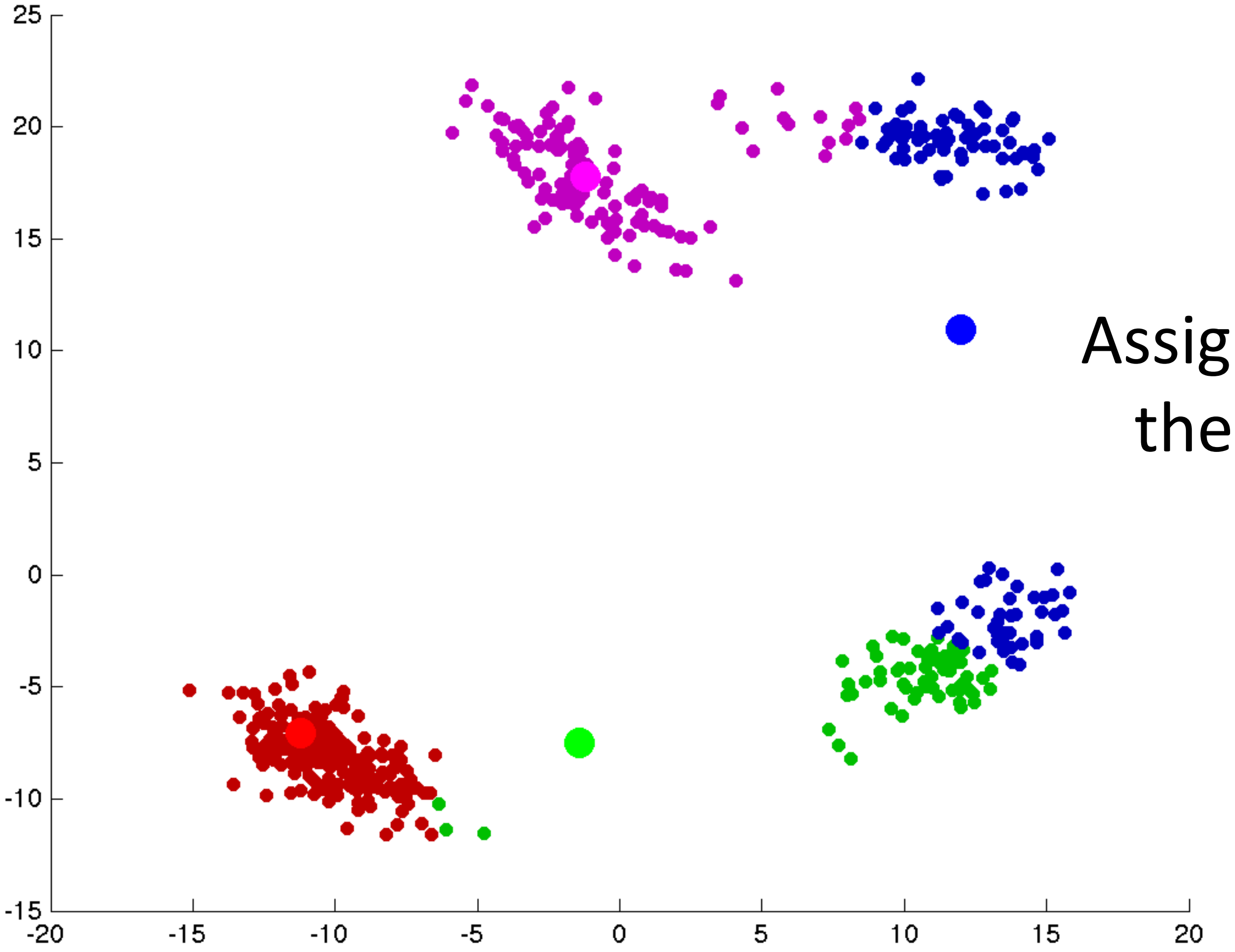
Assign each object to the closest mean.

K-Means Example



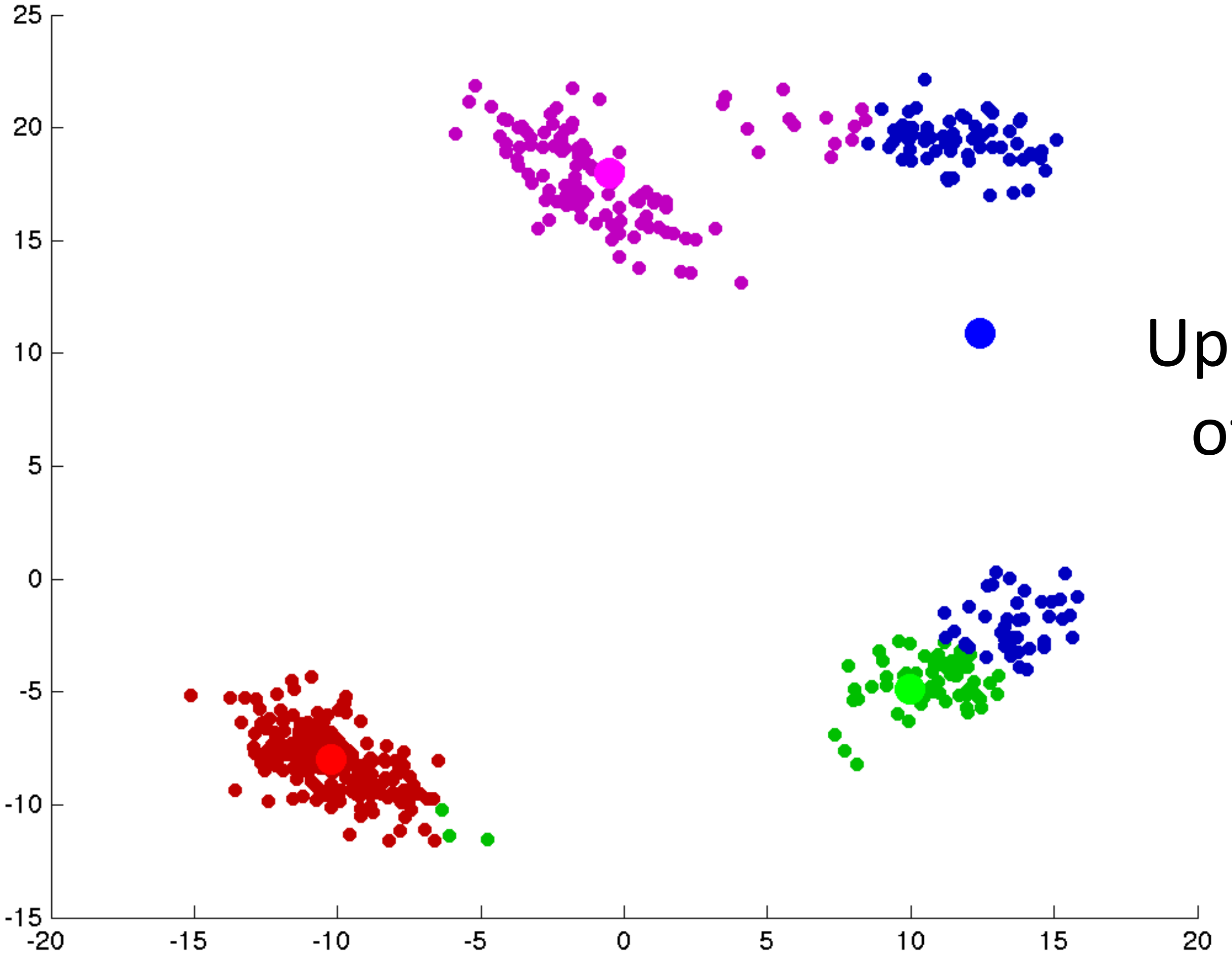
Update the mean of each group.

K-Means Example



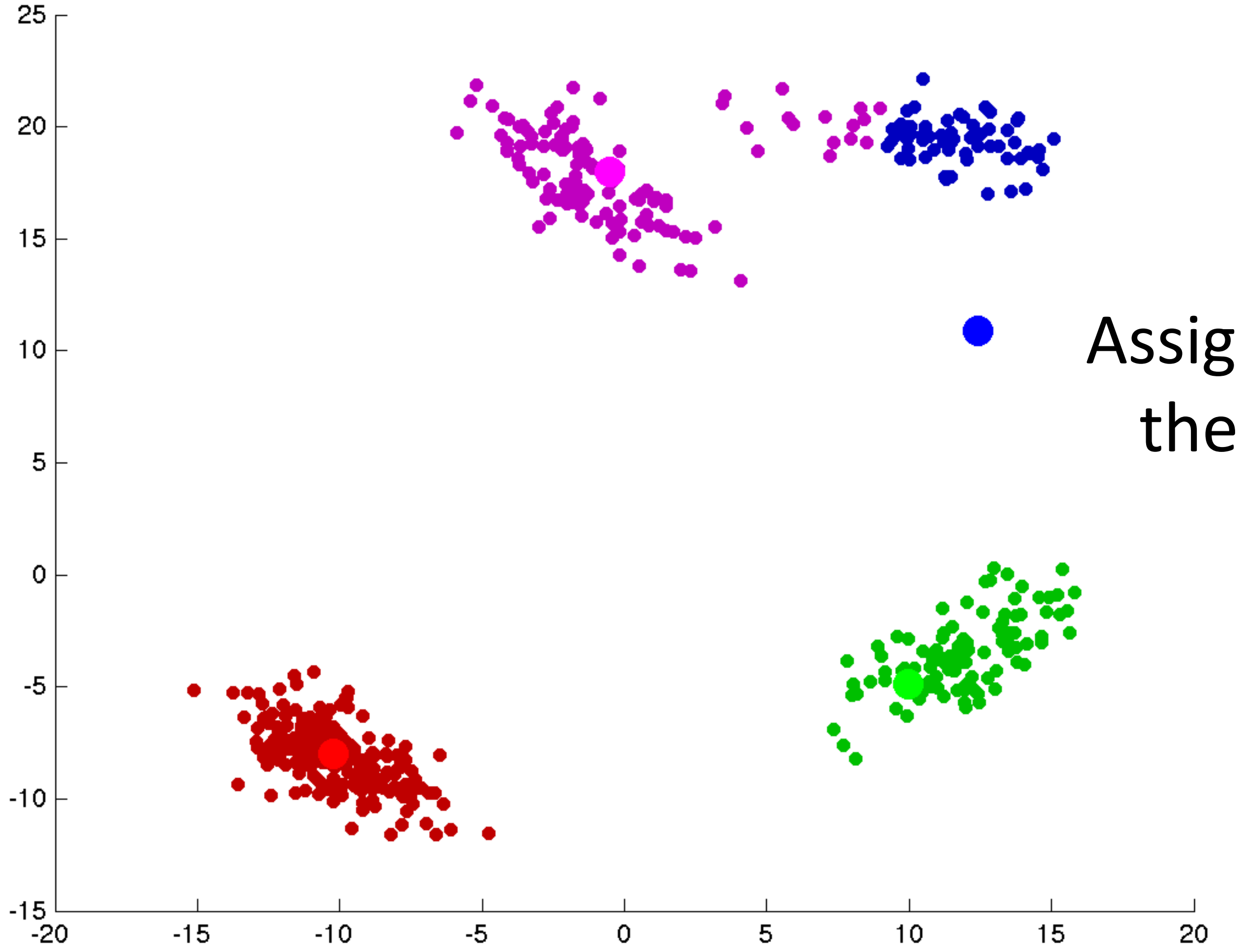
Assign each object to the closest mean.

K-Means Example



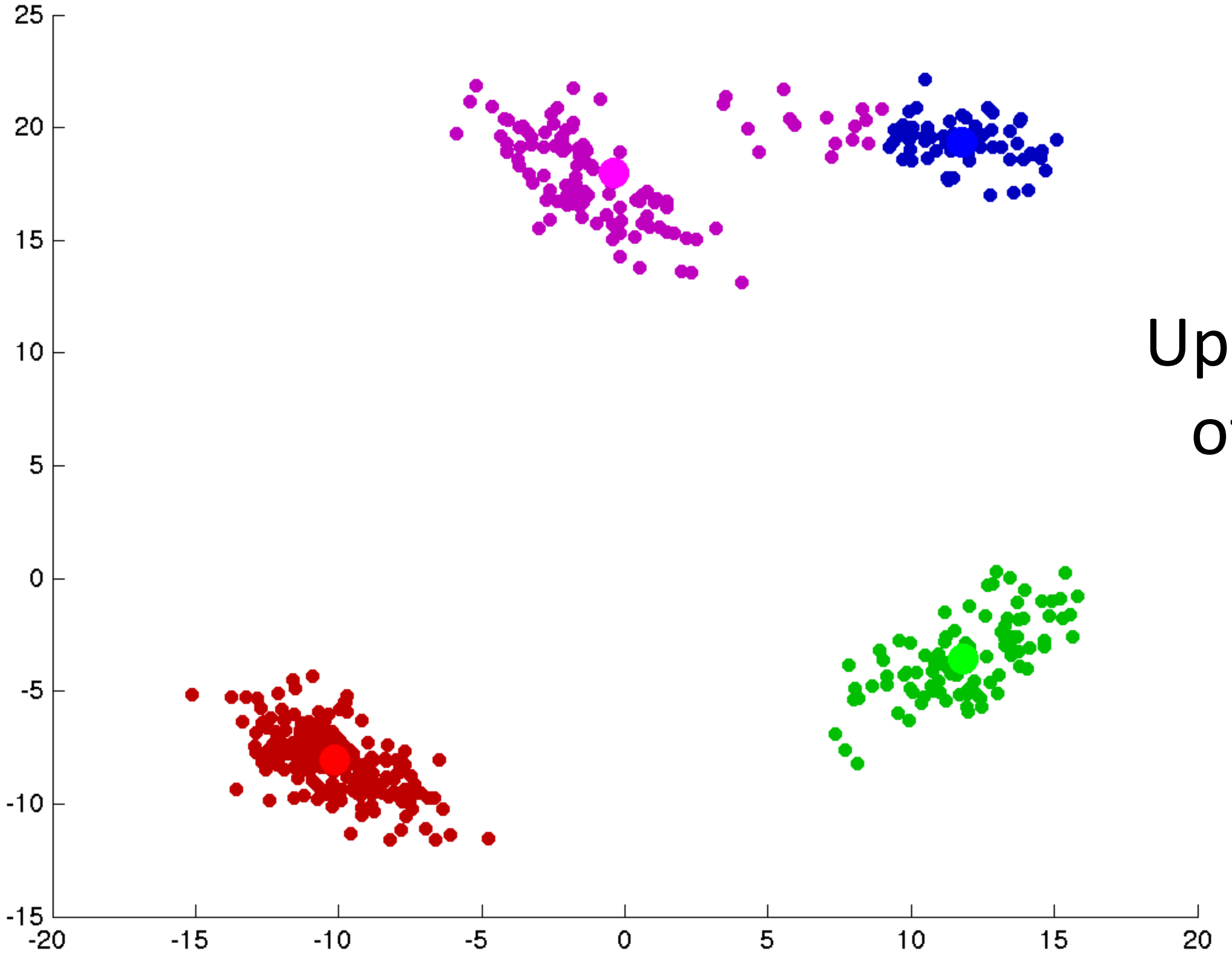
Update the mean of each group.

K-Means Example



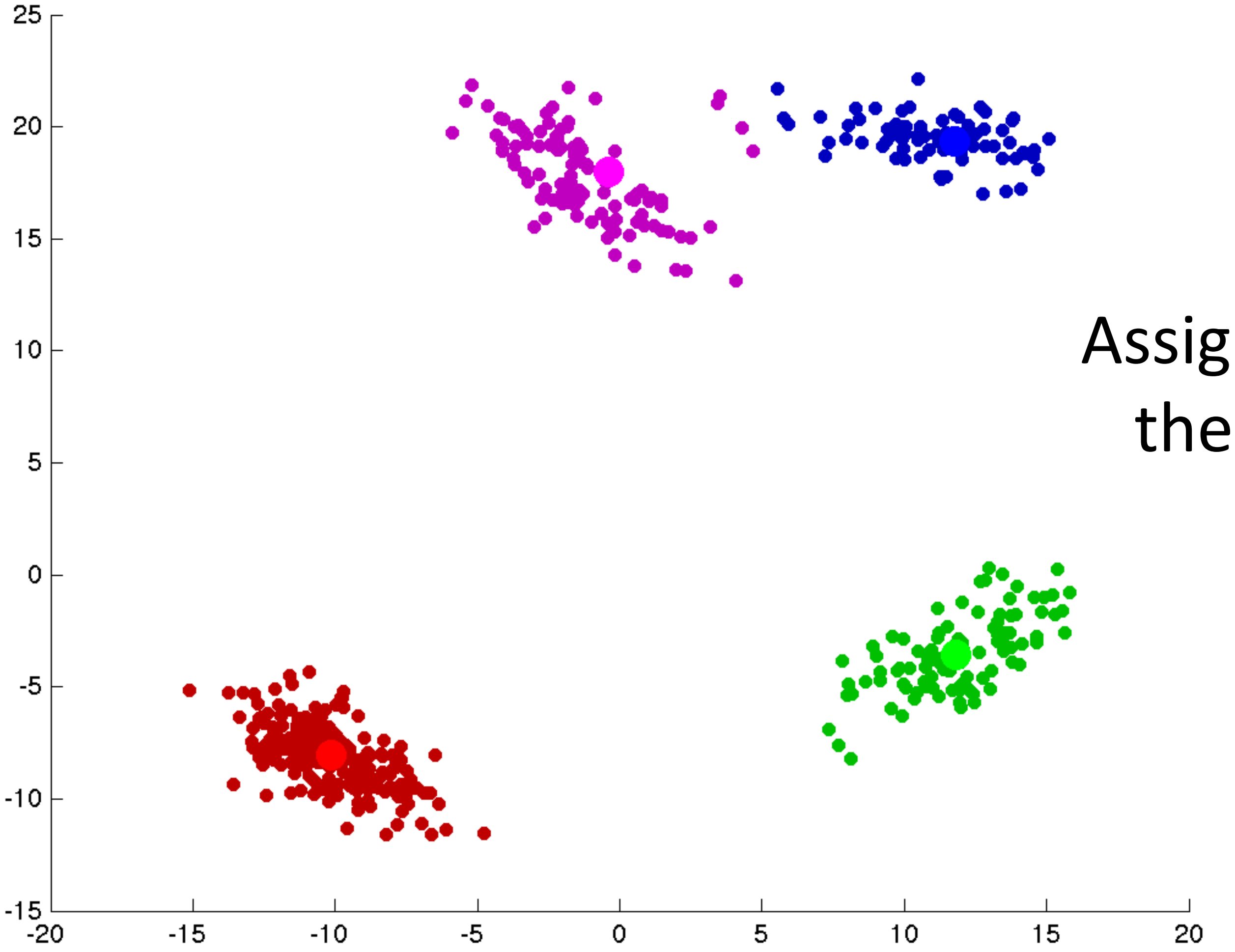
Assign each object to the closest mean.

K-Means Example



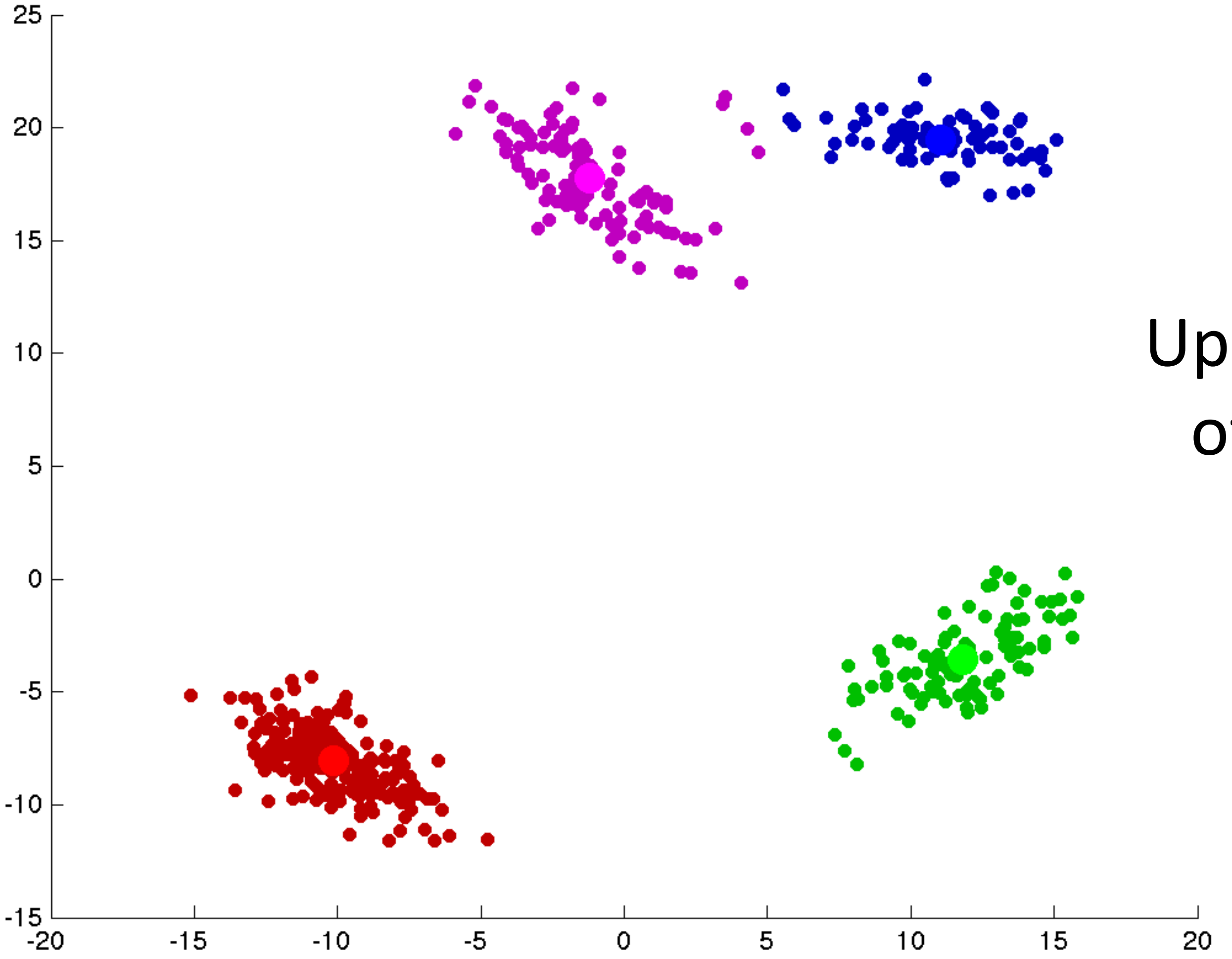
Update the mean of each group.

K-Means Example



Assign each object to the closest mean.

K-Means Example



Update the mean of each group.

Stop if no objects change groups.

Cost of K-means

- The bottleneck is calculating distance from x_i to mean c:

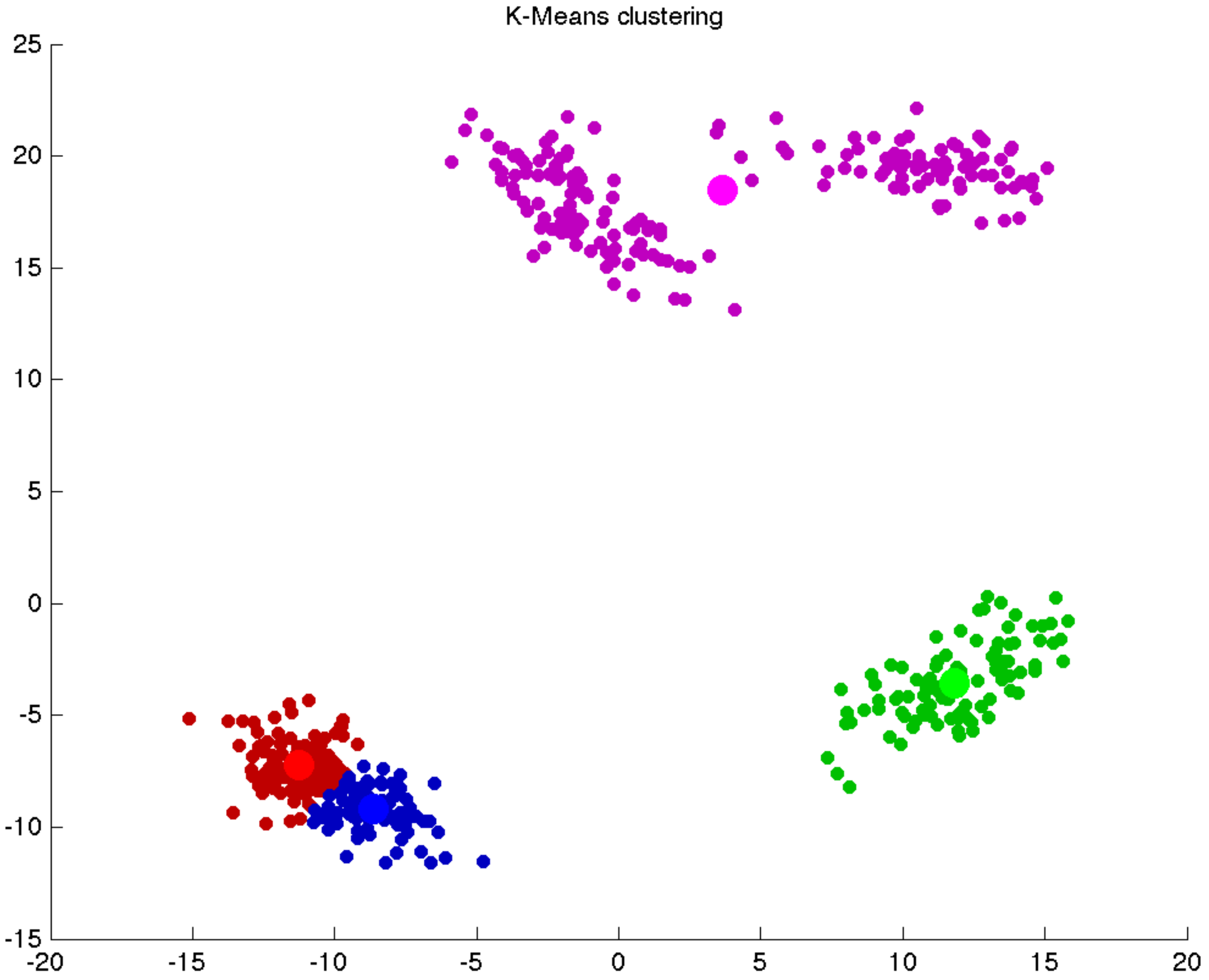
$$\|x_i - \mu_c\| = \sqrt{\sum_{j=1}^{d} (x_{ij} - \mu_{cj})^2}$$

- Each time we do this costs O(d) to go through all features.
- For each of the 'n' objects, we compute the distance to 'k' clusters.
- Total cost of assigning objects to clusters is O(ndk).
  - Fast if k is not too large.
- Updating means is cheaper: O(nd).

K-Means Issues

- Guaranteed to converge when using Euclidean distance.
- Clustering a new object:
  - Assign to the nearest mean.
- Assumes you know ‘k’.
- Each object is assigned to one (and only one) cluster:
  - No possibility to leave objects unassigned.
- It may converge to sub-optimal local solution…

K-Means Clustering with Different Initialization

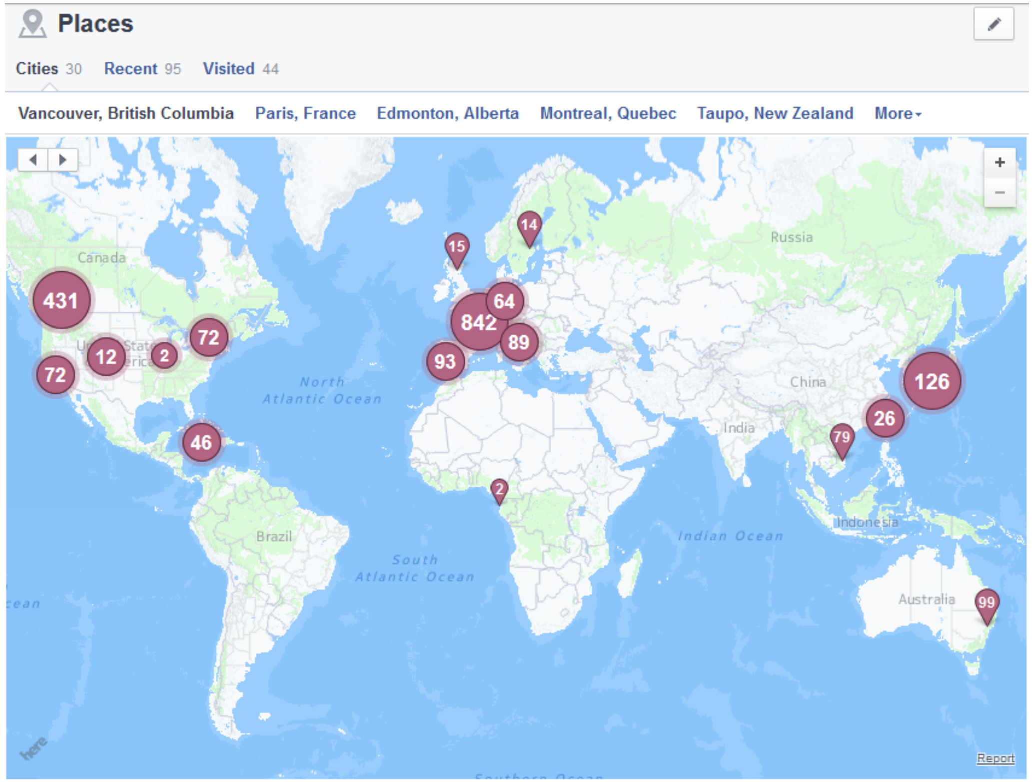


K-Means Initialization

- Classic approach to dealing with sensitivity to initialization:
  - Try several different random starting points, choose the ‘best’.
- Newer approach: K-Means++
  - Choose a random data point as the first mean.
  - Compute the distance of every point to the closets mean.
  - Sample the next proportional to these distances squared.
- K-Means++ tends to give means that are far apart.
  - Can prove it yields an approximation to optimal K-means clustering.

Vector Quantization

- K-means originally comes from signal processing.
- Designed for vector quantization:
  - Replace 'vectors' (objects) with a set of 'prototypes' (means).
- Example: Facebook places:



Vector Quantization: Image Colors

- Usual RGB representation of a pixel's color: three 8-bit numbers.
  - For example, [241 13 50] = .
  - Can apply k-means to find set of prototype colours.

Original:
(24-bits/pixel)

K-Means Quantized:
(6-bits/pixel)

Vector Quantization: Image Colors

- Usual RGB representation of a pixel's color: three 8-bit numbers.
  - For example, [241 13 50] = .
  - Can apply k-means to find set of prototype colours.

Original:
(24-bits/pixel)

K-Means Quantized:
(3-bits/pixel)

Vector Quantization: Image Colors

- Usual RGB representation of a pixel's color: three 8-bit numbers.
  - For example, [241 13 50] = .
  - Can apply k-means to find set of prototype colours.

Original:
(24-bits/pixel)

K-Means Quantized:
(2-bits/pixel)

Vector Quantization: Image Colors

- Usual RGB representation of a pixel's color: three 8-bit numbers.
  - For example, [241 13 50] = .
  - Can apply k-means to find set of prototype colours.

Original:
(24-bits/pixel)

K-Means Quantized:
(1-bits/pixel)

What is K-Means Doing?

- We can interpret K-Means as trying to minimize an objective:
  - Sum of distances from each object xi to its center:

$$f(\mu_1, \mu_2, \dots, \mu_k, c(1), c(2), \dots, c(n)) = \sum_{i=1}^{d} \| x_i - \mu_{c(i)} \|$$

- We alternate between:
  - Updating cluster assignments c(i).
  - Updating means μ_c.
- Convergence follows because
  - Each step does not increase the objective.
  - There are a finite number of assignments to k clusters.

K-Medoids

- With other distances, k-means may not converge.
- However, changing objective function gives convergent algorithms.
- E.g., we can use the L1-norm: $\|x_i - \mu_c\|_1 = \sum_{j=1}^{d} |x_{ij} - \mu_{cj}|$
- A 'k-medoids' algorithm based on the L1-norm optimizes:

$$f(\mu_1, \mu_2, \dots, \mu_k, c(1), c(2), \dots, c(n)) = \sum_{i=1}^{d} \|x_i - \mu_{c(i)}\|_1$$

  - Cluster assignment based on the L1-norm.
  - Update 'medoids' by setting them to the median.
- This approach is more robust to outliers.

Summary

- Unsupervised learning: fitting data without explicit labels.
- Clustering: finding ‘groups’ of related objects.
- K-means: simple iterative clustering strategy.
- Vector quantization: replacing measurements with ‘prototypes’.
- K-medoids: generalization to other distance functions.

- Next time:
  - Non-parametric clustering.