# Unsupervised Learning: Clustering

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Slides adapted from Vibhav Gogate, Carlos Guestrin, Dan Klein & Luke Zettlemoyer

# Machine Learning

Supervised Learning

Unsupervised Learning

Reinforcement Learning

Parametric

Non-parametric

Y Continuous

Y Discrete

Gaussians

Learned in closed form

Linear Functions

1. Learned in closed form
2. Using gradient descent

Decision Trees

Greedy search; pruning

Probability of class | features

1. Learn P(Y), P(X|Y); apply Bayes
2. Learn P(Y|X) w/ gradient descent

Non-probabilistic

Linear: perceptron gradient descent

Nonlinear: neural net: backprop

Support vector machines

# Overview of Learning

Type of Supervision

(eg, Experience, Feedback)

What is Being Learned?

| | Labeled Examples | Reward | Nothing |
|---|---|---|---|
| Discrete Function | Classification | | Clustering |
| Continuous Function | Regression | | |
| Policy | Apprenticeship Learning | Reinforcement Learning | |

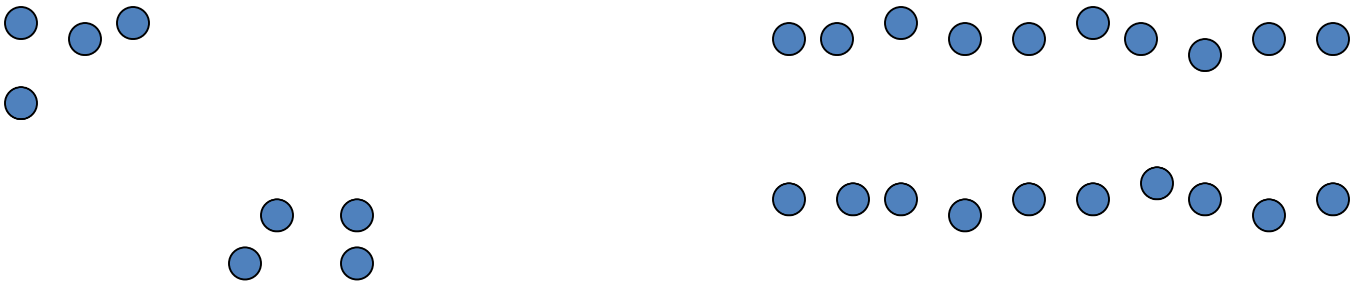
# Clustering

Clustering systems:

- Unsupervised learning
- Requires data, but no labels
- Detect patterns e.g. in
  - Group emails or search results
  - Customer shopping patterns
  - Program executions (intrusion detection)
- Useful when don’t know what you’re looking for
- But: often get gibberish

# Clustering

- Basic idea: group together similar instances
- Example: 2D point patterns



- What could "similar" mean?
  - One option: small (squared) Euclidean distance

$$\text{dist}(x, y) = (x - y)^{\top}(x - y) = \sum_i (x_i - y_i)^2$$

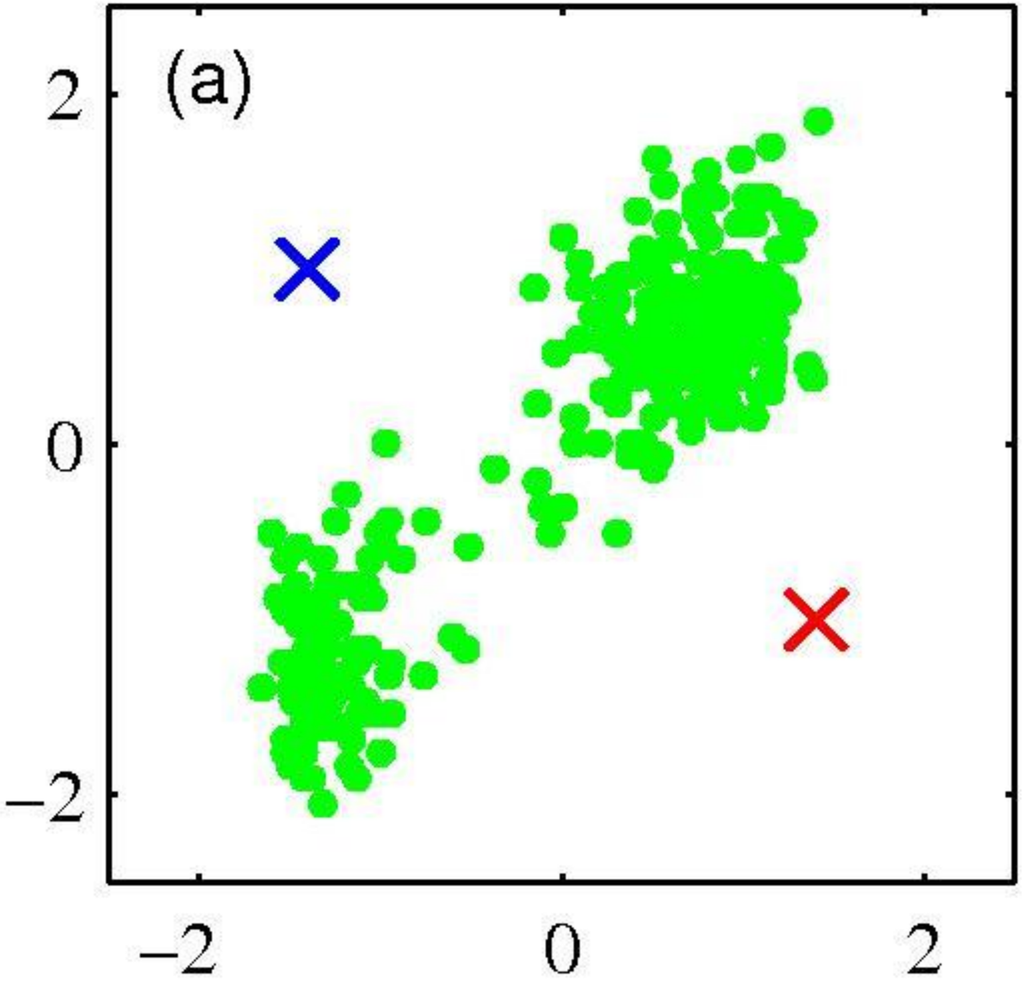
# Outline

- K-means & Agglomerative Clustering
- Agglomerative Clustering
- Expectation Maximization (EM)

# K-Means: Algorithm

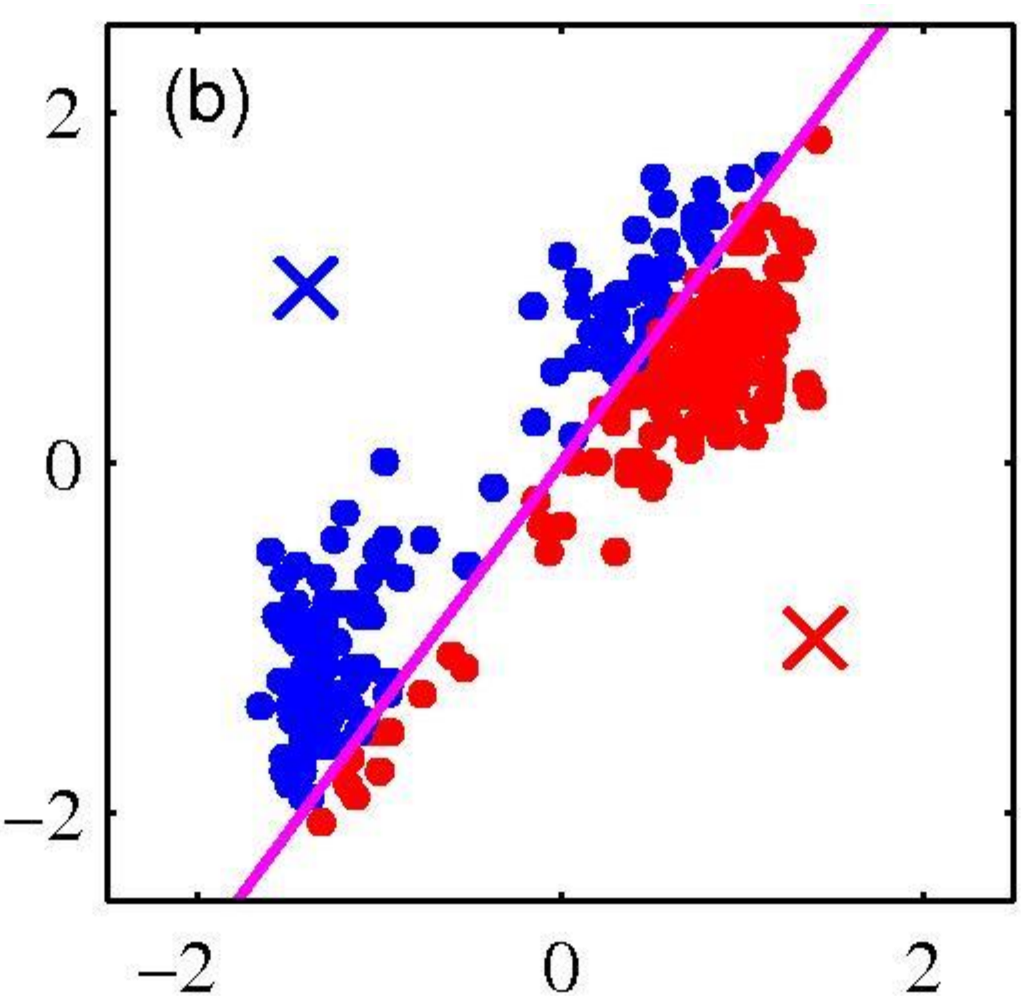
- An iterative clustering algorithm
  - Pick K random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest cluster center
    - Change the cluster center to the average of its assigned points
  - Stop when no points' assignments change

# K-means clustering: Example




- Pick K random points as cluster centers (means)

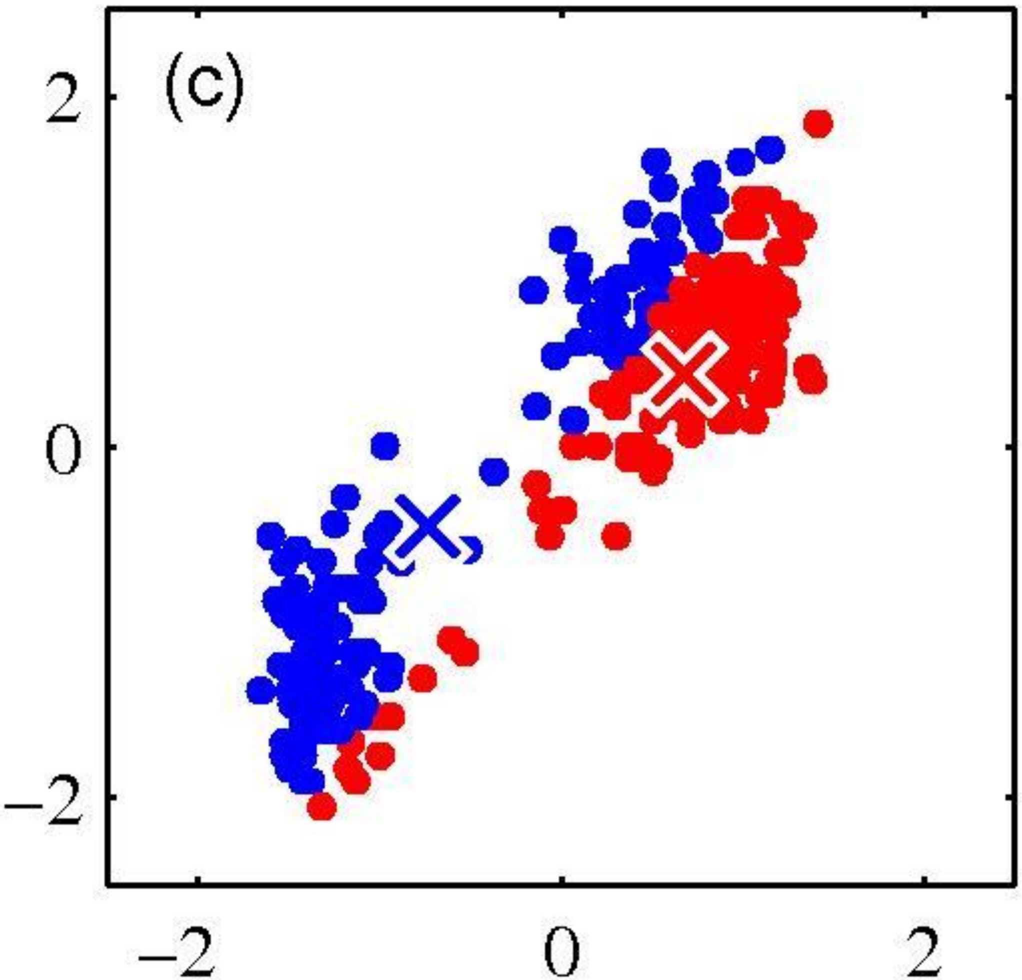
# K-means clustering: Example




Iterative Step 1

- Assign data instances to closest cluster center

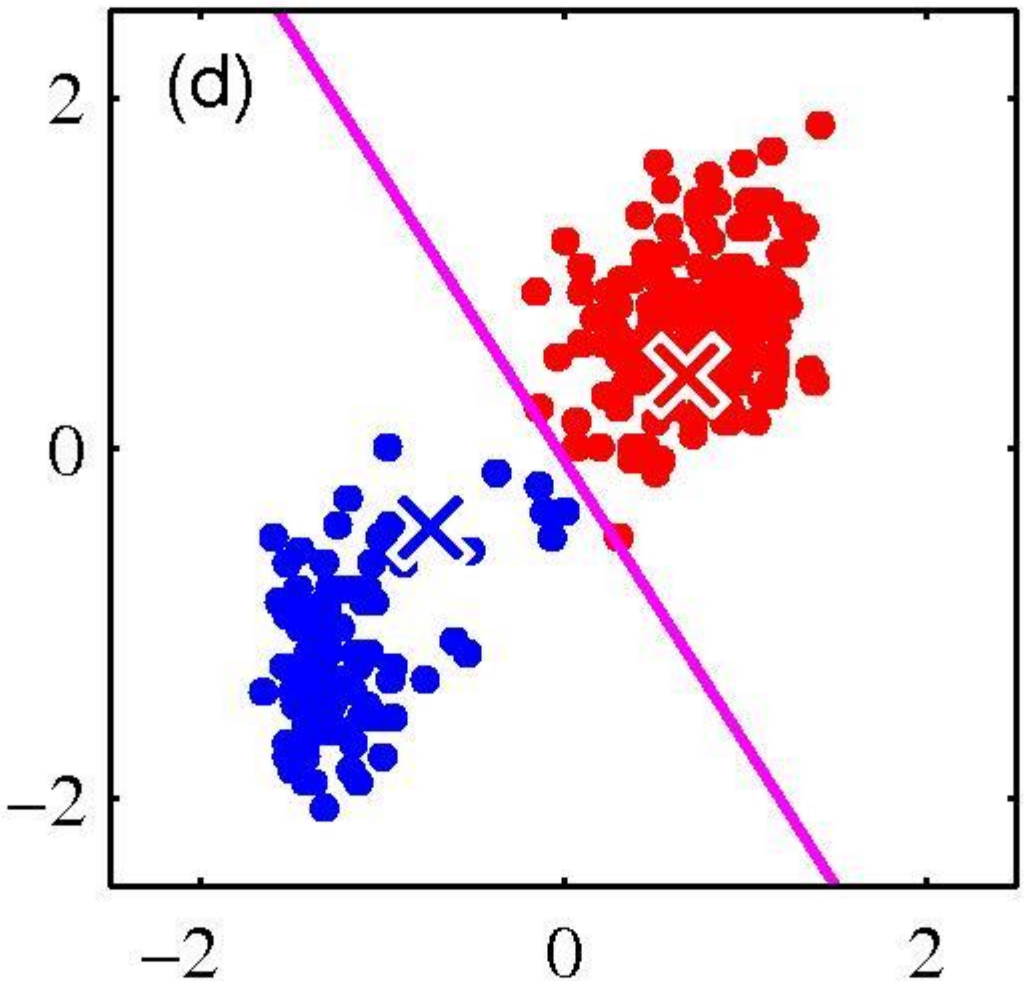
# K-means clustering: Example




Iterative Step 2

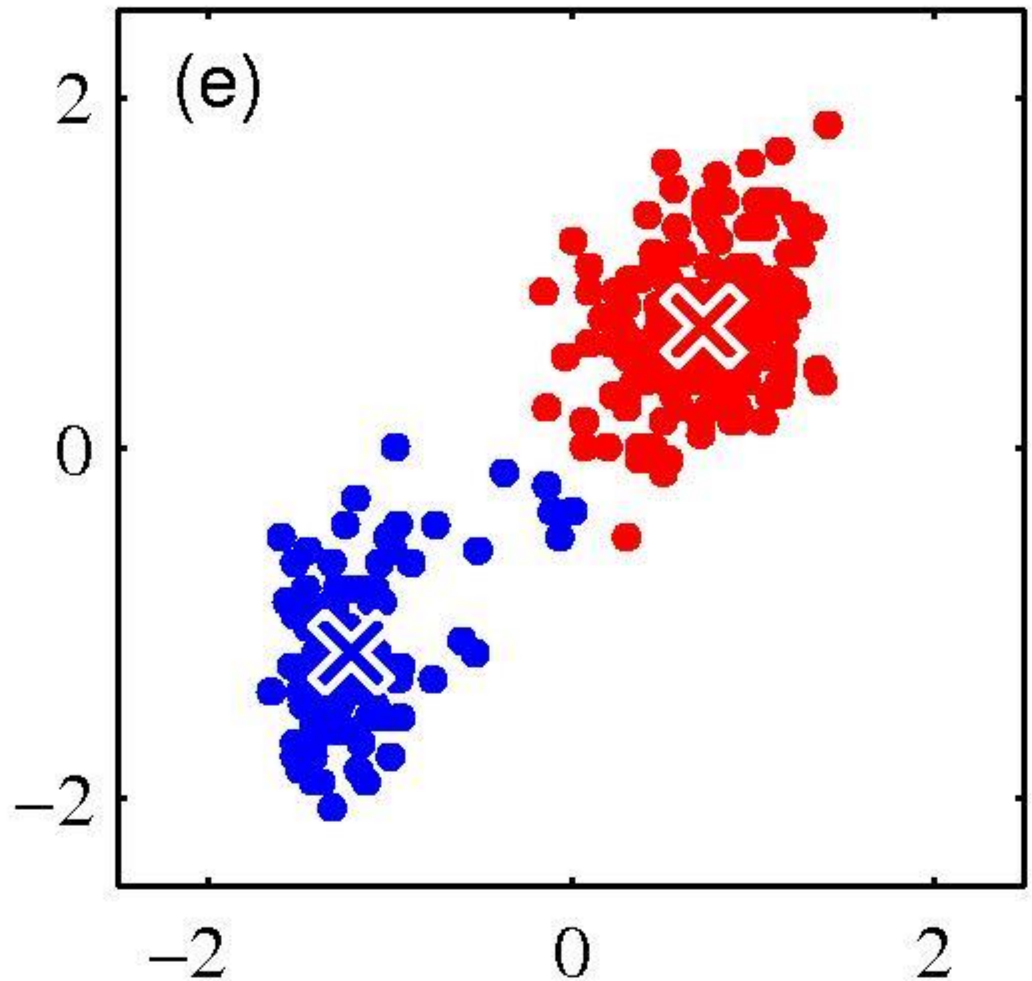
- Change the cluster center to the average of the assigned points

# K-means clustering: Example

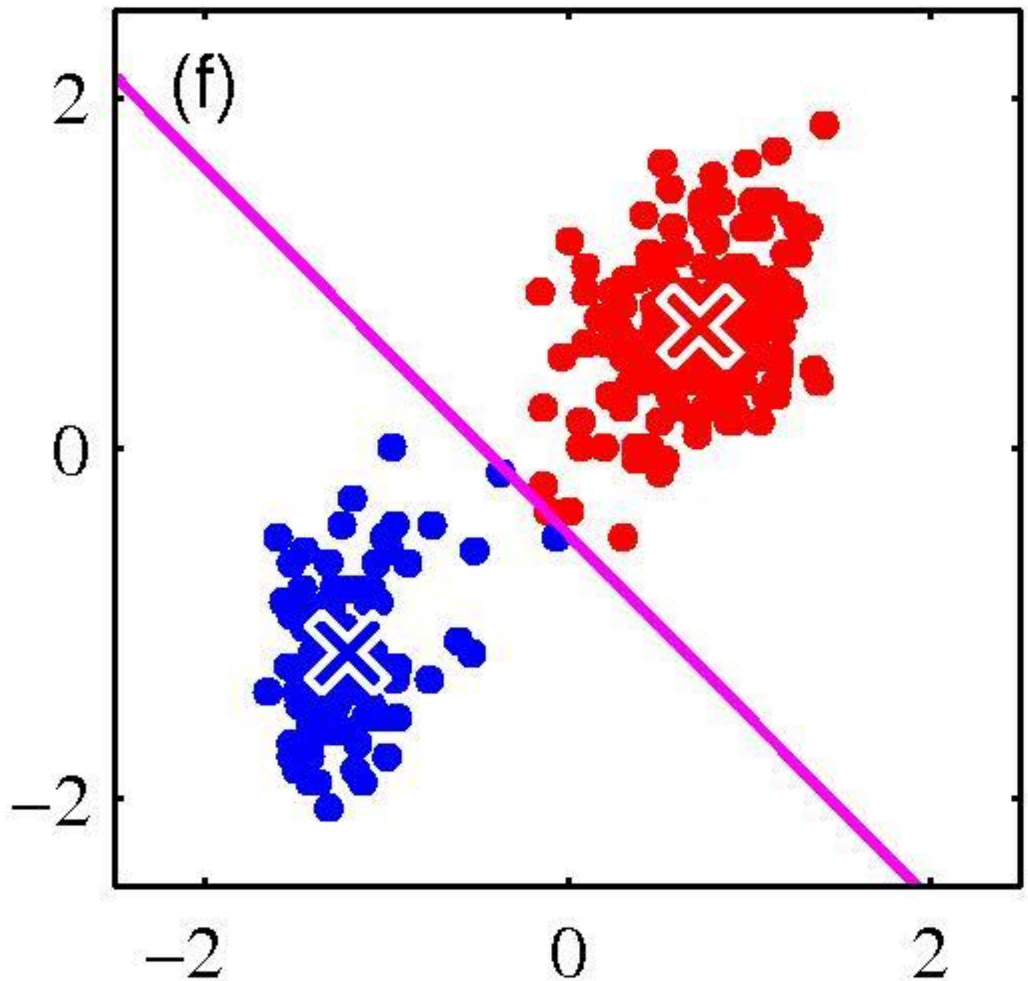



- Repeat until convergence

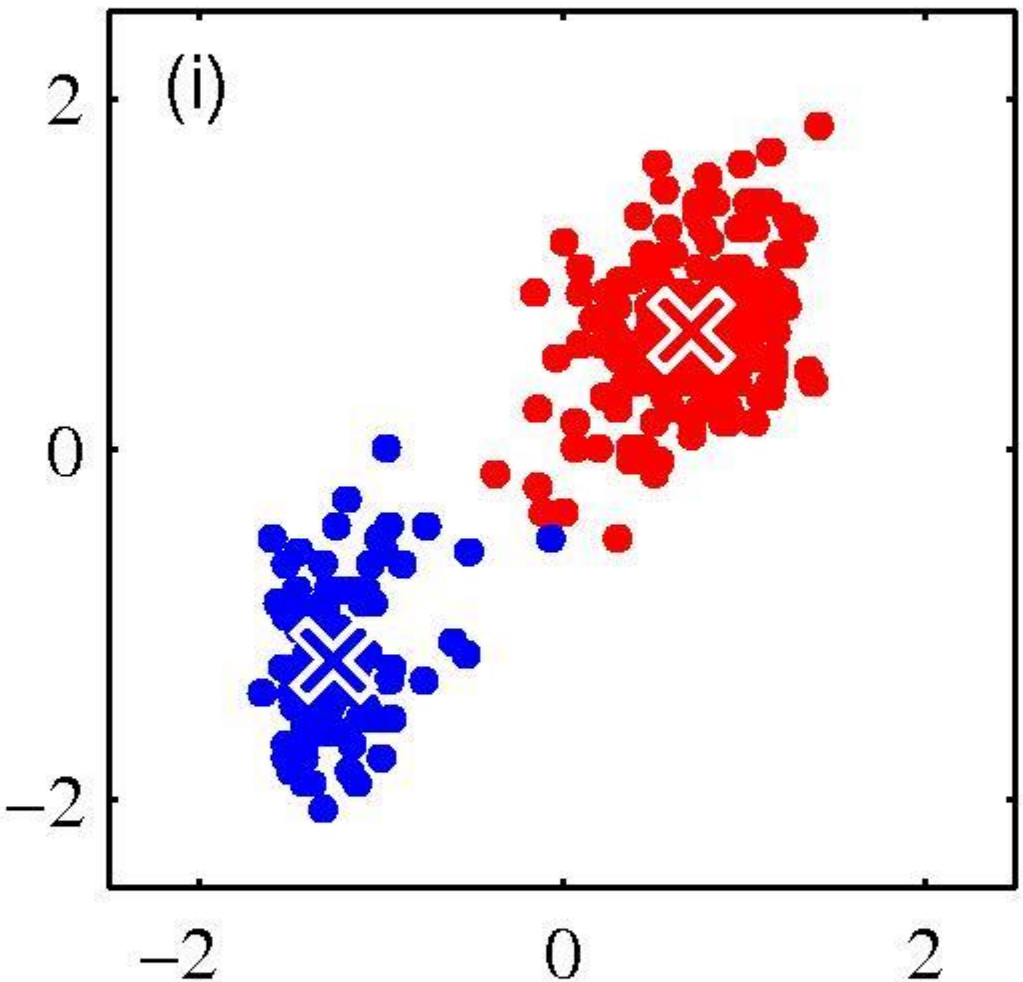
# K-means clustering: Example



# K-means clustering: Example



# K-means clustering: Example



# Example: K-Means for Segmentation

K=2

**Goal of Segmentation is to partition an image into regions each of which has reasonably homogenous visual appearance.**

Original

# Example: K-Means for Segmentation

K=2 K=3 Original





# Example: K-Means for Segmentation

| K=2 | K=3 | K=10 | Original |
|---|---|---|---|
|  |  |  |  |
|  |  |  |  |
| 4% | 8% | 17% | |

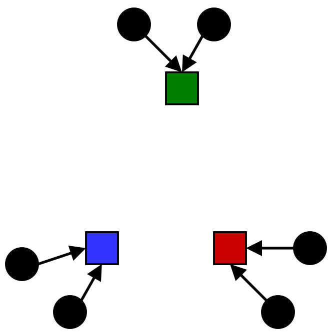
# K-Means as Optimization

- Consider the total distance to the means:

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

points assignments means

- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c



- Co-ordinate Gradient Descent
- Will it converge?
  - Yes!, if you can argue that each update can't increase Φ

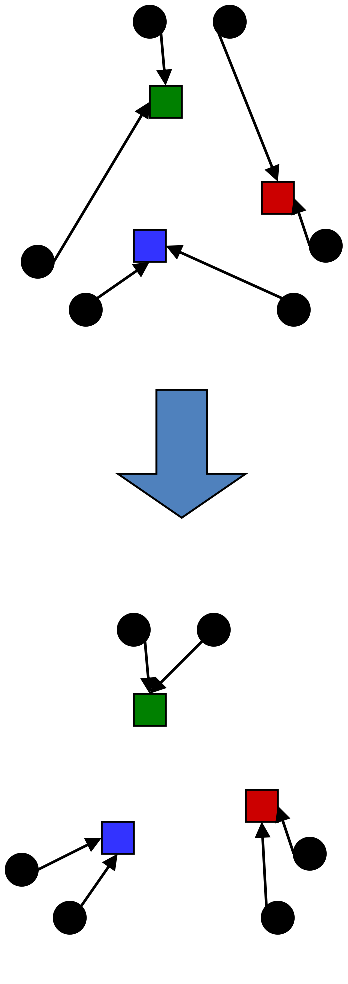
# Phase I: Update Assignments

- For each point, re-assign to closest mean:

$$a_i = \underset{k}{\operatorname{argmin}}\, \text{dist}(x_i, c_k)$$

- Can only decrease total distance phi!

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

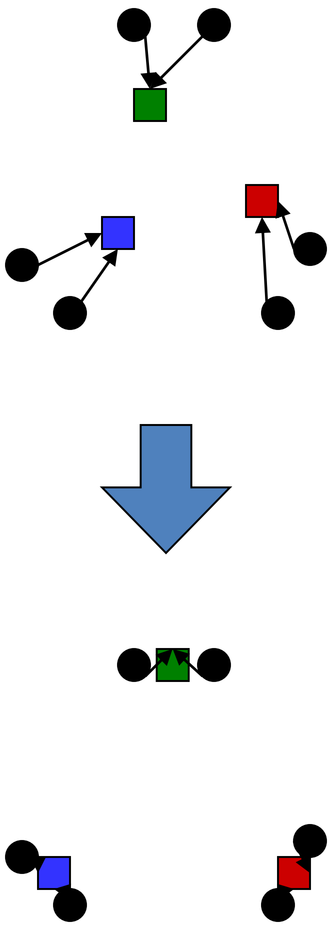


# Phase II: Update Means

- Move each mean to the average of its assigned points:

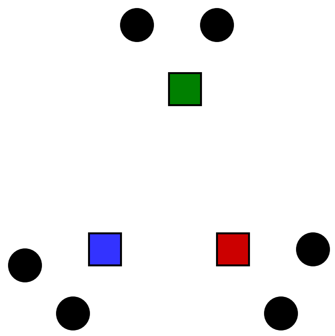
$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

- Also can only decrease total distance… (Why?)
- Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean

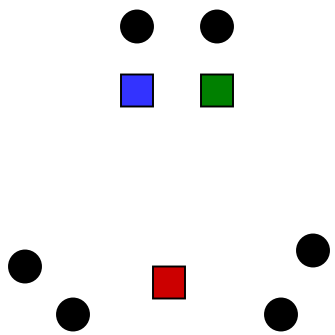


# Initialization

- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!

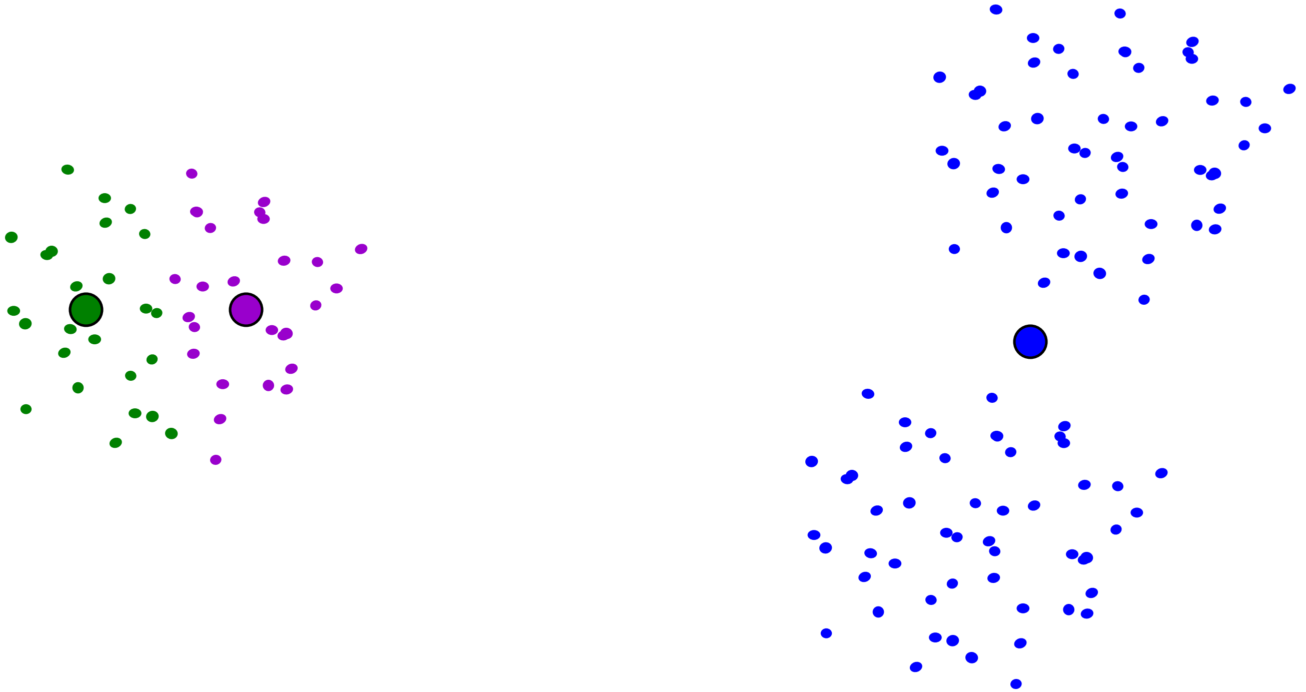


  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



# K-Means Getting Stuck

A local optimum:

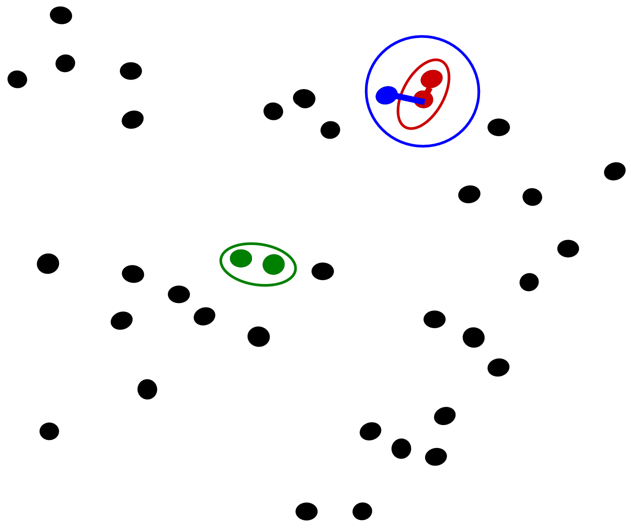


# K-Means Questions

- Will K-means converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
  - If the patterns are very very clear?
- Runtime?
- Do people ever use it?
- How many clusters to pick?

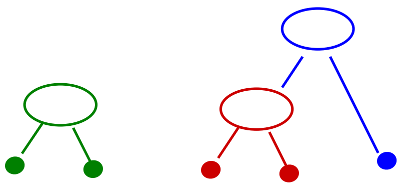
# Agglomerative Clustering

- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters



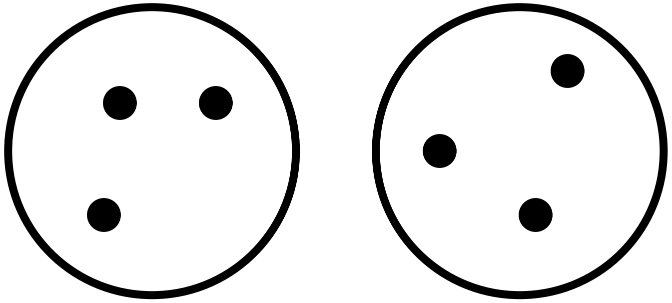
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left

- Produces not one clustering, but a family of clusterings represented by a dendrogram



# Agglomerative Clustering

- How should we define “closest” for clusters with multiple elements?



# Agglomerative Clustering

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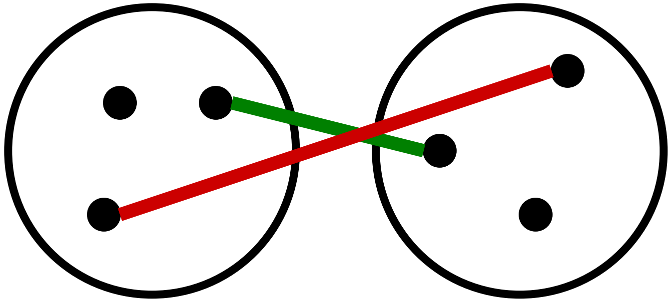
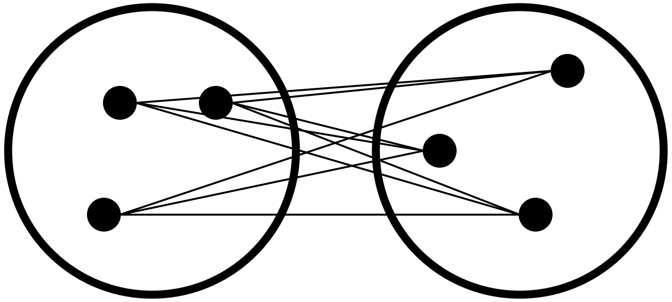
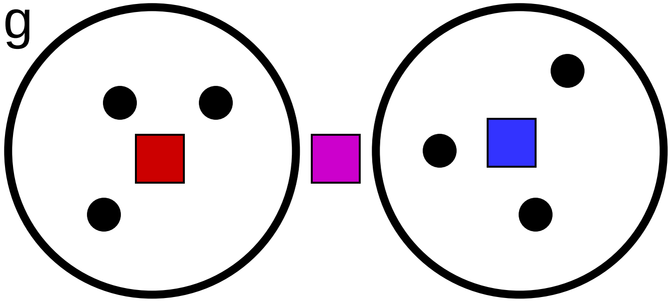


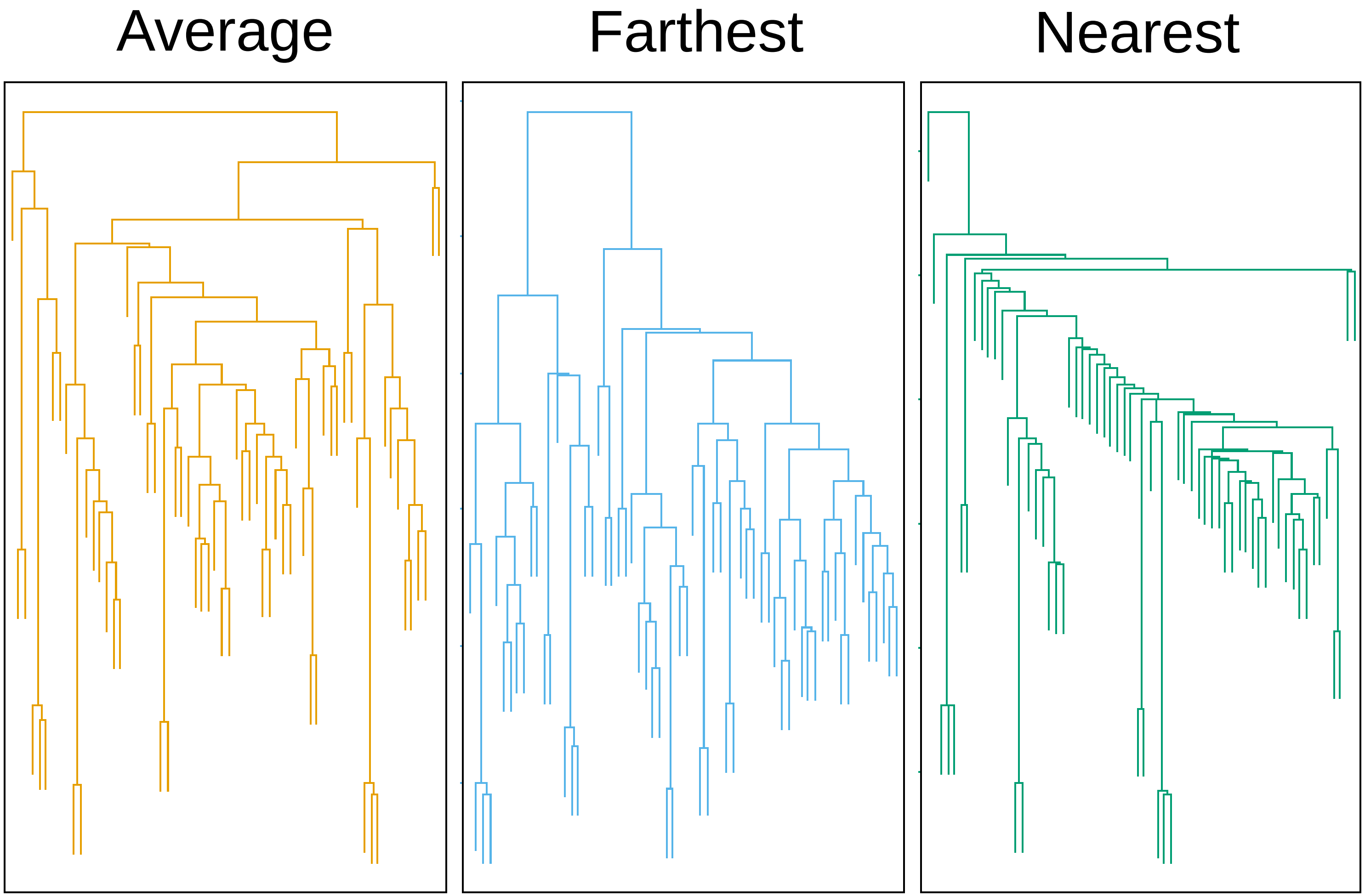
- Many options:
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs
  - Ward’s method (min variance, like k-means)
    - Find pair of clusters that leads to minimum increase in total within cluster distance after merging





- Different choices create different clustering behaviors

# Clustering Behavior




Mouse tumor data from [Hastie]

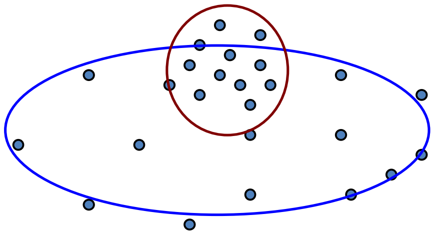
# Agglomerative Clustering Questions

- Will agglomerative clustering converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
- Do people ever use it?
- How many clusters to pick?

# EM: Soft Clustering

- Clustering typically assumes that each instance is given a "hard" assignment to exactly one cluster.
- Does not allow uncertainty in class membership or for an instance to belong to more than one cluster.
  - Problematic because data points that lie roughly midway between cluster centers are assigned to one cluster
- *Soft clustering* gives probabilities that an instance belongs to each of a set of clusters.

# Probabilistic Clustering



- Try a probabilistic model!
  - allows overlaps, clusters of different size, etc.
- Can tell a *generative story* for data
  - $P(X|Z)\ P(Z)$
- Challenge: we need to estimate model parameters without labeled Zs

| Z | $X_1$ | $X_2$ |
|---|---|---|
| ?? | 0.1 | 2.1 |
| ?? | 0.5 | -1.1 |
| ?? | 0.0 | 3.0 |
| ?? | -0.1 | -2.0 |
| ?? | 0.2 | 1.5 |
| … | … | … |

# Finite Mixture Models

$\underline{x}_i$ is a $d$-dimensional vector

- Given a dataset: $D = \{\underline{x}_1, \ldots, \underline{x}_N\}$
- **Mixture model**: $\Theta = \{\alpha_1, \ldots, \alpha_K, \theta_1, \ldots, \theta_K\}$

$$p(\underline{x}|\Theta) = \sum_{k=1}^{K} \alpha_k p_k(\underline{x}|z_k, \theta_k)$$

The $p_k(\underline{x}|z_k, \theta_k)$ are *mixture components*, $1 \leq k \leq K$

$z = (z_1, \ldots, z_K)$ is a vector of $K$ binary indicator variables

Note: only one of them equals 1 at any given point. Each point is assumed to be generated from exactly one mixture component!

**Mixture Weights.** $\alpha_k = p(z_k)$ $\sum_{k=1}^{K} \alpha_k = 1.$

# Finite Mixture Model: Probabilistic View

the "membership weight" of data point $\underline{x}_i$ in cluster $k$, given parameters $\Theta$

$$w_{ik} = p(z_{ik} = 1 | \underline{x}_i, \Theta) = \frac{p_k(\underline{x}_i | z_k, \theta_k) \cdot \alpha_k}{\sum_{m=1}^{K} p_m(\underline{x}_i | z_m, \theta_m) \cdot \alpha_m}$$

- The membership weight express our uncertainty about which of the "K" components generated the vector $\underline{x}_i$.

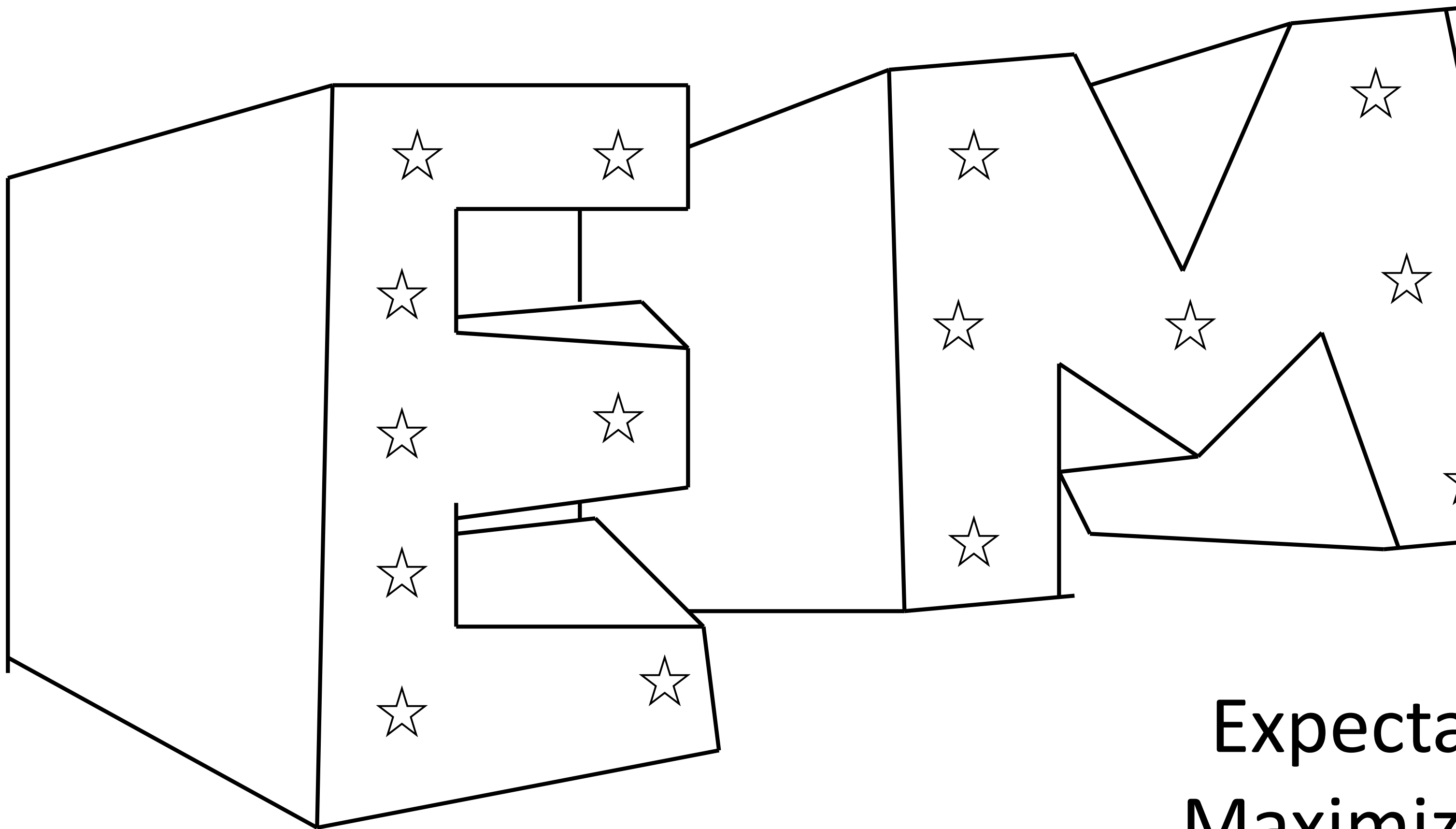
# Gaussian Mixture Models (GMMs)

$$p_k(\underline{x}|\theta_k) \;=\; \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} e^{-\frac{1}{2}(\underline{x}-\underline{\mu}_k)^t \Sigma_k^{-1} (\underline{x}-\underline{\mu}_k)}$$

- We can define a GMM by making each "k-th" component a Gaussian density with parameters:

$$\theta_k = \{\underline{\mu}_k, \Sigma_k\}$$

**Question: How to learn these parameters from data?**



Expectation
Maximization

# EM algorithm: Key Idea

- Start with random parameters
- Find a class for each example (E-step)
  - Since we are using probabilistic classification, each example will be given a vector of probabilities
- Now we have a supervised learning problem. Estimate the parameters of the model using the maximum likelihood method (M-step)
- Iterate between the E-step and M-step until convergence

# EM: Two Easy Steps

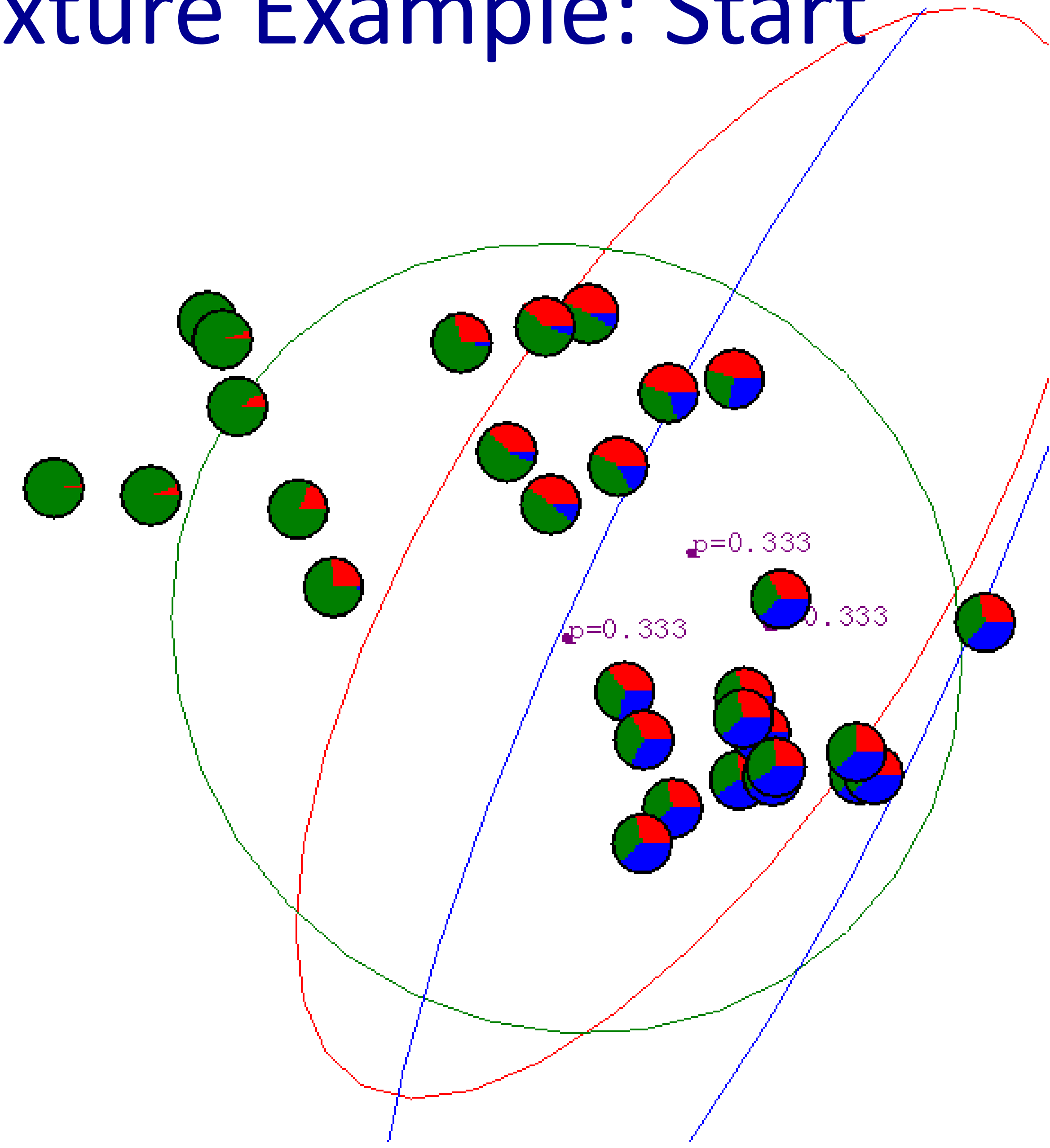
- E-step: (Yields a N x K matrix)
  - Compute $w_{ik}$ for all data points indexed by "i" and all mixture components indexed by "k."
- M-step:
  - Use the membership weights and data to compute the new parameters

$$N_k = \sum_{i=1}^{N} w_{ik} \qquad \alpha_k^{new} = \frac{N_k}{N}$$

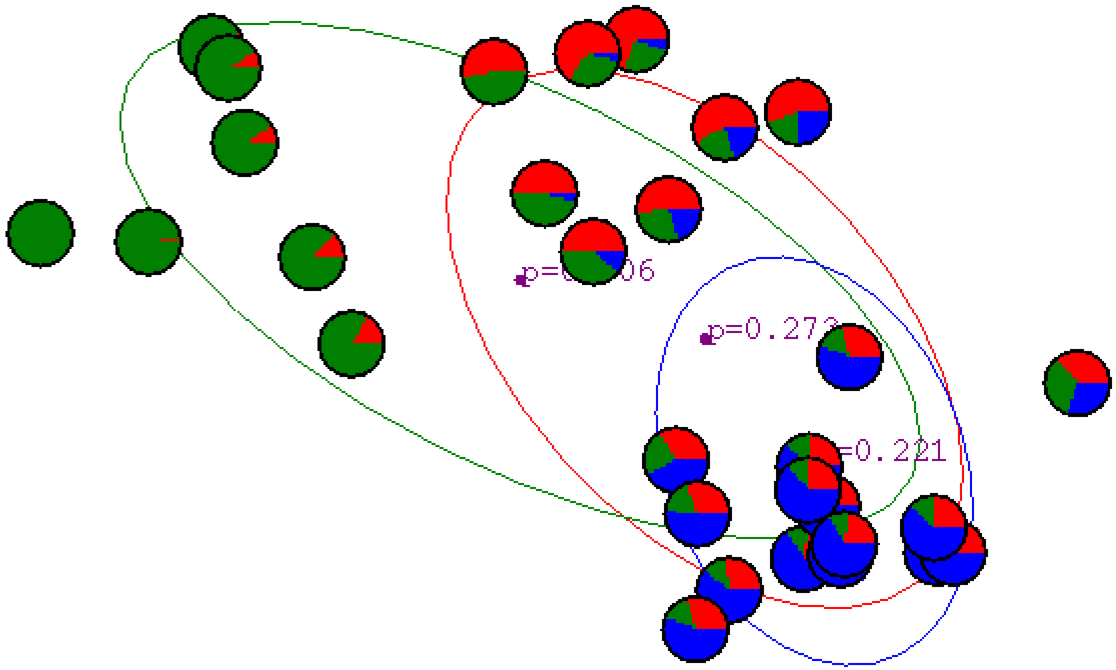
$$\underline{\mu}_k^{new} = \left(\frac{1}{N_k}\right) \sum_{i=1}^{N} w_{ik} \cdot \underline{x}_i$$

$$\Sigma_k^{new} = \left(\frac{1}{N_k}\right) \sum_{i=1}^{N} w_{ik} \cdot (\underline{x}_i - \underline{\mu}_k^{new})(\underline{x}_i - \underline{\mu}_k^{new})^t$$

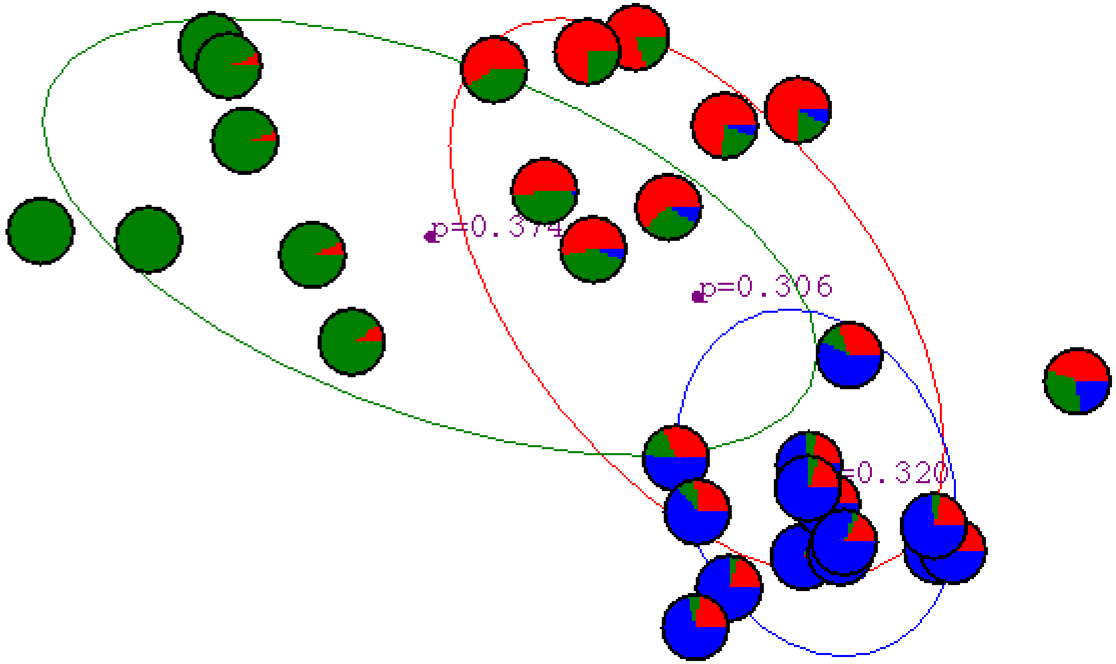
# Gaussian Mixture Example: Start



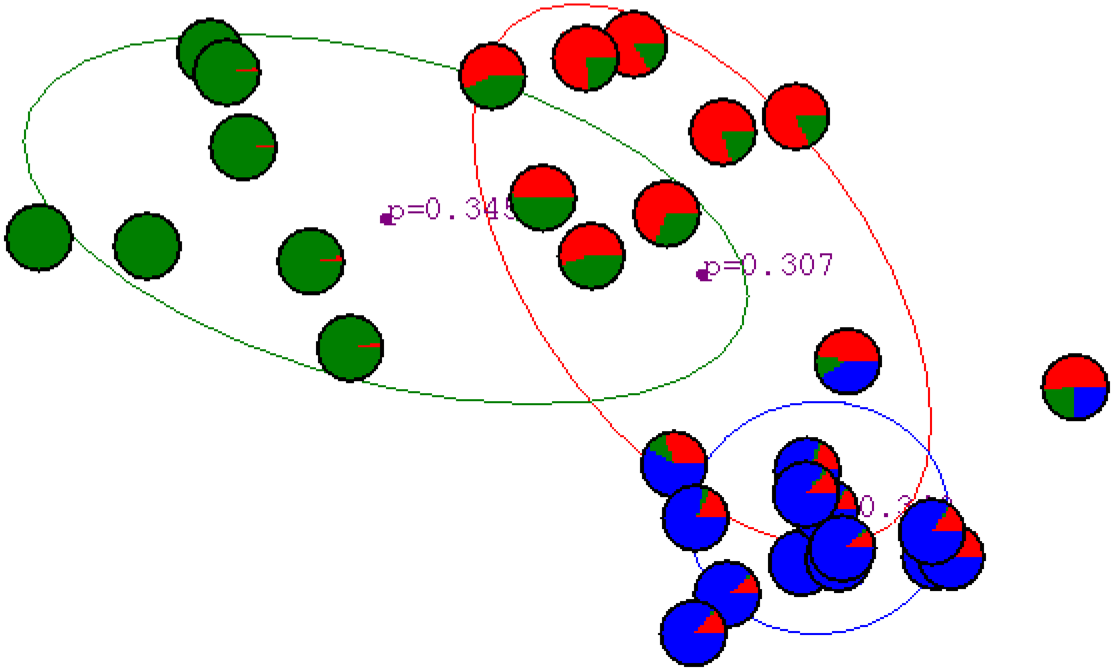
# After first iteration



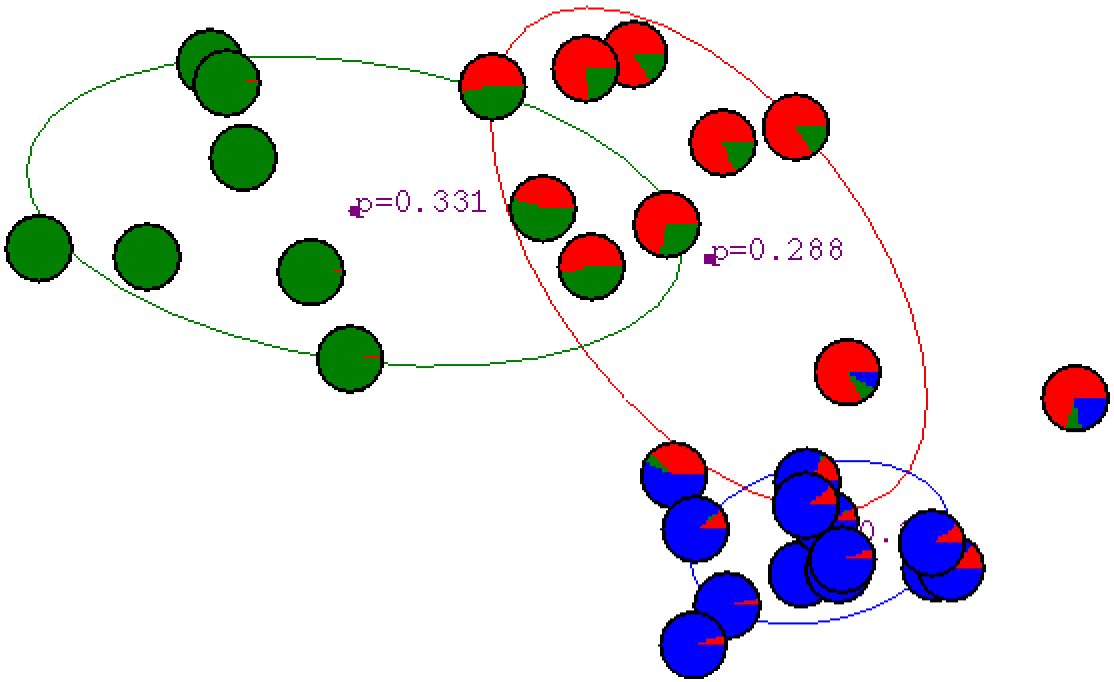
# After 2nd iteration



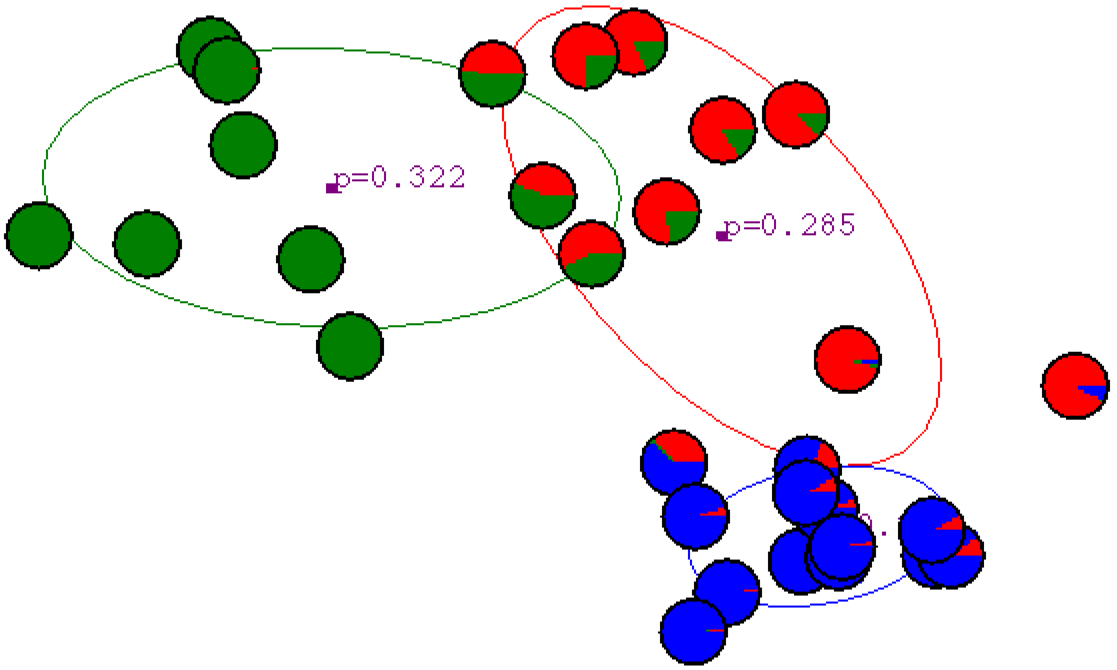
# After 3rd iteration



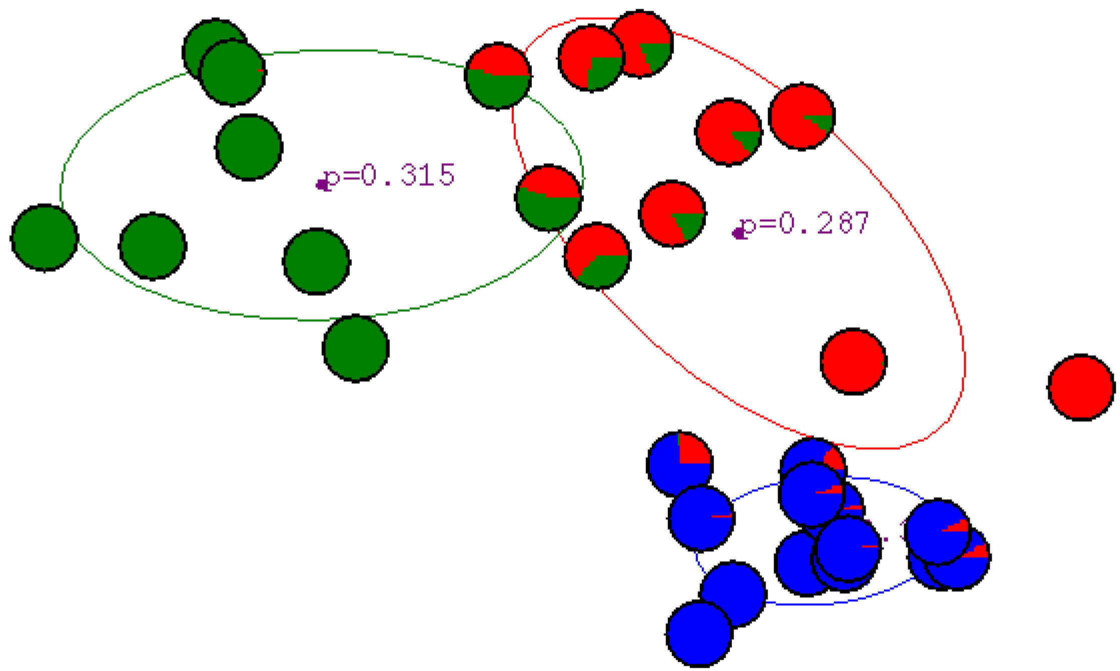
# After 4th iteration



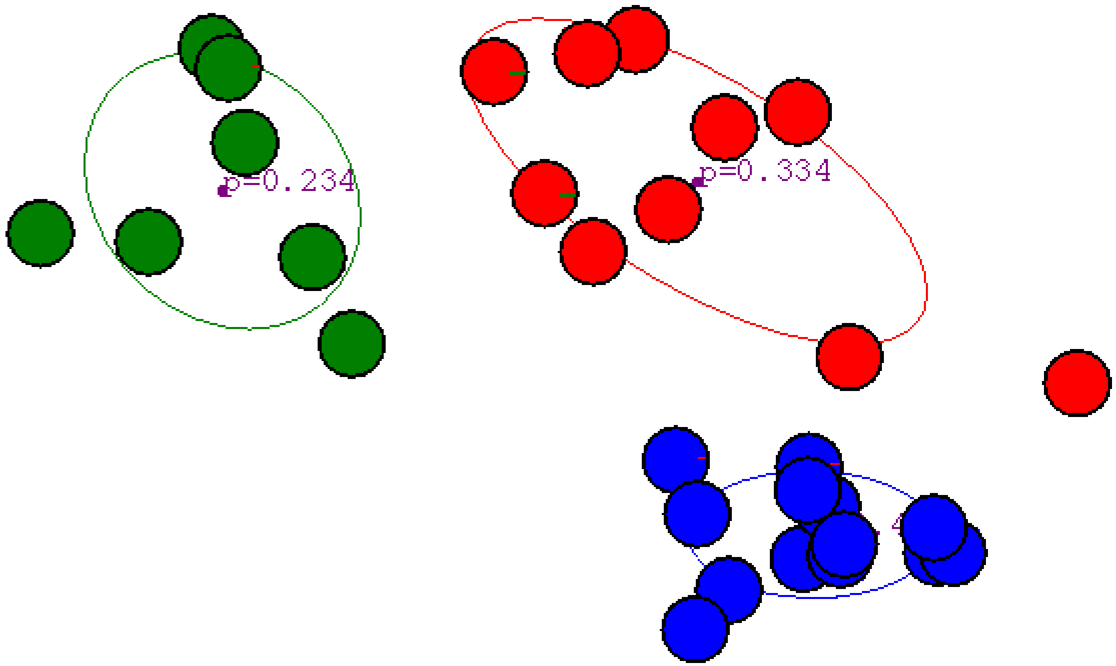
# After 5th iteration



# After 6th iteration



# After 20th iteration



# Properties of EM

- EM converges to a local minima
  - This is because each iteration improves the log-likelihood
  - Proof same as K-means
    - E-step can never decrease likelihood
    - M-step can never decrease likelihood
- If we make hard assignments instead of soft ones. Algorithm is equivalent to K-means!

# What you should know

- K-means for clustering:
  - algorithm
  - converges because it's coordinate ascent
- Know what agglomerative clustering is
- EM for mixture of Gaussians:
- Remember, E.M. can get stuck in local minima,
  - And empirically it ***DOES!***