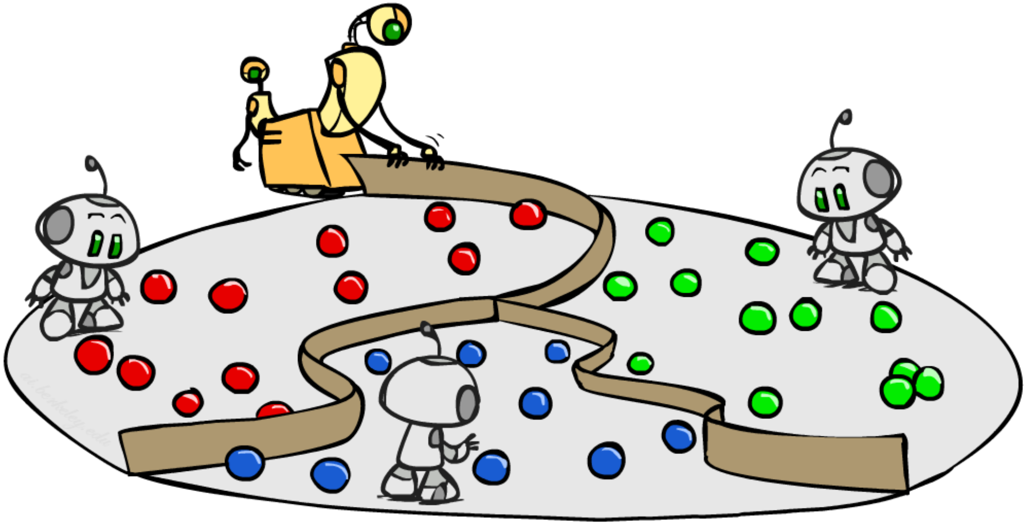
Proposal Presentation

- Proposal presentation
  - 5 min presentation: topic, motivation, possible methods
  - May. 24, in class
  - Presentation schedule & slides submission on BB

Unsupervised Machine Learning



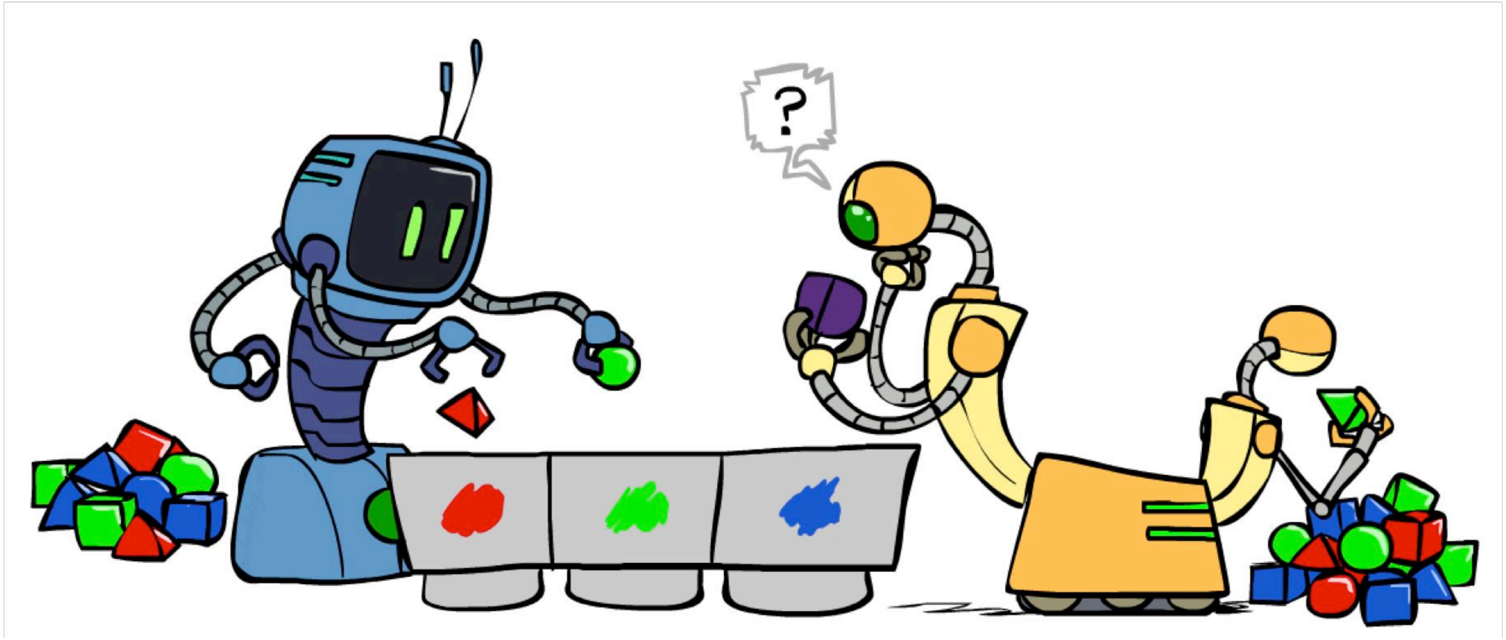
AIMA Chapter 20

[Adapted from slides by Dan Klein and Pieter Abbeel at UC Berkeley and from Daniel Weld, Carlos Guestrin, & Luke Zettlemoyer at U Washington]

Types of Learning

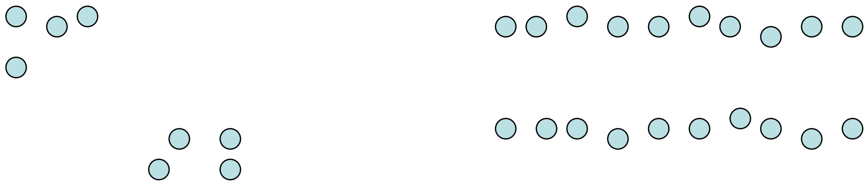
- Supervised learning
  - Training data includes desired outputs
- Unsupervised learning
  - Training data does not include desired outputs
- Semi-supervised learning
  - Training data includes a few desired outputs
- Reinforcement learning
  - Rewards from sequence of actions

Clustering



Clustering

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



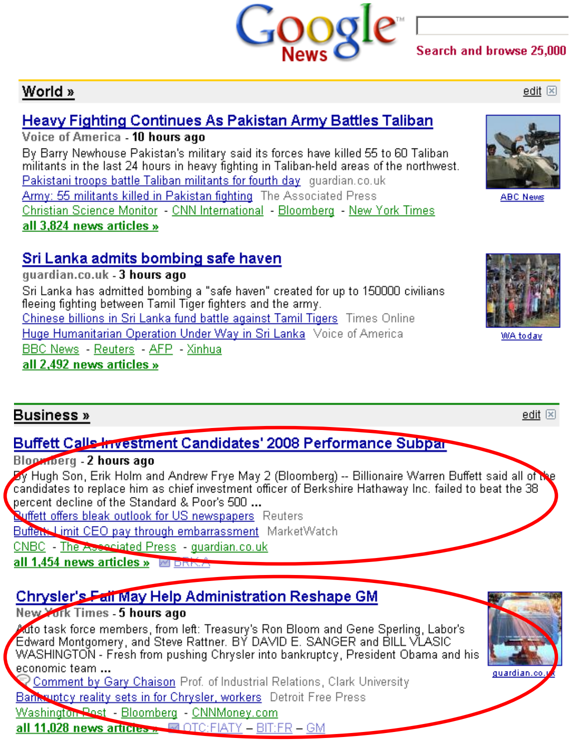
- What could "similar" mean?
  - One option: small (squared) Euclidean distance

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

  - Many other options, often domain specific

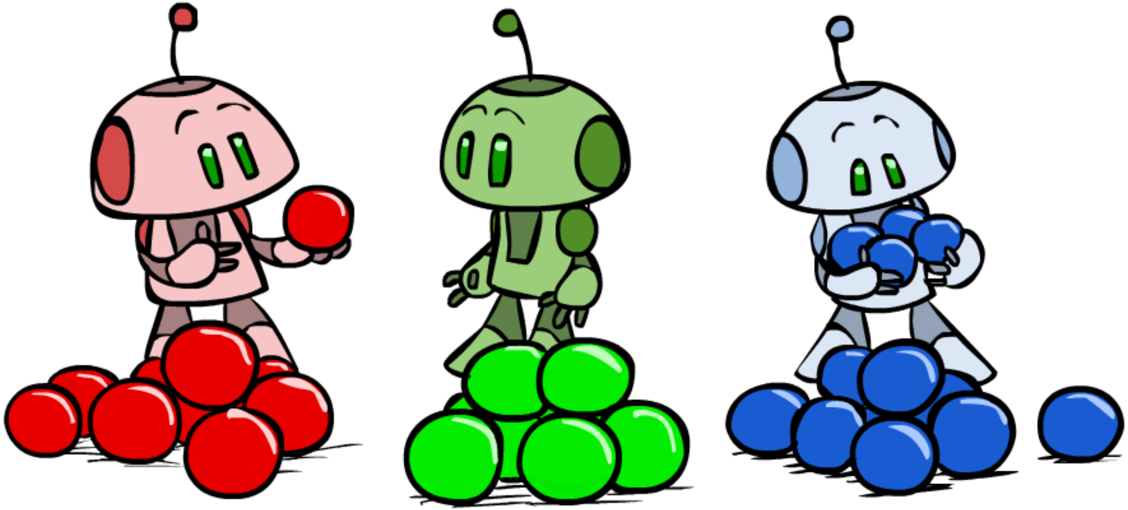
Clustering

- Applications
  - Group emails
  - Group search results
  - Find categories of customers
  - Detect anomalous program executions



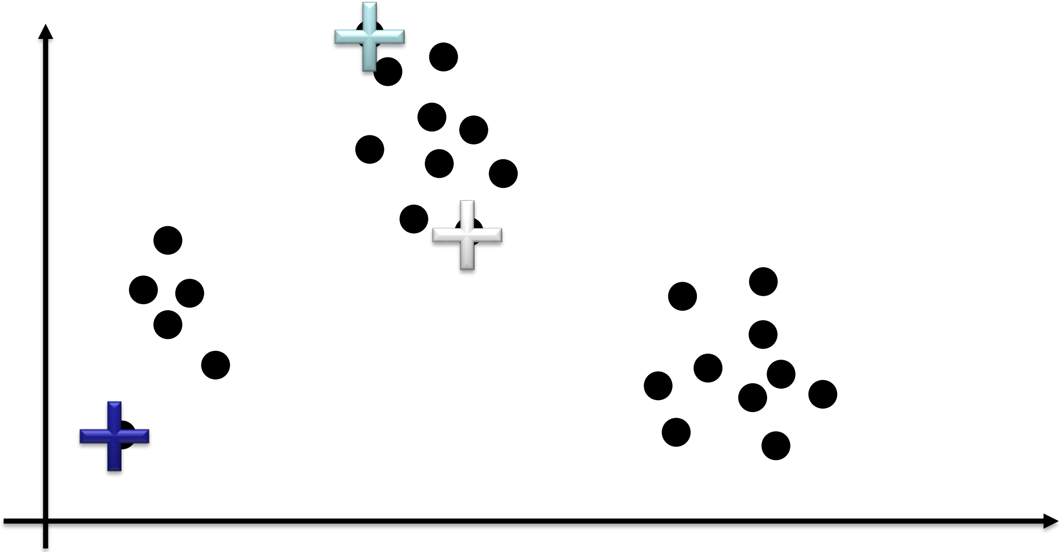
Story groupings:
unsupervised clustering

K-Means



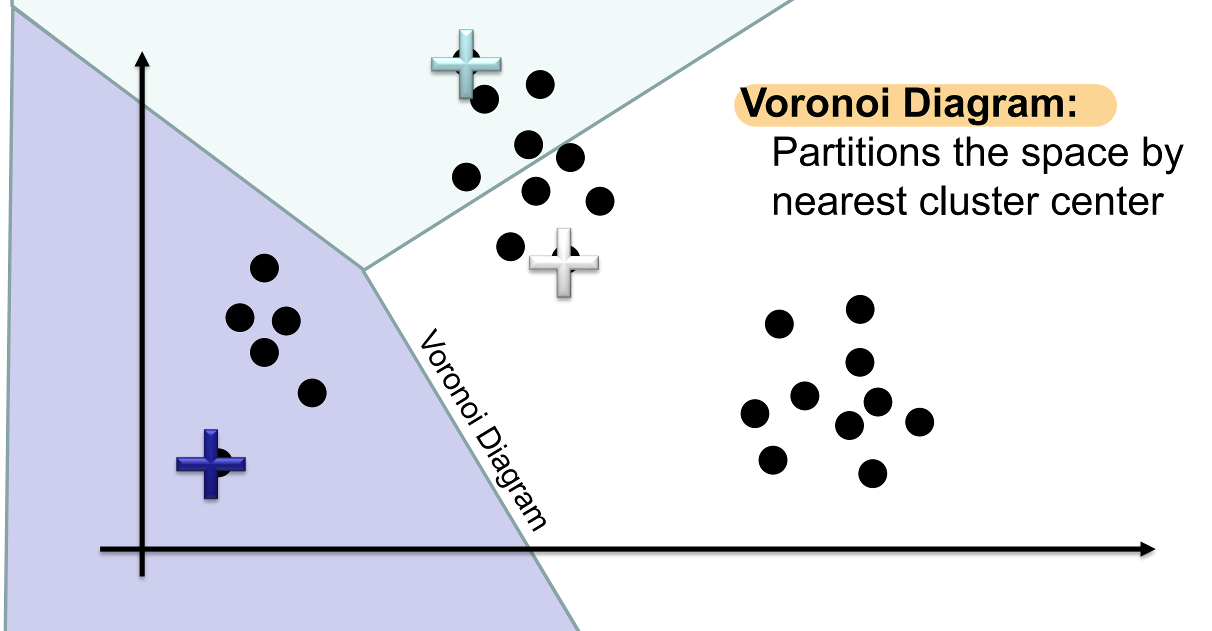
K-Means Clustering: *Intuition*

- Input K: The number of clusters to find
- Pick an initial set of points as cluster centers



K-Means Clustering: *Intuition*

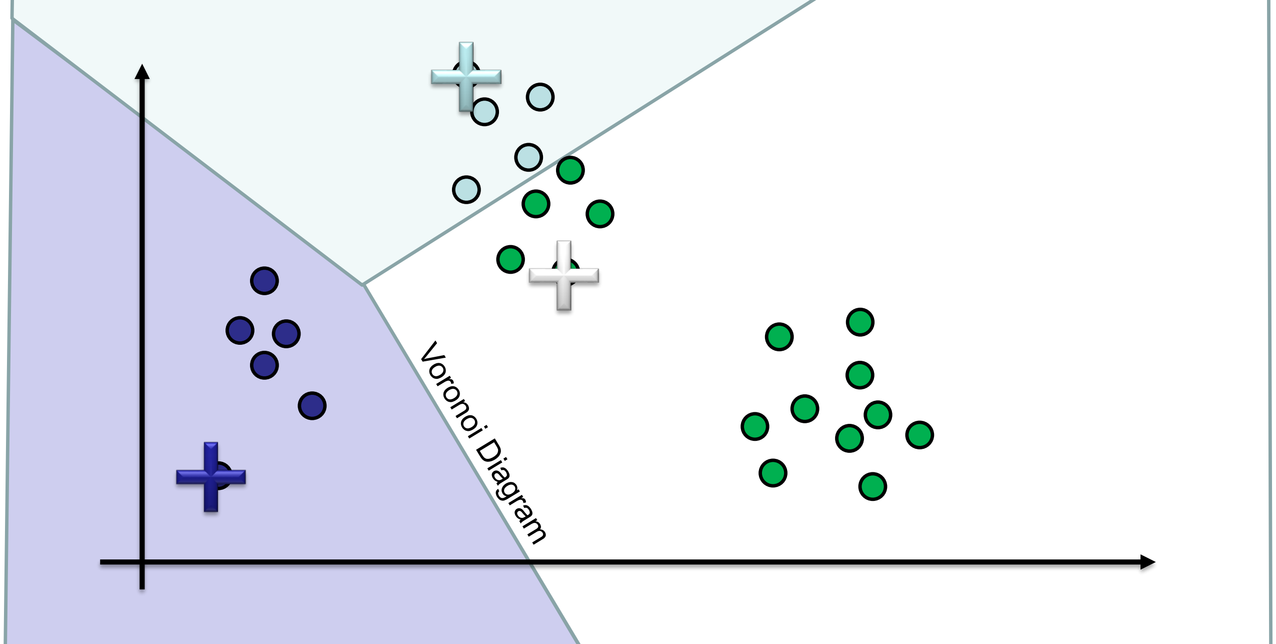
- For each data point find the cluster nearest center



Voronoi Diagram:
Partitions the space by nearest cluster center

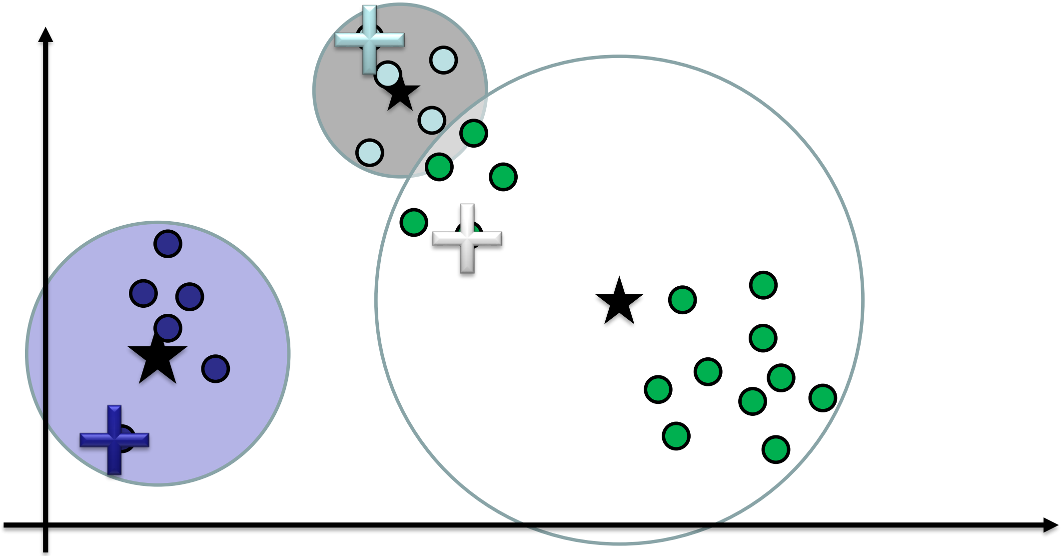
K-Means Clustering: *Intuition*

- For each data point find the cluster nearest center



K-Means Clustering: *Intuition*

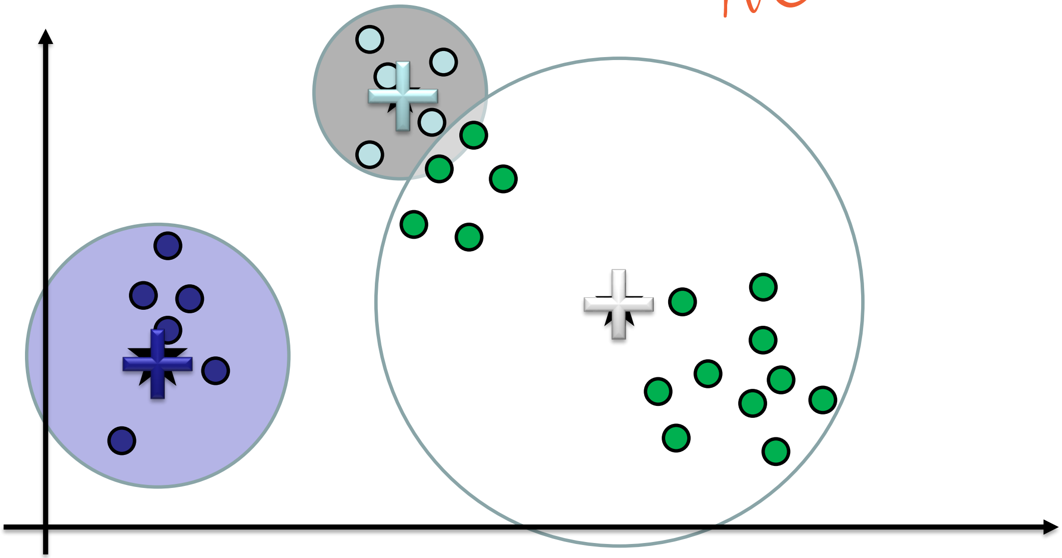
- Compute mean of points in each "cluster"



K-Means Clustering: *Intuition*

- Adjust cluster centers to be the mean of the cluster

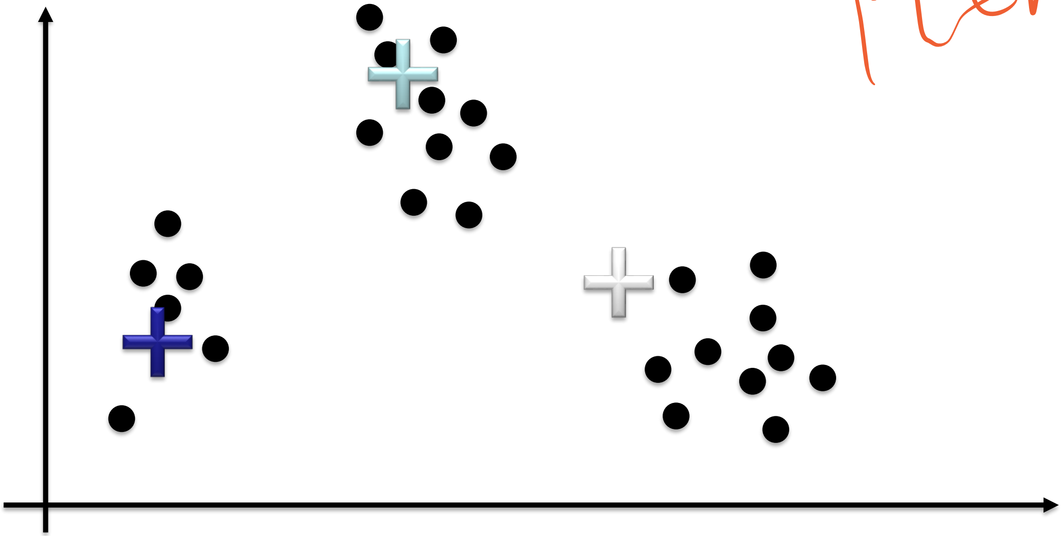
new center!



K-Means Clustering: *Intuition*

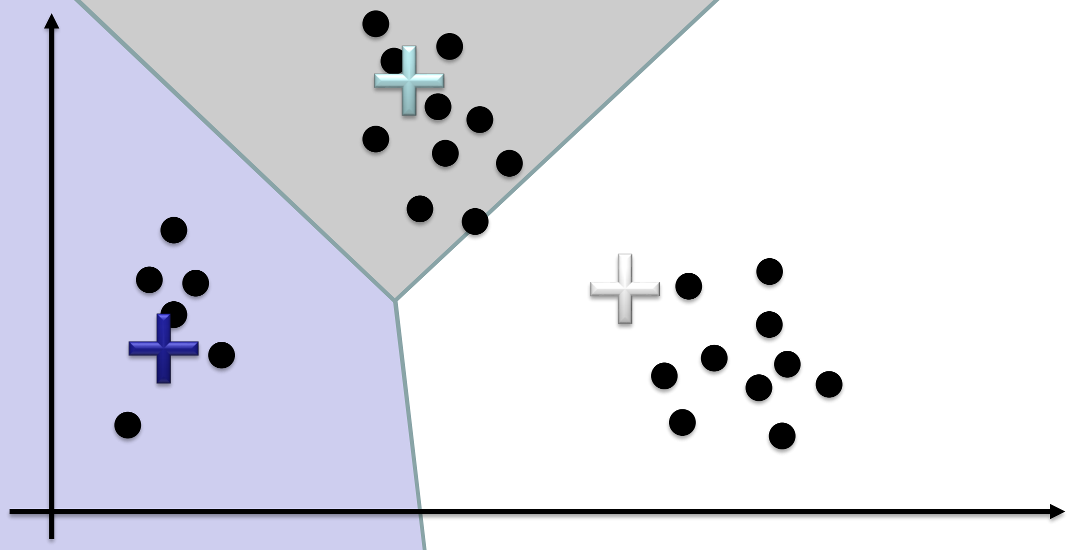
- Improved?
- Repeat

iters



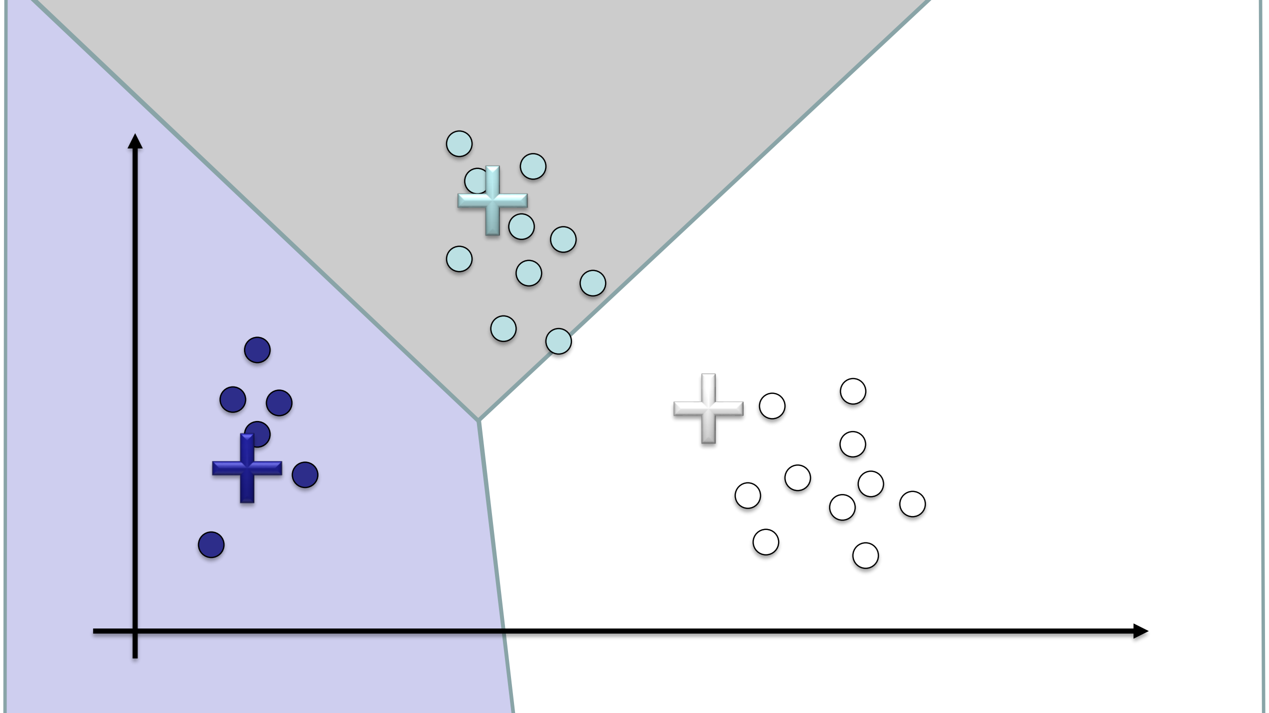
K-Means Clustering: *Intuition*

- Assign Points



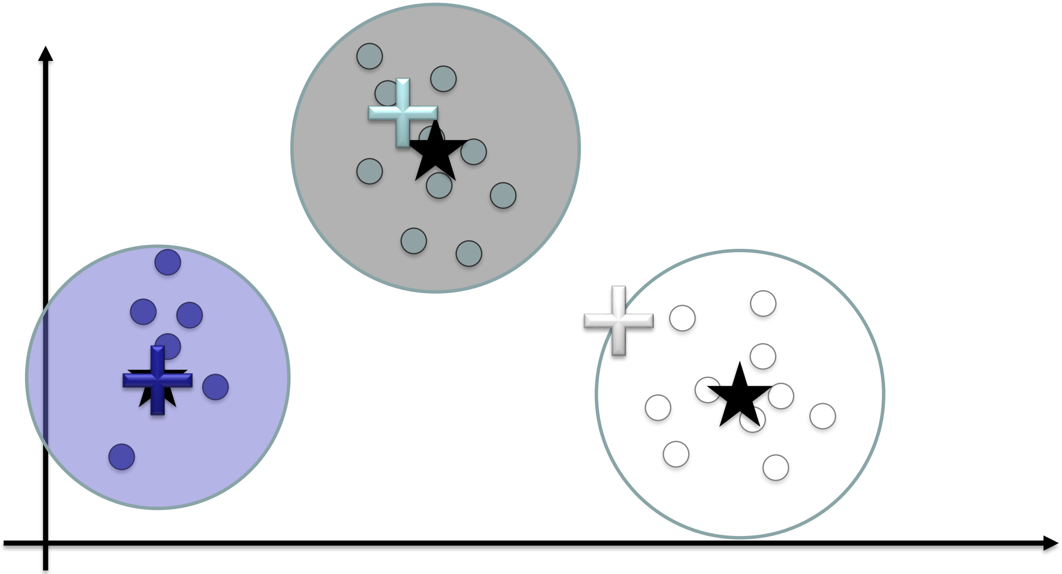
K-Means Clustering: *Intuition*

- Assign Points



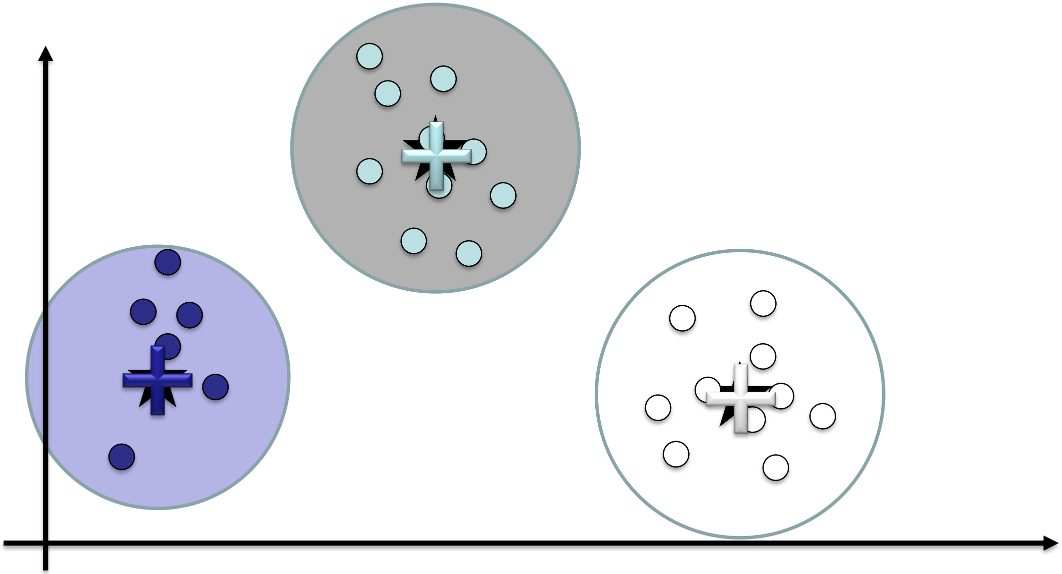
K-Means Clustering: *Intuition*

- Compute cluster means



K-Means Clustering: *Intuition*

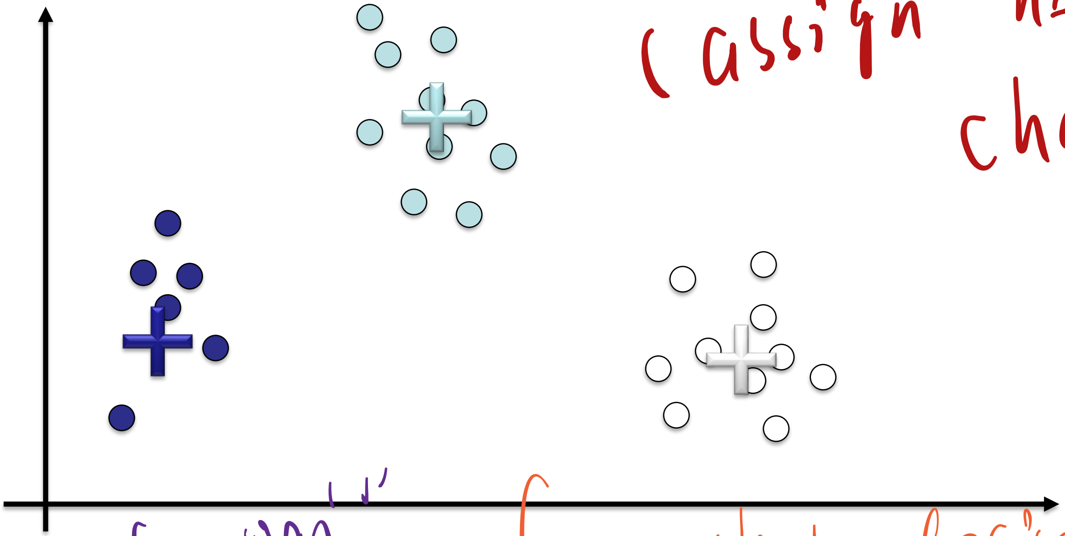
- Update cluster centers



K-Means Clustering: *Intuition*

- Repeat?
  - Yes to check that nothing changes → Converged!

(assign not chage)



function → func that desired to

objective

K-Means as Optimization

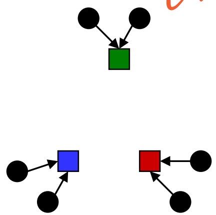
max

min

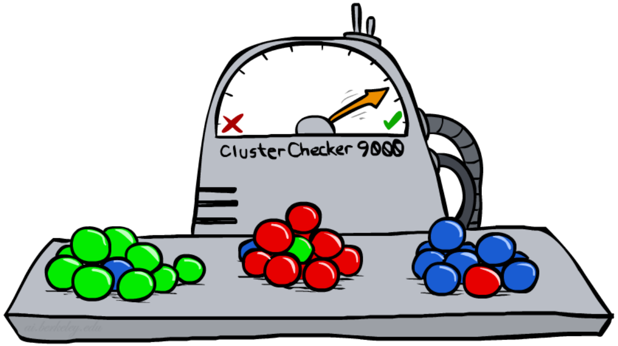
- Consider the total distance to the means:

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

points, assignments, means, squared Euclidean distance



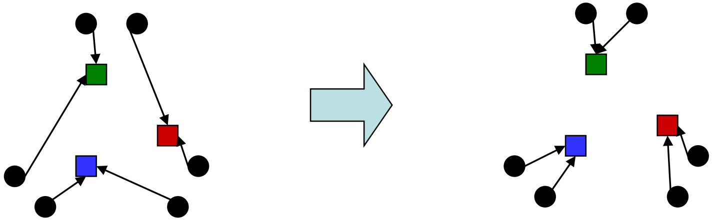
- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c
- Each step cannot increase phi



Phase I: Update Assignments

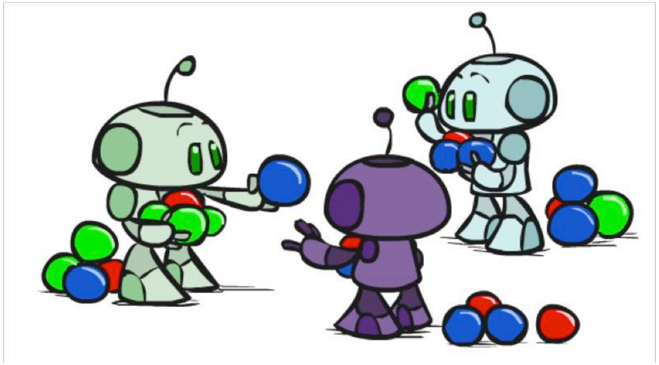
- For each point, re-assign to closest mean:

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



- Cannot increase total distance phi!

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

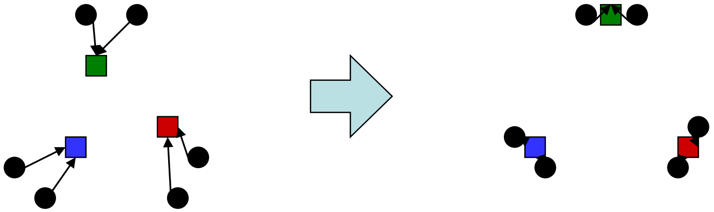


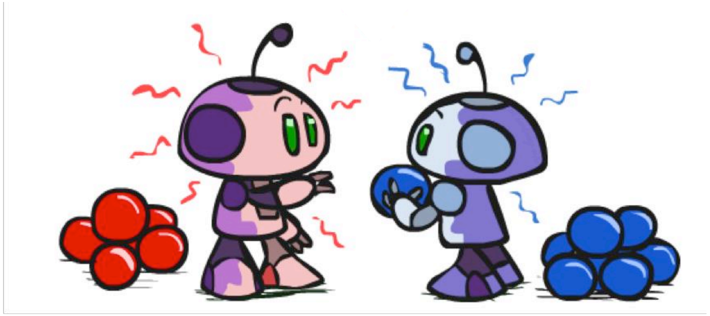
Phase II: Update Means

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

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

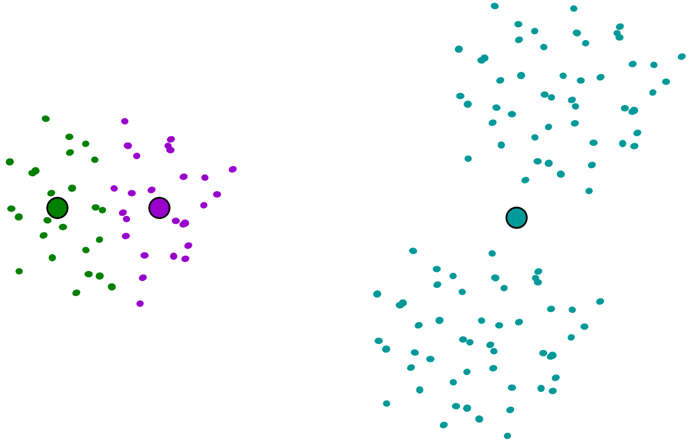
- Also cannot increase total distance
  - Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean

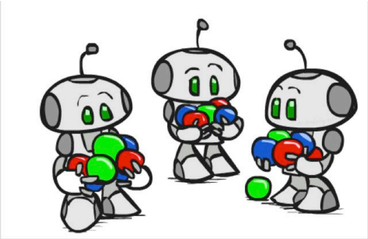


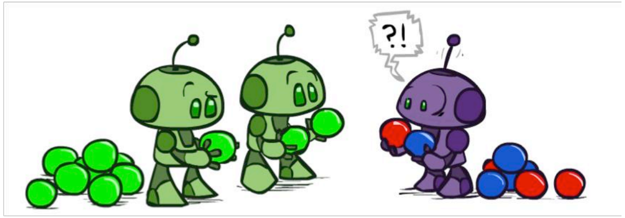


Bad Initialization

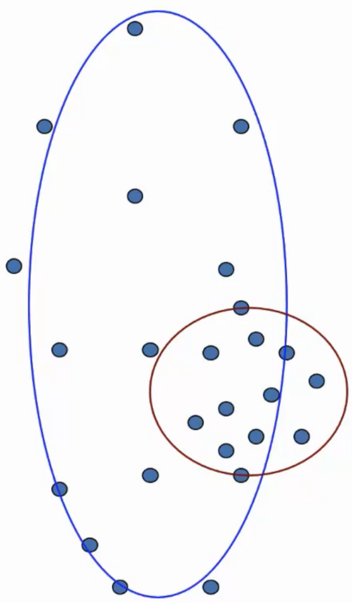
- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
    - Local optima





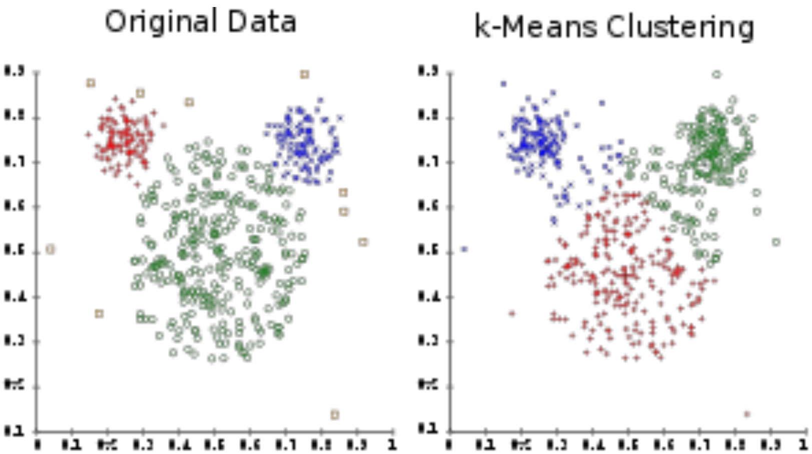


Problems with k-means

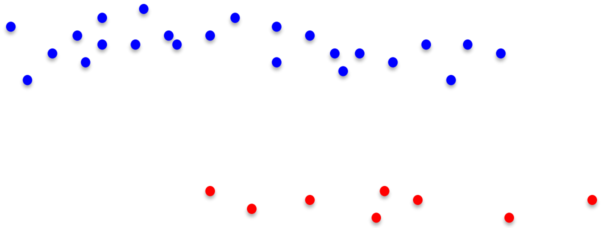


- Assigning data to closest centers
  - But some clusters may be “wider” than others
  - Distances can be deceiving!
- Hard Assignments
  - But clusters may overlap

Inductive Bias



Equally Sized Clusters



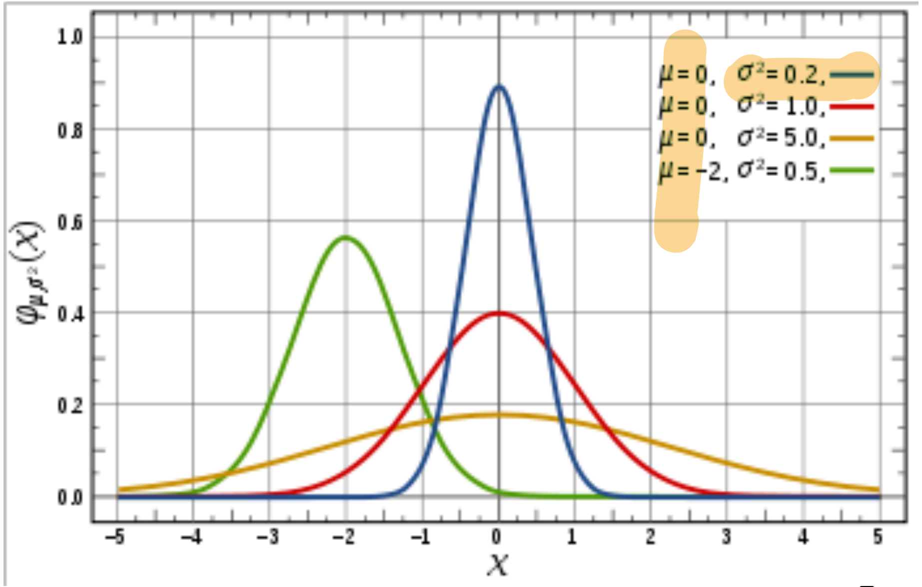
Circular Clusters

Probabilistic Clustering

- Try a probabilistic model!
  - allows overlaps, clusters of different sizes/shapes, etc.

- Gaussian mixture model (GMM)
  - also called Mixture of Gaussians

Review: Gaussians



μ, σ^2

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Learning Gaussian Parameters

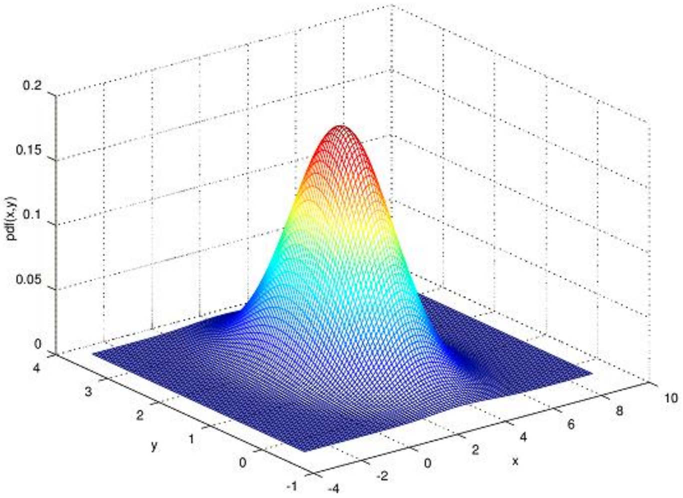
Given fully-observable data:

$$\hat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\hat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N} (x_i - \hat{\mu})^2$$

最大似然...

Multivariate Gaussians

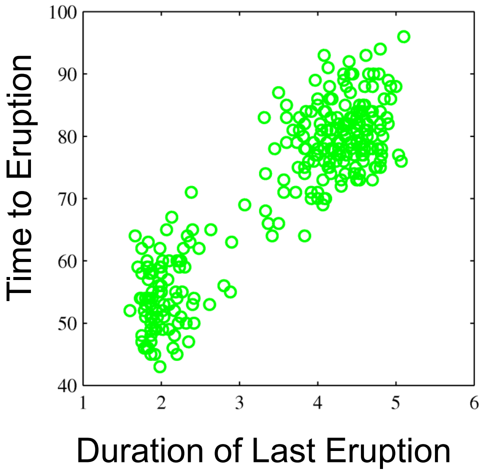


Covariance matrix Σ: degree to which x_i vary together

$$P(X = \mathbf{x}) = \frac{1}{(2\pi)^{m/2}||\Sigma||^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma^{-1}(\mathbf{x}-\mu)\right]$$

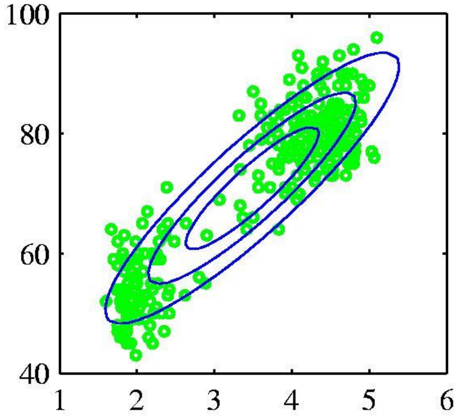
Mixtures of Gaussians

- Old Faithful Data Set

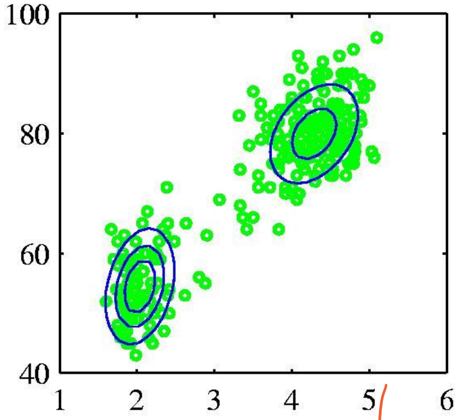


Mixtures of Gaussians

- Old Faithful Data Set



Single Gaussian



Mixture of two Gaussians

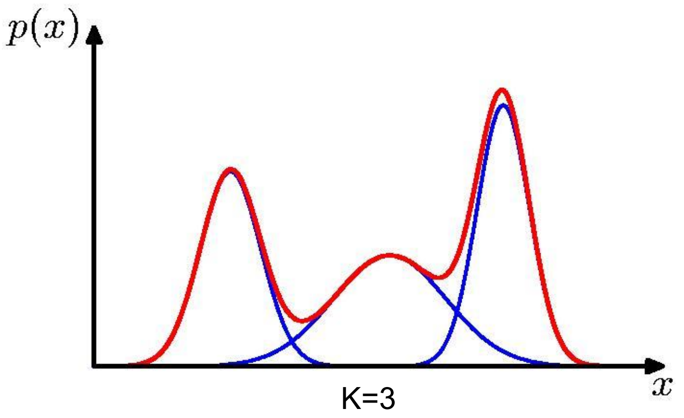
Mixtures of Gaussians

K gaussian

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \underbrace{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

Mixing coefficient

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

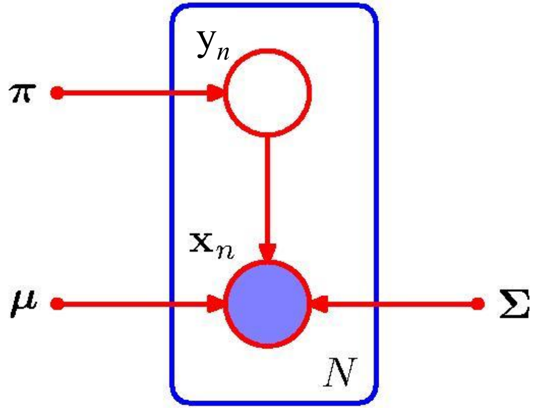


Gaussian mixture model

- P(Y): Distribution over *k* components (clusters)
- P(X|Y): Each component generates data from a **multivariate Gaussian** with mean μ_i and covariance matrix Σ_i

Each data point is sampled from a ***generative process*:**

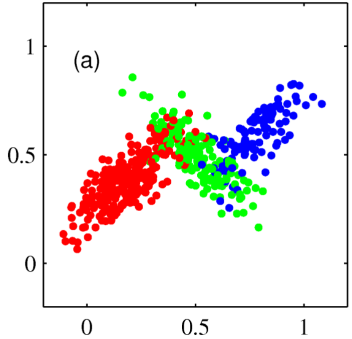
1. Choose component *i* with probability π_i
2. ~~Generate data~~ point from $N(\mathbf{x}|\mu_i, \Sigma_i)$



Supervised learning for GMM

- We observe both the data points and their labels (generated from which Gaussian components)
- How do we estimate parameters of GMM?

$\pi \quad \begin{cases} \sigma_1 \ \mu_1 \\ \sigma_2 \ \mu_2 \\ \ldots \end{cases}$



Supervised learning for GMM

- We observe both the data points and their labels (generated from which Gaussian components)
- How do we estimate parameters of GMM?
- Objective: maximize the likelihood

$$\prod_j P(y_j = i, \mathbf{x}_j) = \prod_j \pi_i N(\mathbf{x}_j | \mu_i, \Sigma_i)$$

- Closed form solution:
  - *m* data points. For component *i*, suppose we have *n* data points with label *i*.

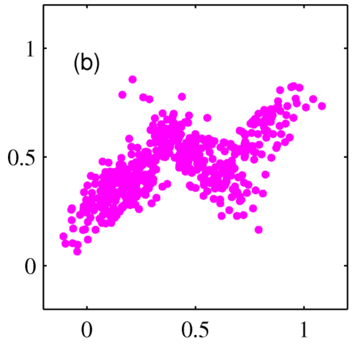
$$\mu_i = \frac{1}{n} \sum_{j=1}^{n} \mathbf{x}_j \qquad \Sigma_i = \frac{1}{n} \sum_{j=1}^{n} (\mathbf{x}_j - \mu_i)(\mathbf{x}_j - \mu_i)^T \qquad \pi_i = \frac{n}{m}$$

Unsupervised learning for GMM

- In clustering, we don't know the labels Y!
- Maximize marginal likelihood:

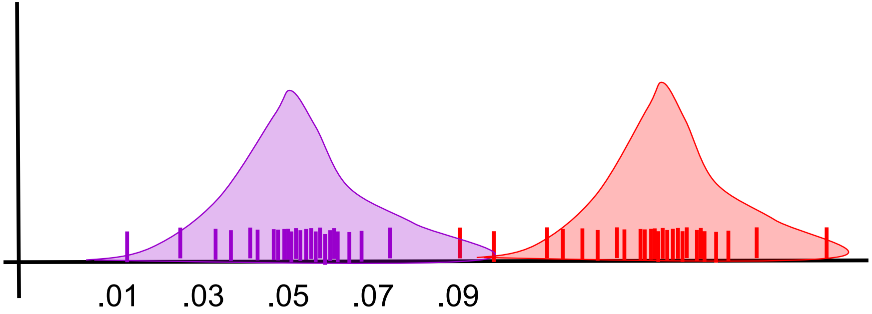
$$\prod_j P(\mathbf{x}_j) = \prod_j \sum_i P(y_j = i, \mathbf{x}_j) = \prod_j \sum_i \pi_i N(\mathbf{x}_j | \mu_i, \Sigma_i)$$

- How do we optimize it?
  - No closed form solution

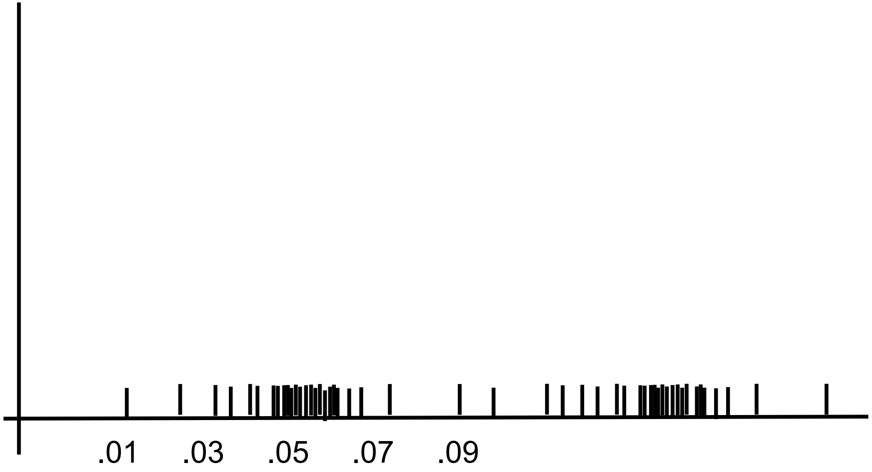


Simplest Example

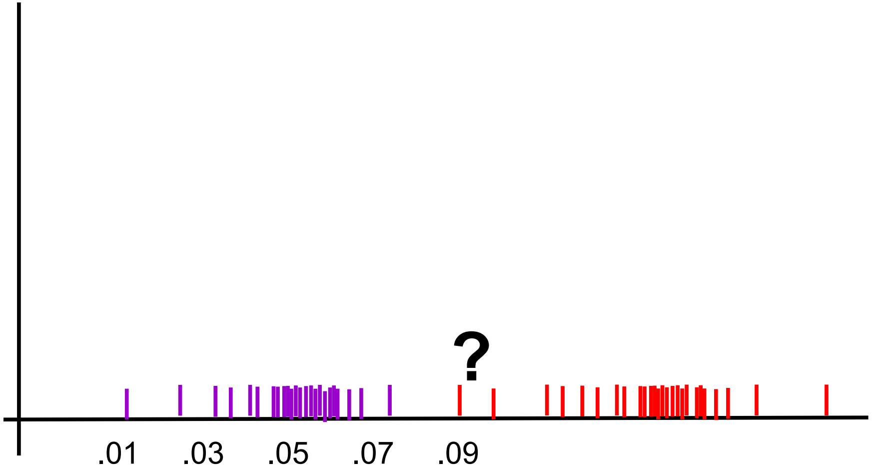
Mixture of two distributions



Input Looks Like

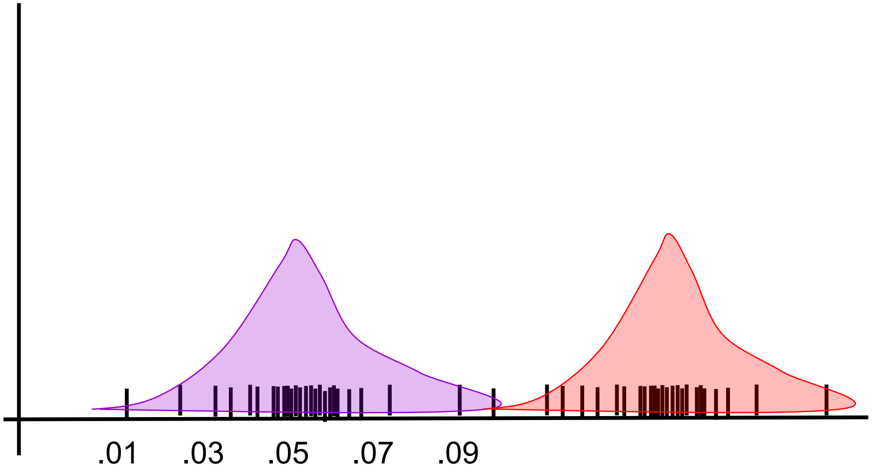


We Want to Predict



Chicken & Egg

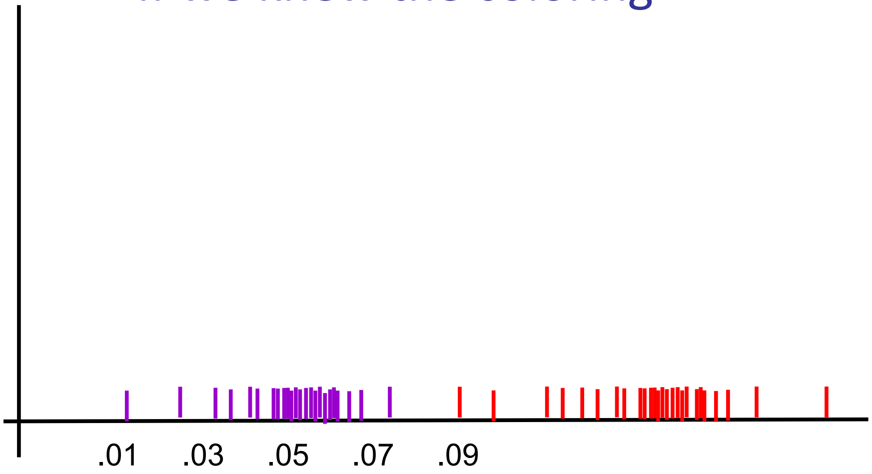
Note that coloring instances would be easy
if we knew Gaussians….



Chicken & Egg

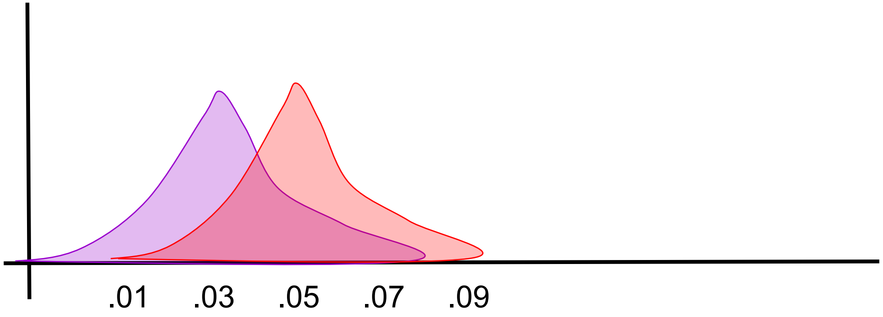
And finding the Gaussians would be easy

If we knew the coloring



Expectation Maximization (EM)

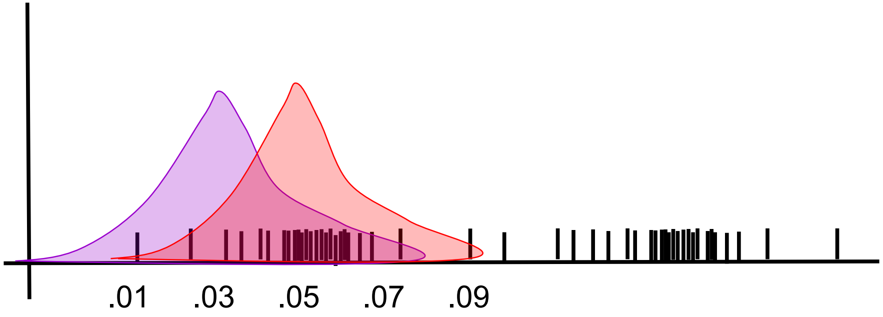
- Pretend we do know the parameters
  - Initialize randomly



Expectation Maximization (EM)

- [E step] Compute probability of each instance having each possible label

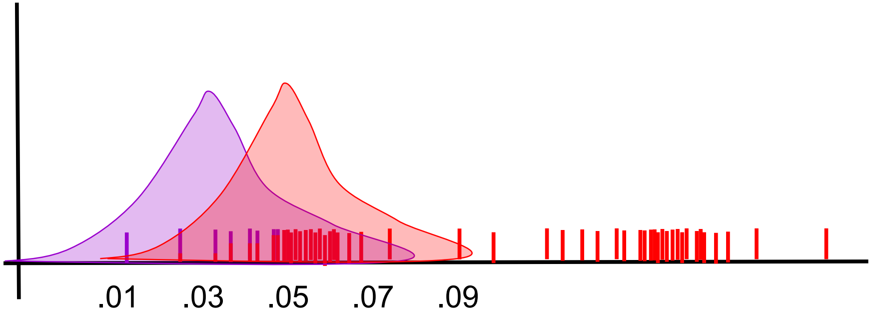
(by each possible G model).



Expectation Maximization (EM)

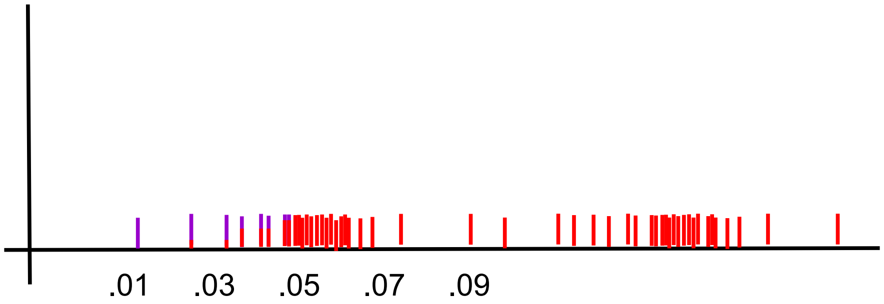
- [E step] Compute probability of each instance having each possible label

(AKA. generated by each model)



Expectation Maximization (EM)

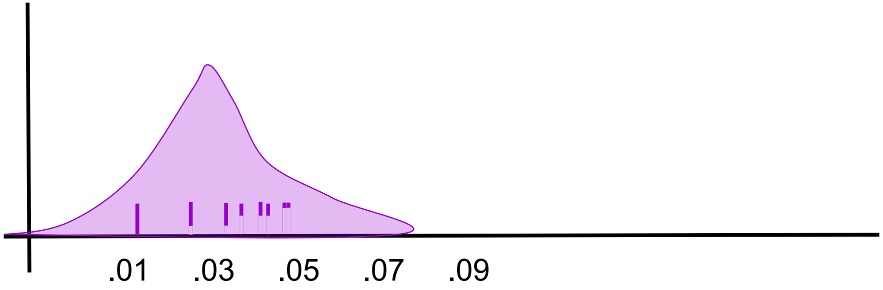
- [E step] Compute probability of each instance having each possible label
- [M step] Treating each instance as fractionally having both labels, compute the new parameter values



Expectation Maximization (EM)

- [E step] Compute probability of each instance having each possible label
- [M step] Treating each instance as fractionally having both labels, compute the new parameter values

(New Gs)



Expectation Maximization (EM)

- [E step] Compute probability of each instance having each possible label
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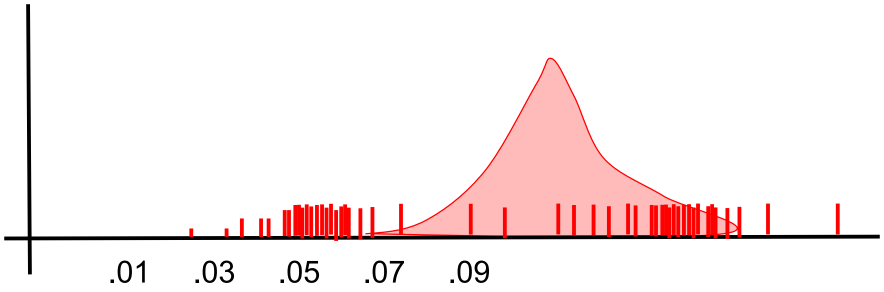
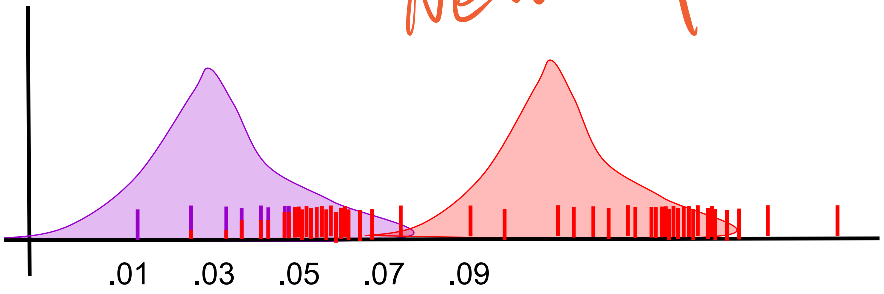


Expectation Maximization (EM)

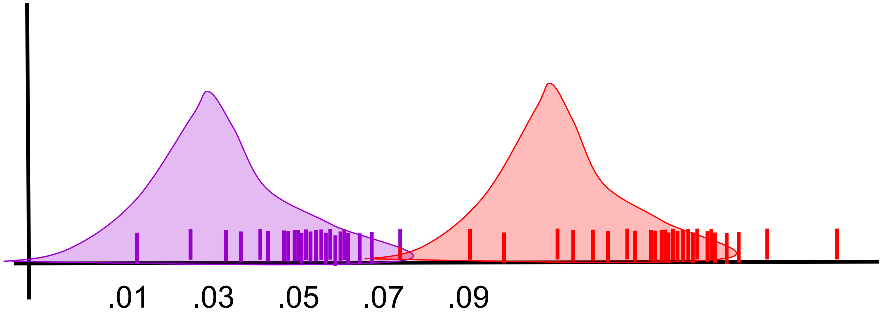
- [E step] Compute probability of each instance having each possible label
- [M step] Treating each instance as fractionally having both labels, compute the new parameter values

New G



Expectation Maximization (EM)

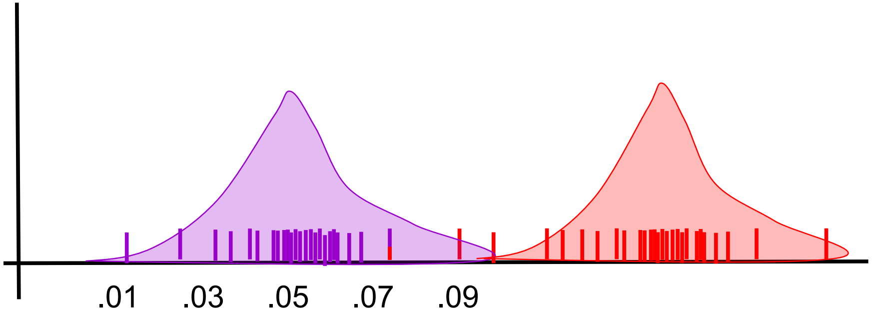
- Repeat E-step



Expectation Maximization (EM)

- Repeat E-step
- Repeat M-step

… until convergence



Expectation Maximization (EM)

- Pick K random cluster models (Gaussians)
- Alternate:
  - Assign data instances proportionately to different models
  - Revise each cluster model based on its (proportionately) assigned points
- Stop when no changes

EM: Two Easy Steps

Objective: $\text{argmax}_\theta \prod_j \sum_{i=1}^{k} P(y_j=i,x_j|\theta) = \sum_j \log \sum_{i=1}^{k} P(y_j=i,x_j|\theta)$

Data: $\{x_j \mid j=1 .. n\}$

Notation a bit inconsistent
Parameters = θ=λ

- **E-step**: Compute expectations to "fill in" missing y values according to current parameters, θ
  - For all examples j and values i for y, compute: $P(y_j=i \mid x_j, \theta)$
- **M-step**: Re-estimate the parameters with "weighted" MLE estimates
  - Set $\theta = \text{argmax}_\theta \sum_j \sum_{i=1}^{k} P(y_j=i \mid x_j, \theta) \log P(y_j=i,x_j|\theta)$

Especially useful when the E and M steps have closed form solutions!!!

EM for GMM

Iterate: On the *t*'th iteration let our estimates be

$$\theta^{(t)} = \{ \mu_1^{(t)}, \mu_2^{(t)} \dots \mu_k^{(t)}, \Sigma_1^{(t)}, \Sigma_2^{(t)} \dots \Sigma_k^{(t)}, \pi_1^{(t)}, \pi_2^{(t)} \dots \pi_k^{(t)} \}$$

E-step

Compute label distribution of each data point

$$\mathrm{P}\left(y_j = i \,\middle|\, x_j, \theta^{(t)}\right) \propto \pi_i^{(t)} N\left(x_j \,\middle|\, \mu_i^{(t)}, \Sigma_i^{(t)}\right)$$

Just evaluate a Gaussian at x_j

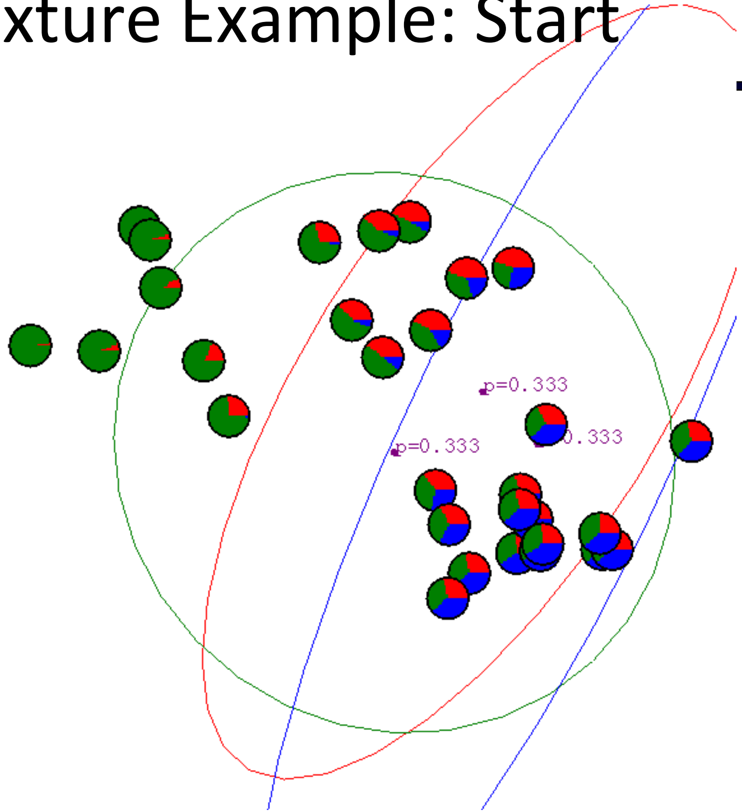
M-step

Compute weighted MLE of parameters given label distributions

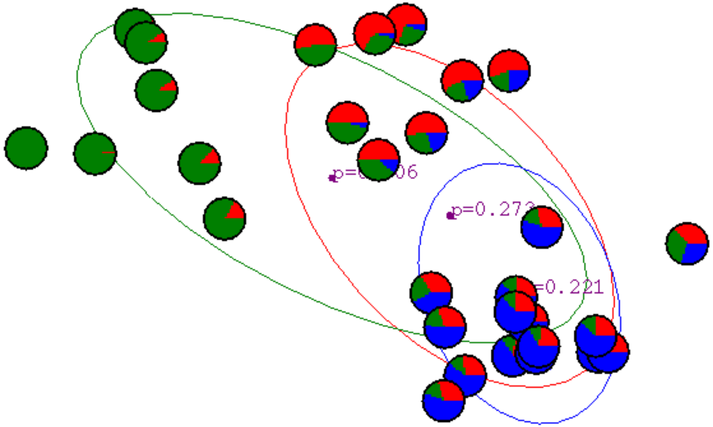
$$\mu_i^{(t+1)} = \frac{\sum_j \mathrm{P}\left(y_j = i \,\middle|\, x_j, \theta^{(t)}\right) x_j}{\sum_{j'} \mathrm{P}\left(y_{j'} = i \,\middle|\, x_{j'}, \theta^{(t)}\right)} \qquad \Sigma_i^{(t+1)} = \frac{\sum_j \mathrm{P}\left(y_j = i \,\middle|\, x_j, \theta^{(t)}\right) \left[x_j - \mu_i^{(t+1)}\right]\left[x_j - \mu_i^{(t+1)}\right]^T}{\sum_{j'} \mathrm{P}\left(y_{j'} = i \,\middle|\, x_{j'}, \theta^{(t)}\right)} \qquad \pi_i^{(t+1)} = \frac{\sum_j \mathrm{P}\left(y_j = i \,\middle|\, x_j, \theta^{(t)}\right)}{m}$$

m = #training examples

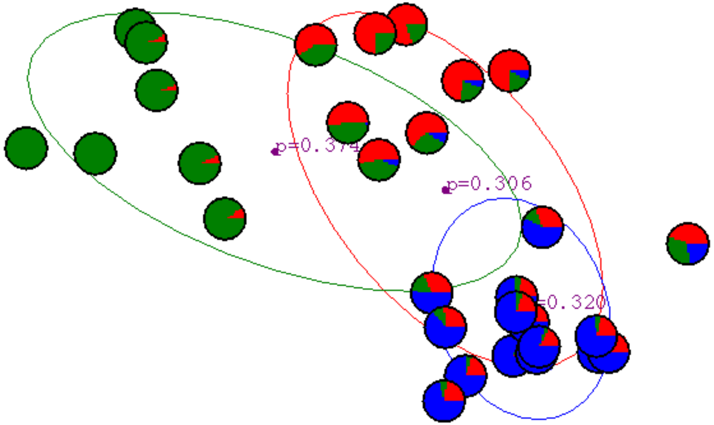
Gaussian Mixture Example: Start



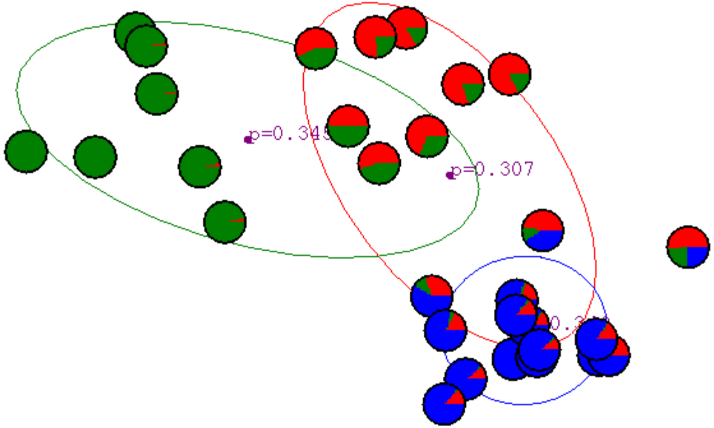
After first iteration



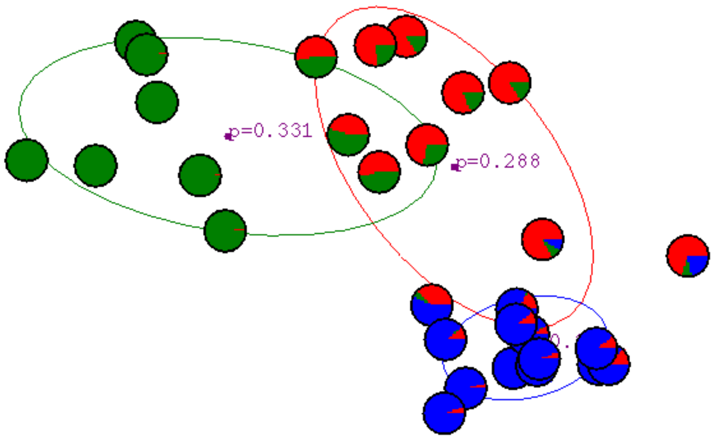
After 2nd iteration



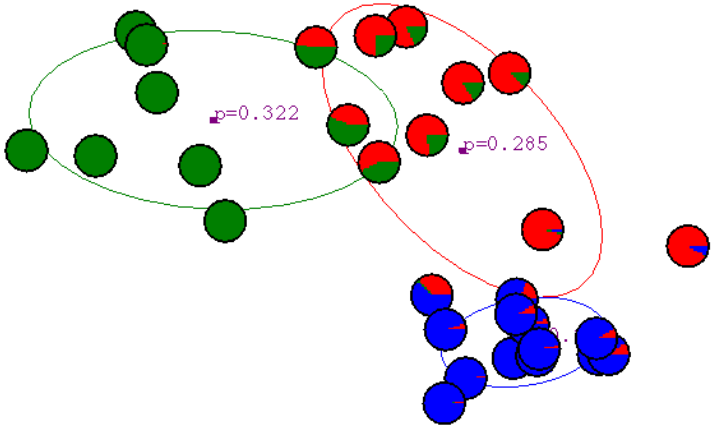
After 3rd iteration



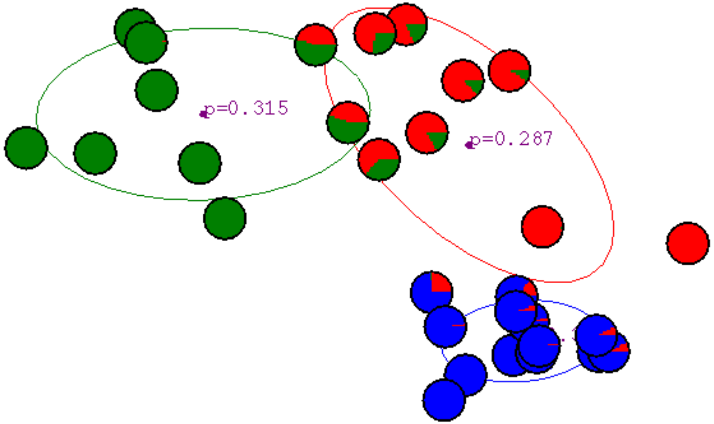
After 4th iteration



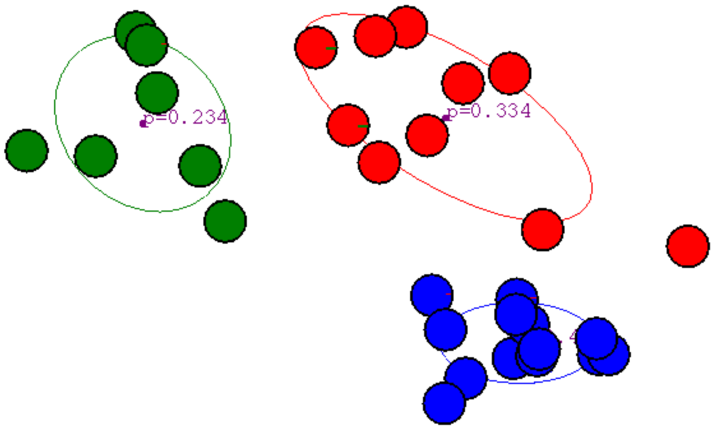
After 5th iteration



After 6th iteration



After 20th iteration



(kMeans

EM

EM and K-means

- EM degrades to k-means if we assume
  - All the Gaussians are spherical and have identical weights and covariances
    - i.e., the only parameters are the means
  - The label distributions computed at E-step are point-estimations
    - i.e., hard-assignments of data points to Gaussians
    - Alternatively, assume the variances are close to zero

k means: hard-assign

EM: prob

EM in General

$\pi \quad \sigma \quad \mu$

- Can be used to learn any model with hidden variables (missing data)
- Alternate:
  - Compute distributions over hidden variables based on current parameter values
  - Compute new parameter values to maximize expected log likelihood based on distributions over hidden variables
- Stop when no changes

Summary

- Clustering
  - Group together similar instances
- K-means
  - Assign data instances to closest mean
  - Assign each mean to the average of its assigned points
- EM
  - Assign data instances proportionately to different Gaussian models
  - Revise each model based on its (proportionately) assigned points