Introduction to Machine Learning,

Clustering and EM

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- Clustering
  - K-means
  - Mixture of Gaussians
- Expectation Maximization
- Variational Methods

Clustering

What is clustering?

Clustering:

The process of grouping a set of objects into classes of similar objects

–high intra-class similarity

–low inter-class similarity

–It is the most common form of unsupervised learning

Clustering is Subjective

What is clustering?

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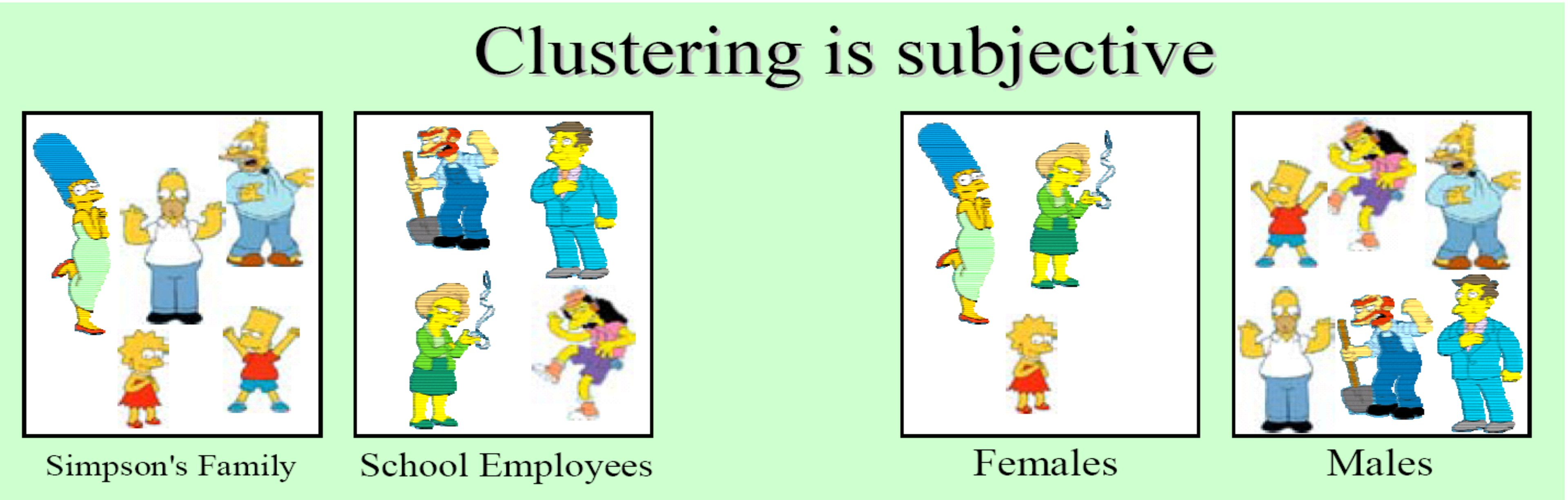


What is Similarity?

Hard to define! *…but we know it when we see it*

The K- means Clustering Problem

K-means Clustering Problem

Given a set of observations $(x_1, x_2, \ldots, x_n)$, where $x_i \in \mathbb{R}^d$

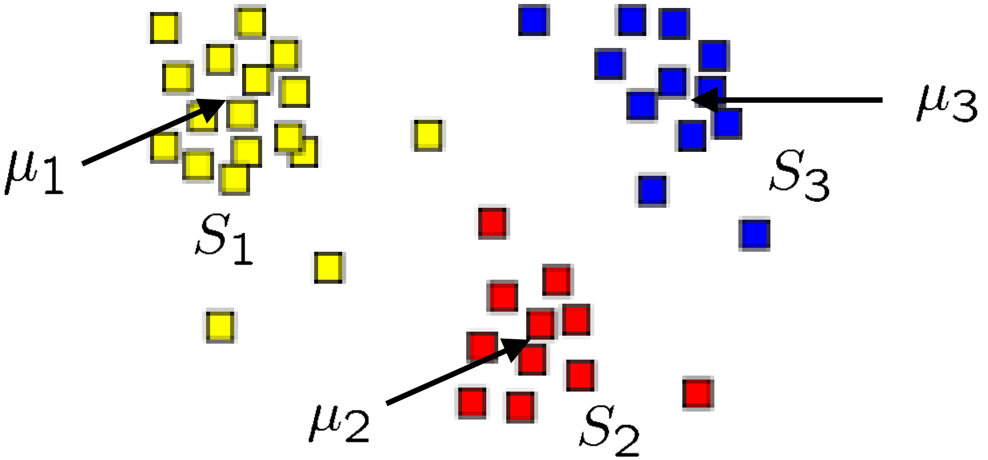
***K*-means clustering problem:**

Partition the n observations into K sets ($K \leq n$) $\mathbf{S} = \{S_1, S_2, \ldots, S_K\}$ such that the sets minimize the within-cluster sum of squares:

$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{K} \sum_{\mathbf{x}_j \in S_i} \left\| \mathbf{x}_j - \boldsymbol{\mu}_i \right\|^2$$

where μ_i is the mean of points in set S_i.

K=3



K-means Clustering Problem

Given a set of observations $(x_1, x_2, \ldots, x_n)$, where $x_i \in \mathbb{R}^d$

***K*-means clustering problem:**

Partition the *n* observations into *K* sets ($K \leq n$) $\mathbf{S} = \{S_1, S_2, \ldots, S_K\}$ such that the sets minimize the within-cluster sum of squares:

$$\underset{\mathbf{S}}{\arg\min} \sum_{i=1}^{K} \sum_{\mathbf{x}_j \in S_i} \left\| \mathbf{x}_j - \boldsymbol{\mu}_i \right\|^2$$

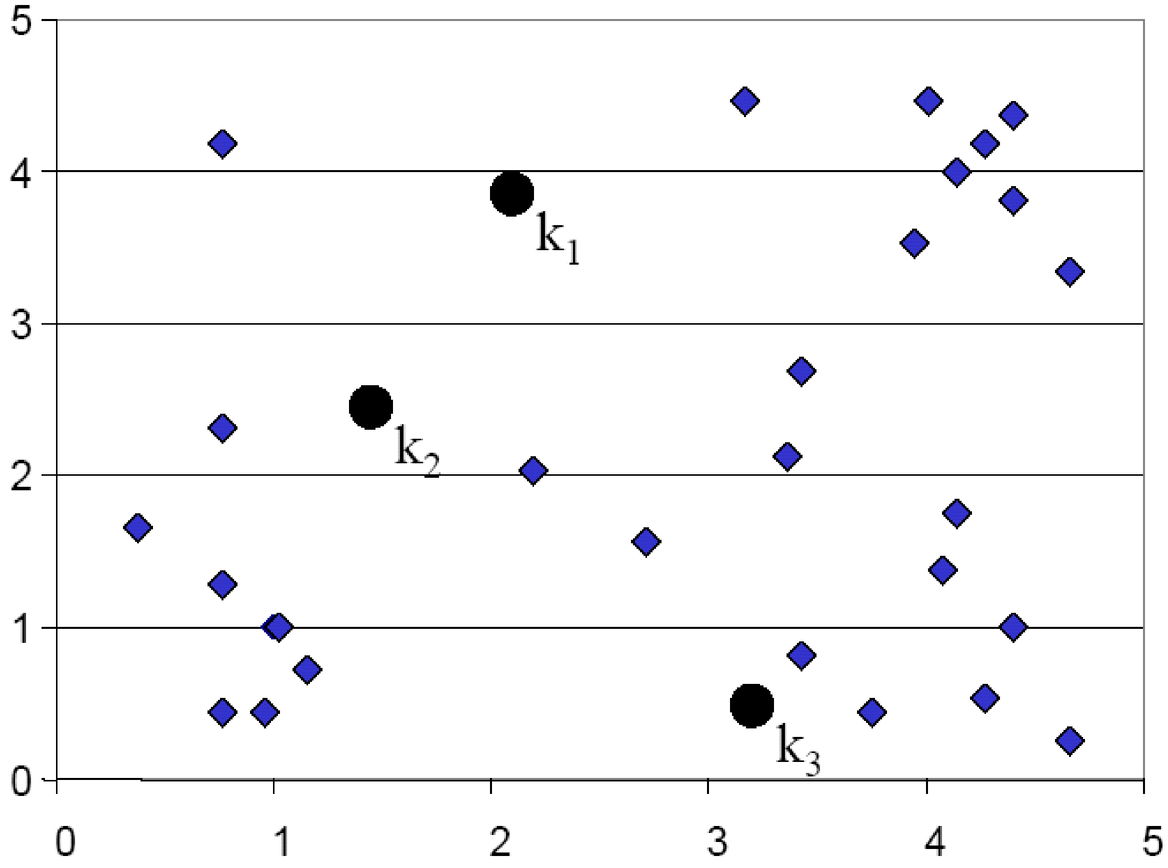
where μ_i is the mean of points in set S_i.

How hard is this problem?

The problem is NP hard, but there are good heuristic algorithms that seem to work well in practice:

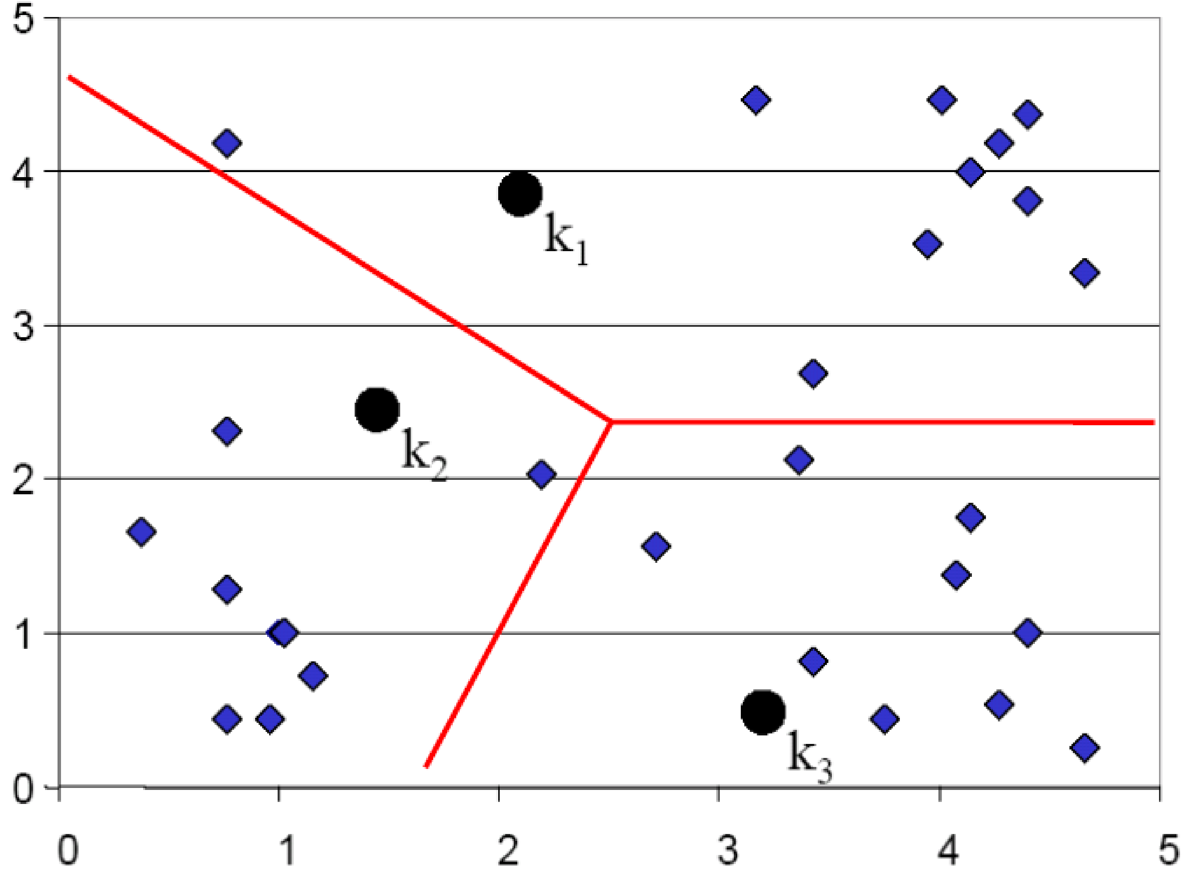
- K–means algorithm
- mixture of Gaussians

K-means Clustering Alg: Step 1



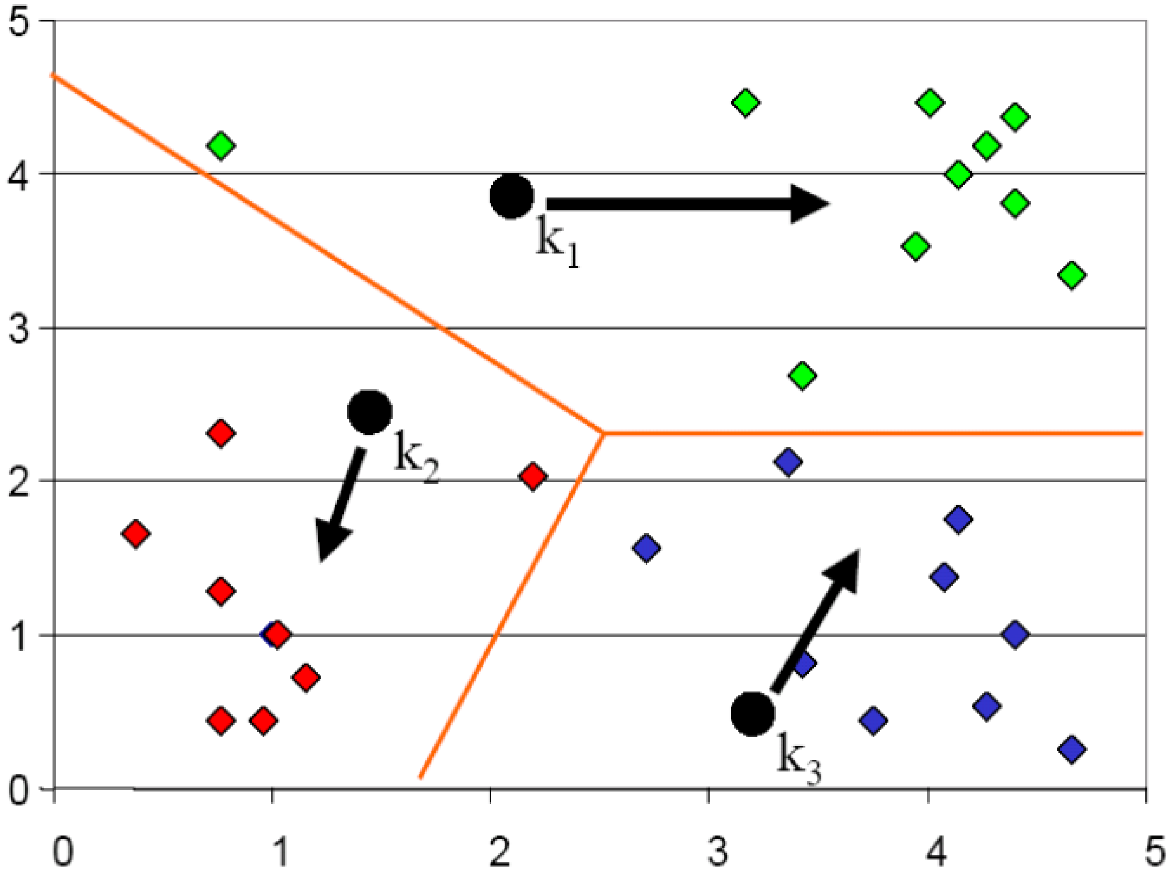
- Given n objects.
- Guess the cluster centers (k_1, k_2, $k_{3.}$ They were μ_1, μ_2,μ_3 in the previous slide)

K-means Clustering Alg: Step 2



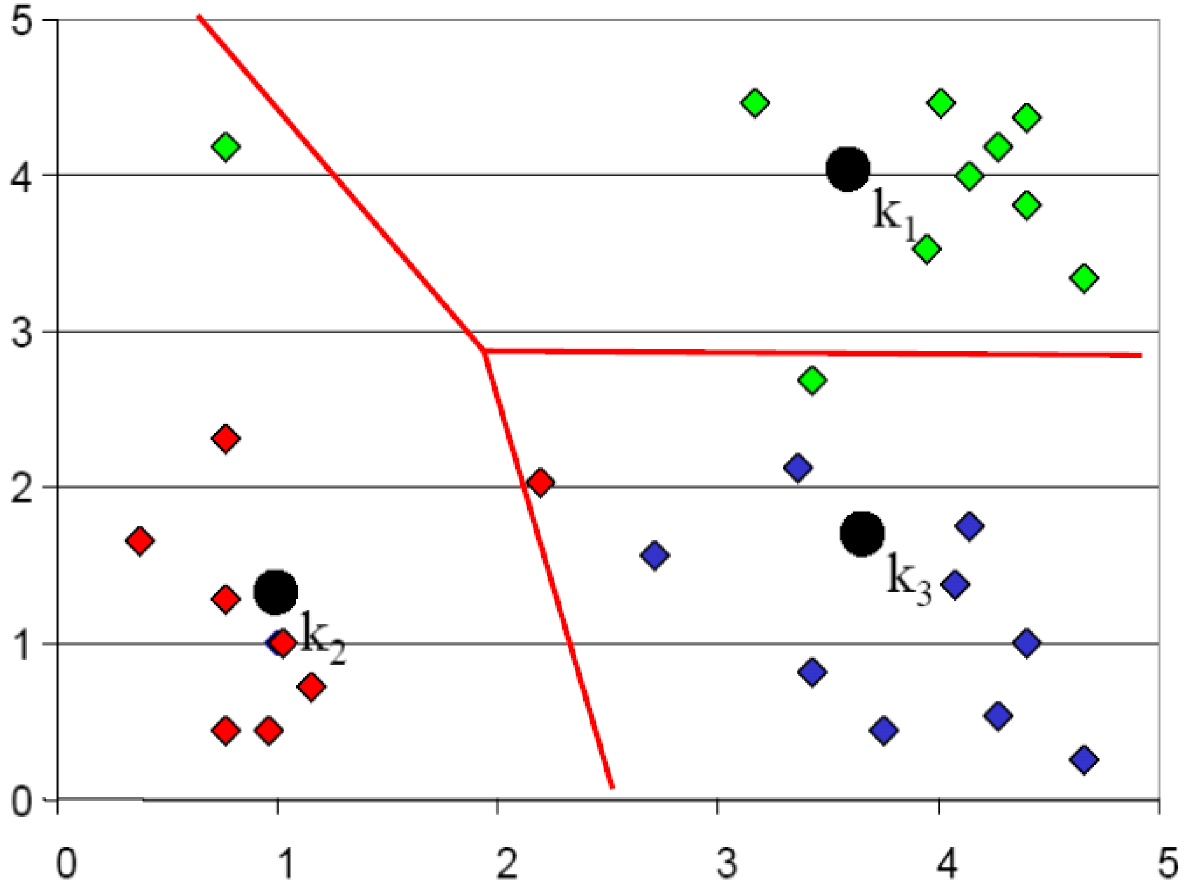
Decide the class memberships of the n objects by assigning them to the nearest cluster centers k_1, k_2, k_3.
(= Build a Voronoi diagram based on the cluster centers k_1, k_2, k_3.)

K-means Clustering Alg: Step 3



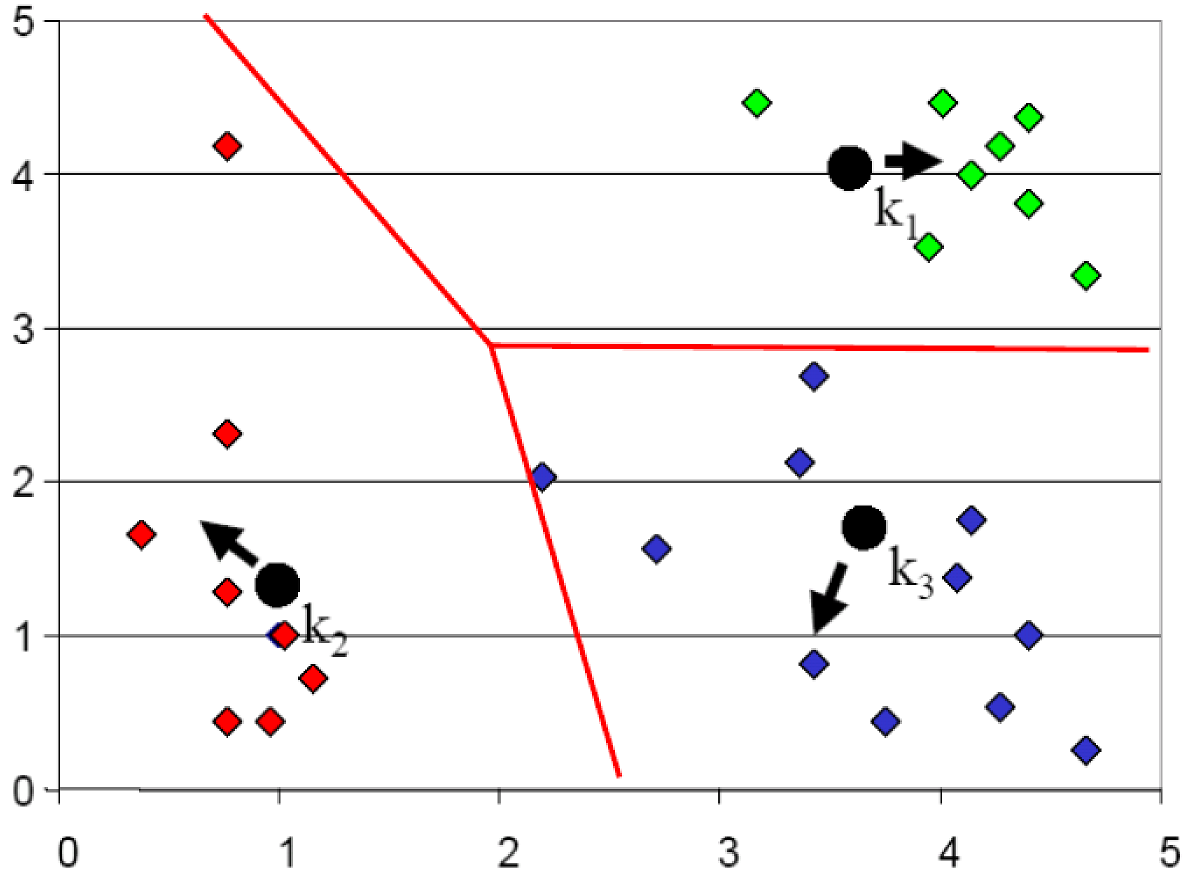
- Re-estimate the cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

K-means Clustering Alg: Step 4



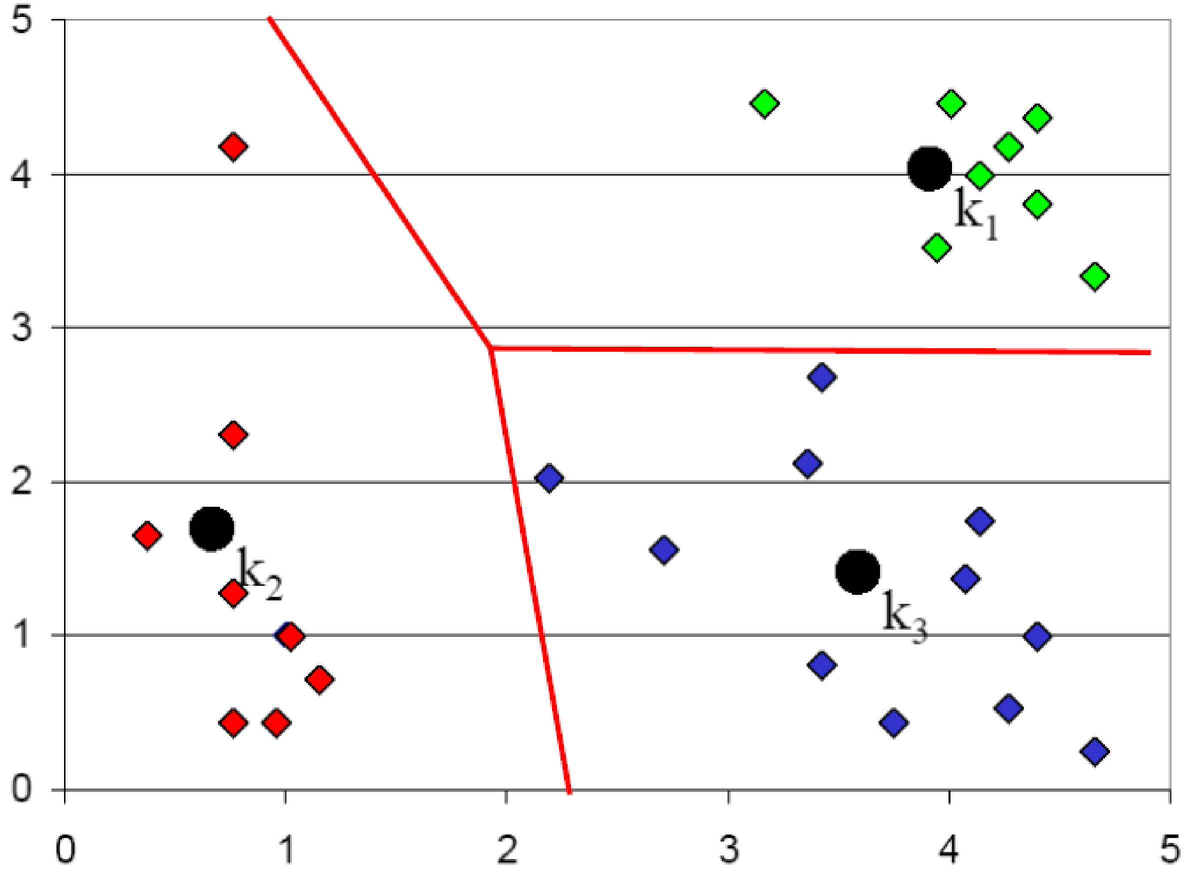
- Build a new Voronoi diagram based on the new cluster centers.
- Decide the class memberships of the n objects based on this diagram

K-means Clustering Alg: Step 5



- Re-estimate the cluster centers.

K-means Clustering Alg: Step 6



- Stop when everything is settled.
  (The Voronoi diagrams don’t change anymore)

K- means Clustering Algorithm

Algorithm

Input

– Data + Desired number of clusters, K

Initialize

– the K cluster centers (randomly if necessary)

Iterate

1. Decide the class memberships of the n objects by assigning them to the nearest cluster centers

2. Re-estimate the K cluster centers (aka the centroid or mean), by assuming the memberships found above are correct.

Termination

– If none of the n objects changed membership in the last iteration, exit.

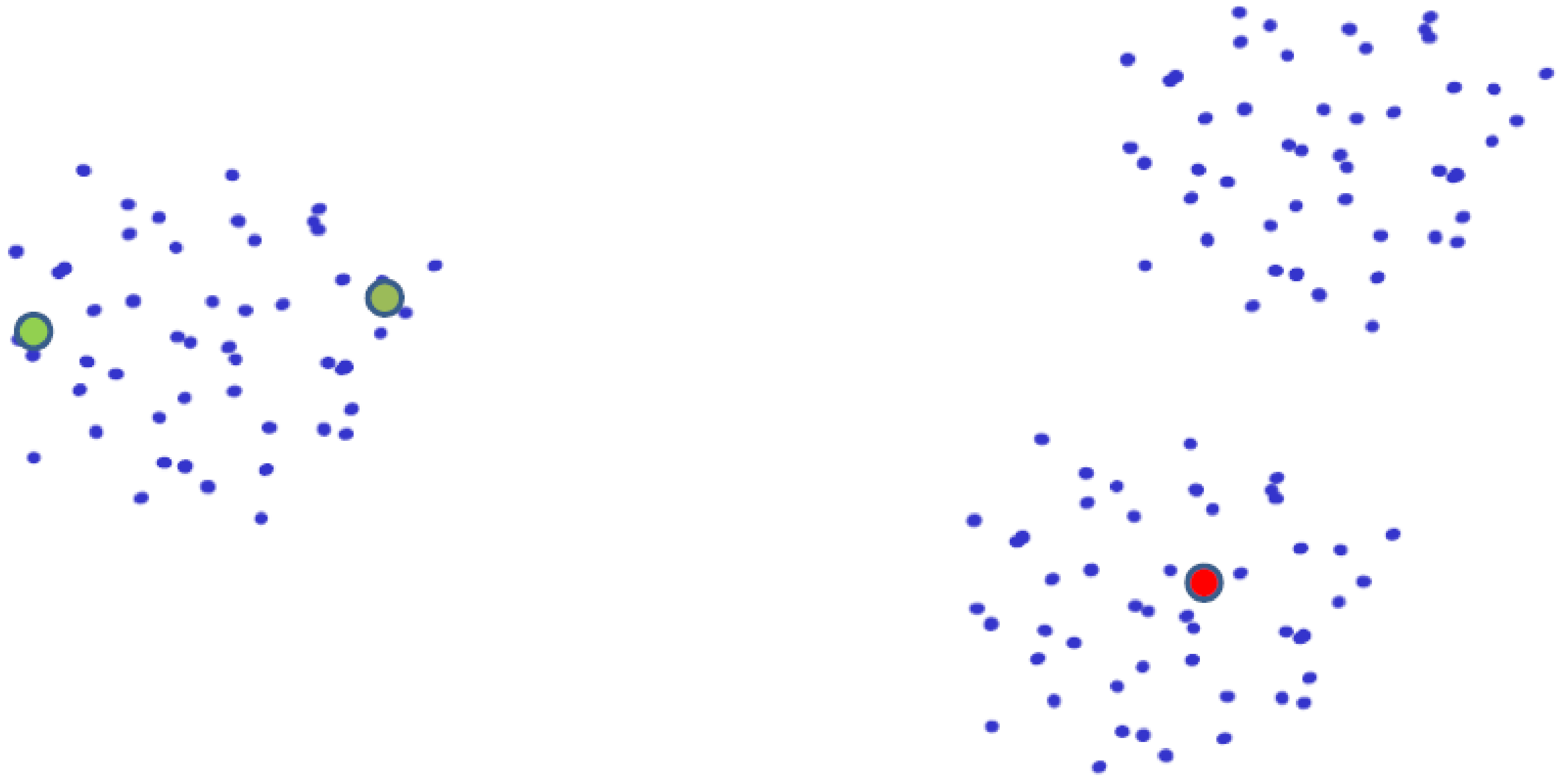
Otherwise go to 1.

K- means Algorithm Computation Complexity

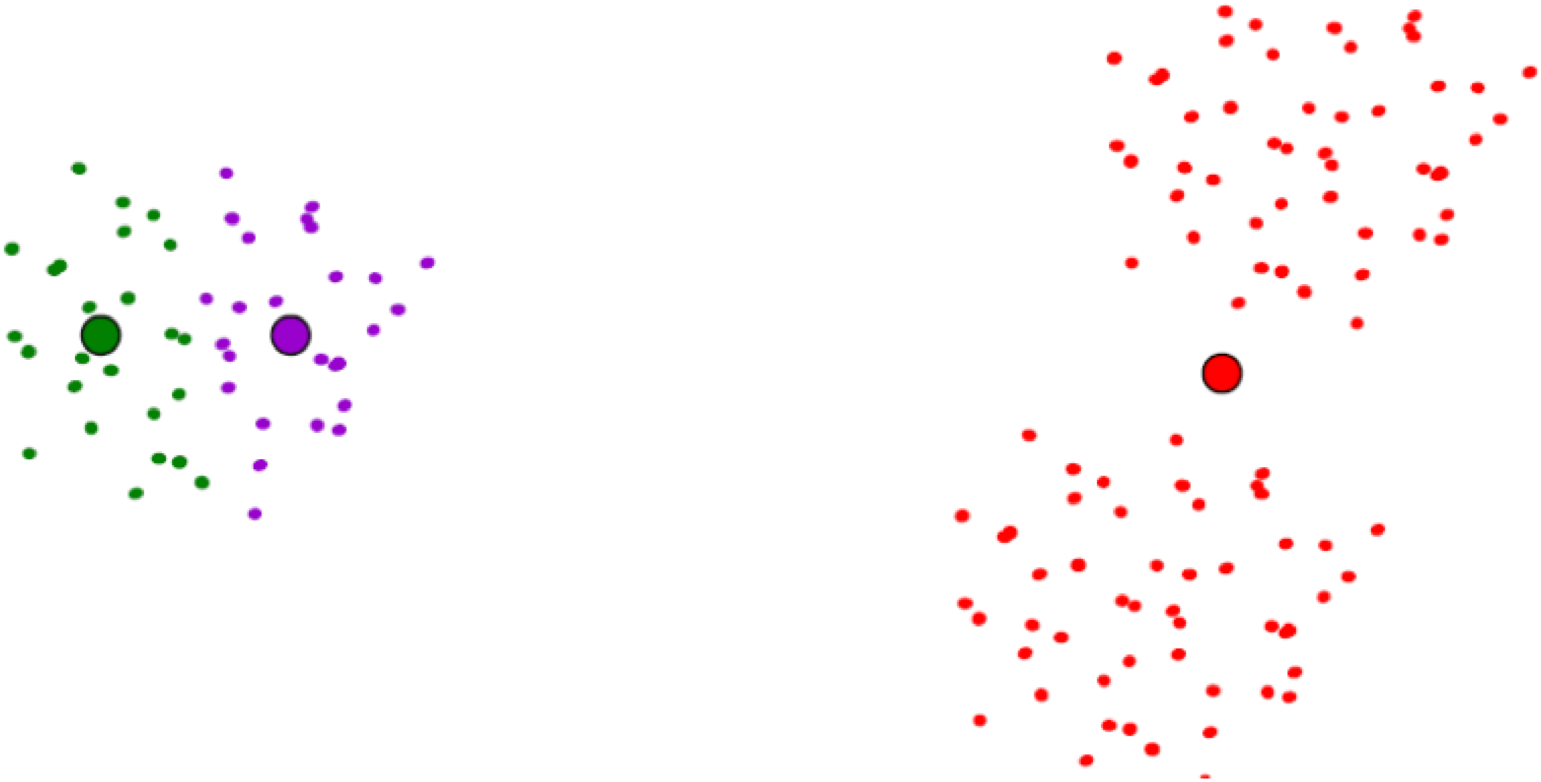
- At each iteration,
  - – Computing distance between each of the n objects and the K cluster centers is $O(Kn)$.
  - – Computing cluster centers: Each object gets added once to some cluster: $O(n)$.

- Assume these two steps are each done once for ℓ iterations: $O(\ell Kn)$.

Seed Choice



Seed Choice



Seed Choice

The results of the K- means Algorithm can vary based on random seed selection.

- Some seeds can result in **poor convergence rate**, or convergence to **sub-optimal** clustering.
- K-means algorithm can get stuck easily in **local minima.**
  - Select good seeds using a heuristic (e.g., object least similar to any existing mean)
  - Try out **multiple** starting points (very important!!!)
  - Initialize with the results of another method.

Alternating Optimization

K- means Algorithm (more formally)

- **Randomly initialize k centers**

$$\mu^0 = (\mu_1^0, \ldots, \mu_K^0)$$

- **Classify**: At iteration t, assign each point x_j ($j \in \{1,\ldots,n\}$) to the nearest center:

Classification at iteration *t*

$$\{1, 2, \ldots, K\} \ni C^t(j) \leftarrow \arg\min_i \|\mu_i^t - x_j\|^2$$

- **Recenter**: $\mu_i^{(t+1)}$ is the centroid of the new set:

$$\mu_i^{(t+1)} \leftarrow \arg\min_{\mu} \sum_{j:C^t(j)=i} \|\mu - x_j\|^2$$

Re-assign new cluster centers at iteration *t*

What is the K-means algorithm optimizing?

- Define the following **potential function** F of centers μ and point allocation C

$$\mu = (\mu_1, \ldots, \mu_K)$$

$$C = (C(1), \ldots, C(n))$$

$$\left.\begin{aligned} F(\mu, C) &= \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|^2 \\ &= \sum_{i=1}^{K} \sum_{j:C(j)=i} \|\mu_i - x_j\|^2 \end{aligned}\right\} \text{Two equivalent versions}$$

- It's easy to see that the optimal solution of the K-means **problem** is:

$$\min_{\mu, C} F(\mu, C)$$

K-means Algorithm

Optimize the potential function:

$$\min_{\mu,C} F(\mu,C) = \min_{\mu,C} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|^2 = \min_{\mu,C} \sum_{i=1}^{K} \sum_{j:C(j)=i} \|\mu_i - x_j\|^2$$

K-means algorithm:

(1) Fix μ, Optimize C

$$\min_{C(1),C(2),\ldots,C(n)} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|^2 = \sum_{j=1}^{n} \underbrace{\min_{C(j)} \|\mu_{C(j)} - x_j\|^2}_{\text{Exactly the first step}}$$

Assign each point to the nearest cluster center

(2) Fix C, Optimize μ

$$\min_{\mu_1,\ldots,\mu_K} \sum_{i=1}^{K} \sum_{j:C(j)=i} \|\mu_i - x_j\|^2 = \sum_{i=1}^{K} \underbrace{\min_{\mu_i} \sum_{j:C(j)=i} \|\mu_i - x_j\|^2}_{\text{Exactly the 2nd step (re-center)}}$$

K-means Algorithm

Optimize the potential function:

$$\min_{\mu,C} F(\mu, C) = \min_{\mu,C} \sum_{j=1}^{n} \|\mu_{C(j)} - x_j\|^2$$

K-means algorithm: (coordinate descent on F)

(1) Fix μ, Optimize C **"Expectation step"**

(2) Fix C, Optimize μ **"Maximization step"**

Today, we will see a generalization of this approach:

EM algorithm

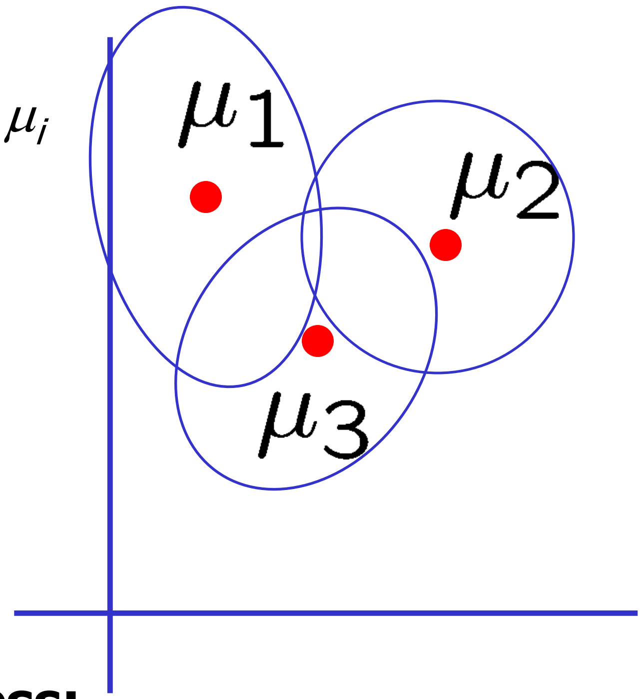
Gaussian Mixture Model

Generative Gaussian Mixture Model

Mixture of K Gaussians distributions: (Multi-modal distribution)

- There are K components
- Component *i* has an associated mean vector μ_i

Component *i* generates data from $N(\mu_i, \Sigma_i)$



Each data point is generated using this process:

1) Choose component i with probability $\pi_i = P(y = i)$

2) Datapoint $x \sim N(\mu_i, \Sigma_i)$

Gaussian Mixture Model

Mixture of K Gaussians distributions: (Multi-modal distribution)

Hidden variable

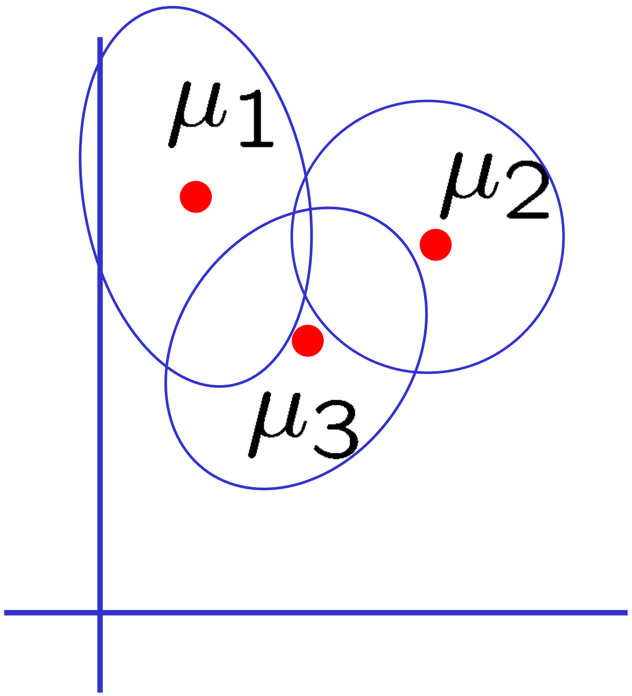
$$p(x|y = i) = N(\mu_i, \Sigma_i)$$

$$p(x) = \sum_{i=1}^{K} p(x|y = i)P(y = i)$$

Observed data

Mixture component

Mixture proportion



Mixture of Gaussians Clustering

Assume that

$\Sigma_i = \sigma^2 \mathbf{I}$, for simplicity.

$p(x|y=i) = N(\mu_i, \sigma^2 \mathbf{I})$

$p(y=i) = \pi_i$

All prameters $\mu_1, \ldots, \mu_K, \sigma^2, \pi_1, \ldots, \pi_K$ are known.

For a given x we want to decide if it belongs to cluster i or cluster j

Cluster x based on the ratio of posteriors:

$$\log \frac{P(y=i|x)}{P(y=j|x)}$$

$$= \log \frac{p(x|y=i)P(y=i)/p(x)}{p(x|y=j)P(y=j)/p(x)}$$

$$= \log \frac{p(x|y=i)\pi_i}{p(x|y=j)\pi_j} = \log \frac{\pi_i \exp(\frac{-1}{2\sigma^2}\|x-\mu_i\|^2)}{\pi_j \exp(\frac{-1}{2\sigma^2}\|x-\mu_j\|^2)}$$

Mixture of Gaussians Clustering

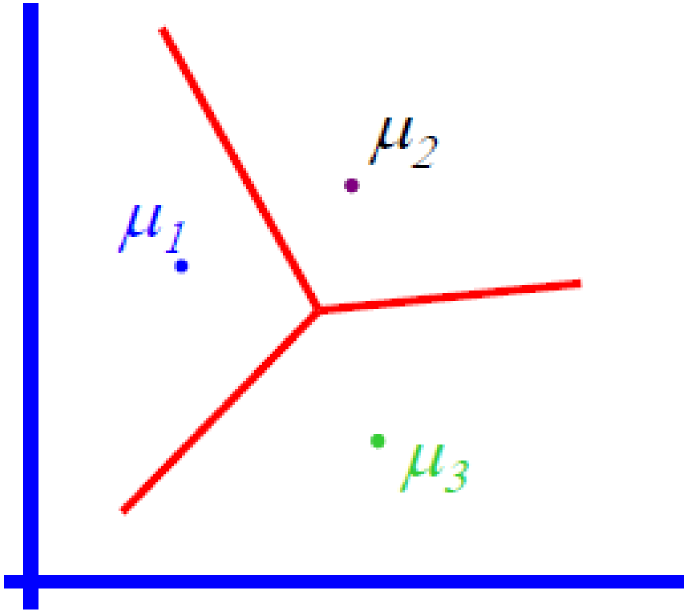
Assume that

$\Sigma_i = \sigma^2 \mathbf{I}$, for simplicity. $\quad p(x|y=i) = N(\mu_i, \sigma^2 \mathbf{I})$

$p(y=i) = \pi_i \quad \mu_1, \ldots, \mu_K, \sigma^2, \pi_1, \ldots, \pi_K$ are known.

$$\log \frac{P(y=i|x)}{P(y=j|x)} = \log \frac{p(x|y=i)\pi_i}{p(x|y=j)\pi_j} = \log \frac{\pi_i \exp(\frac{-1}{2\sigma^2}\|x-\mu_i\|^2)}{\pi_j \exp(\frac{-1}{2\sigma^2}\|x-\mu_j\|^2)}$$

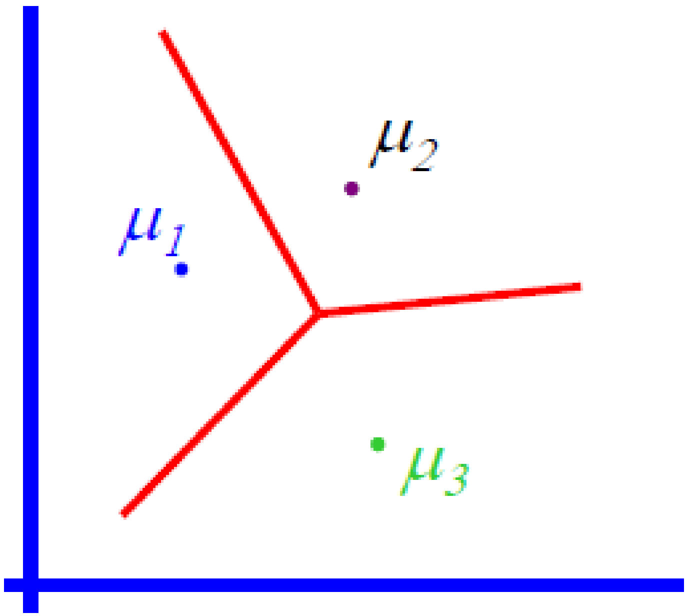
Piecewise linear decision boundary



MLE for GMM

What if we don't know the parameters? $\mu_1, \ldots, \mu_K, \sigma^2, \pi_1, \ldots, \pi_K?$

$\Rightarrow$ **Maximum Likelihood Estimate (MLE)**



$$\theta = [\mu_1, \ldots, \mu_K, \sigma^2, \pi_1, \ldots, \pi_K]$$

$$\arg\max_\theta \prod_{j=1}^{n} P(x_j|\theta)$$

$$= \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i, x_j|\theta)$$

$$= \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i|\theta) p(x_j|y_j = i, \theta)$$

$$= \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} \pi_i \frac{1}{\sqrt{2\pi\sigma^2}} \exp(\frac{-1}{2\sigma^2}\|x_j - \mu_i\|^2)$$

General GMM

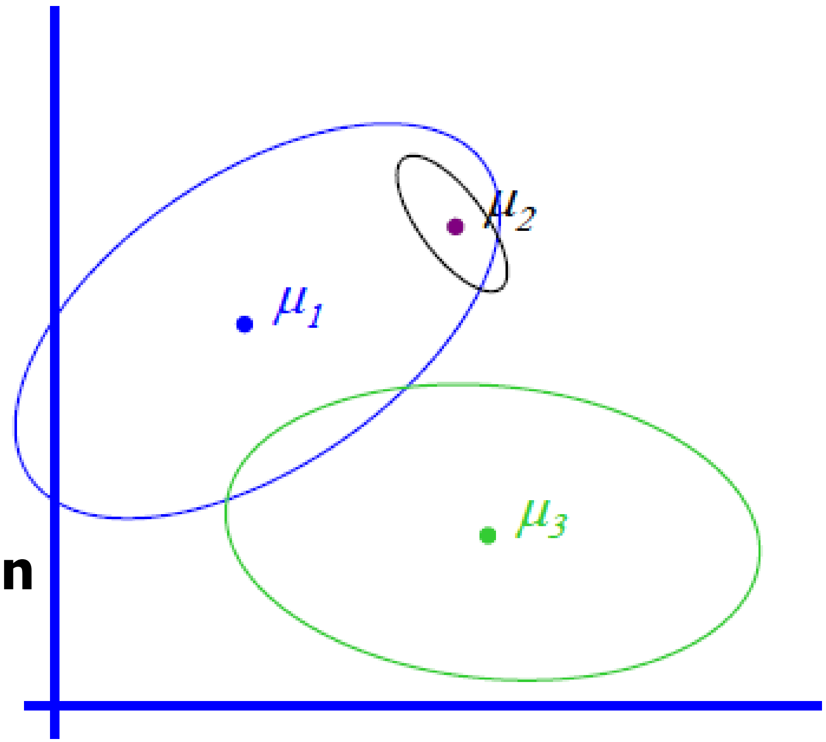
GMM –Gaussian Mixture Model

$$p(x|y=i) = N(\mu_i, \Sigma_i)$$

$$p(x) = \sum_{i=1}^{K} p(x|y=i)P(y=i)$$

Mixture component

Mixture proportion



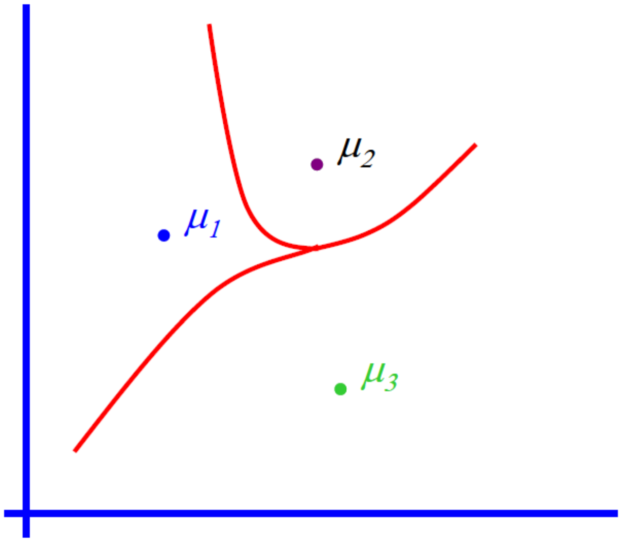
General GMM

Assume that

$$\theta = [\mu_1, \dots, \mu_K, \Sigma_1, \dots, \Sigma_K, \pi_1, \dots, \pi_K] \text{ are known.}$$

$$p(x|y = i) = N(\mu_i, \Sigma_i)$$

$$p(y = i) = \pi_i$$



Clustering based on ratios of posteriors:

$$\log \frac{P(y = i|x)}{P(y = j|x)}$$

$$= \log \frac{p(x|y = i)P(y = i)/p(x)}{p(x|y = j)P(y = j)/p(x)}$$

$$= \log \frac{p(x|y = i)\pi_i}{p(x|y = j)\pi_j} = \log \frac{\pi_i \frac{1}{\sqrt{|2\pi\Sigma_i|}} \exp\left[-\frac{1}{2}(x - \mu_i)^T \Sigma_i^{-1} (x - \mu_i)\right]}{\pi_j \frac{1}{\sqrt{|2\pi\Sigma_j|}} \exp\left[-\frac{1}{2}(x - \mu_j)^T \Sigma_j^{-1} (x - \mu_j)\right]}$$

$$= x^T W x + w^T x + c$$

Depends on $\mu_1, \dots, \mu_K, \Sigma_1, \dots, \Sigma_K, \pi_1, \dots, \pi_K$

"Quadratic Decision boundary" – second-order terms don't cancel out

General GMM MLE Estimation

What if we don't know $\theta = [\mu_1, \ldots, \mu_K, \Sigma_1, \ldots, \Sigma_K, \pi_1, \ldots, \pi_K]$?

$\Rightarrow$ **Maximize marginal likelihood (MLE):**

$$\arg\max_\theta \prod_{j=1}^{n} P(x_j|\theta) = \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i, x_j|\theta)$$

$$= \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i|\theta) p(x_j|y_j = i|\theta)$$

$$= \arg\max_\theta \prod_{j=1}^{n} \sum_{i=1}^{K} \pi_i \frac{1}{\sqrt{|2\pi\Sigma_i|}} \exp\left[-\frac{1}{2}(x_j - \mu_i)^T \Sigma_i^{-1} (x_j - \mu_i)\right]$$

* Set $\frac{\partial}{\partial \mu_i} \log \text{Prob}(\ldots) = 0$, and solve for μ_i.

Non-linear, non-analytically solvable

* Use gradient descent. Doable, but often slow

* Use EM.

The EM algorithm

What is EM in the general case, and why does it work?

Expectation-Maximization (EM)

A general algorithm to deal with hidden data, but we will study it in the context of unsupervised learning (hidden class labels = clustering) first.

- EM is an optimization strategy for objective functions that can be interpreted as likelihoods in the presence of missing data.
- In the following examples EM is "simpler" than gradient methods: No need to choose step size.
- EM is an iterative algorithm with two linked steps:
  - E-step: fill-in hidden values using inference
  - M-step: apply standard MLE/MAP method to completed data
- We will prove that this procedure monotonically improves the likelihood (or leaves it unchanged).

General EM algorithm

Notation

Observed data: $D = \{x_1, \ldots, x_n\}$

Unknown variables: y

For example in clustering: $y = (y_1, \ldots, y_n)$

Paramaters: θ

For example in MoG: $\theta = [\mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, \Sigma_1, \ldots, \Sigma_K]$

Goal: $\widehat{\theta}_n = \arg\max_{\theta} \log P(D|\theta)$

General EM algorithm

Goal: $\arg\max_{\theta} \log P(D|\theta)$

$$\log P(D|\theta^t) = \int dy\, q(y) log P(D|\theta^t)$$

$$= \int dy\, q(y) log \left[\frac{P(y,D|\theta^t)}{P(y|D,\theta^t)} \frac{q(y)}{q(y)} \right] \quad \text{since } P(y,D|\theta^t) = P(D|\theta^t)P(y|D,\theta^t)$$

$$= \underbrace{\int dy\, q(y) log P(y,D|\theta^t) \underbrace{- \int dy\, q(y) \log q(y)}_{H(q)}}_{\text{Free energy: } F_{\theta^t}(q(\cdot),D)} + \underbrace{\int dy\, q(y) \log \frac{q(y)}{P(y|D,\theta^t)}}_{KL(q(y)\|P(y|D,\theta^t))}$$

E Step: $Q(\theta^t|\theta^{t-1}) = \mathbb{E}_y[\log P(y,D|\theta^t)|D,\theta^{t-1}]$

$$= \int dy\, P(y|D,\theta^{t-1}) \log P(y,D|\theta^t)$$

M Step: $\theta^t = \arg\max_{\theta} Q(\theta|\theta^{t-1})$

We are going to discuss why this approach works

General EM algorithm

$$\log P(D|\theta^t) = \underbrace{\int dy\, q(y) log P(y, D|\theta^t) \underbrace{- \int dy\, q(y) \log q(y)}_{H(q)}}_{\text{Free energy: } F_{\theta^t}(q(\cdot), D)} + \underbrace{\int dy\, q(y) \log \frac{q(y)}{P(y|D, \theta^t)}}_{KL(q(y)\|P(y|D,\theta^t))}$$

E Step: $Q(\theta|\theta^t) = \int dy\, P(y|D, \theta^t) \log P(y, D|\theta)$

Let $q(y) = P(y|D, \theta^t)$

$\Rightarrow KL(q(y)\|P(y|D, \theta^t)) = 0$

$$\Rightarrow \log P(D|\theta^t) = F_{\theta^t}(P(y|D, \theta^t), D)$$

$$= \overbrace{\int dy\, P(y|D, \theta^t) log P(y, D|\theta^t)}^{Q(\theta^t|\theta^t)} - \int dy\, P(y|D, \theta^t) \log P(y|D, \theta^t)$$

M Step: $\leq \int dy\, P(y|D, \theta^t) log P(y, D|\theta^{t+1}) - \int dy\, P(y|D, \theta^t) \log P(y|D, \theta^t)$

$\theta^{t+1} = \arg\max_\theta Q(\theta|\theta^t)$

We maximize only here in θ!!!

General EM algorithm

$$\log P(D|\theta^t) = \underbrace{\int dy\, q(y) log P(y, D|\theta^t) \underbrace{- \int dy\, q(y) \log q(y)}_{H(q)}}_{\text{Free energy: } F_{\theta^t}(q(\cdot), D)} + \underbrace{\int dy\, q(y) \log \frac{q(y)}{P(y|D, \theta^t)}}_{KL(q(y) \| P(y|D, \theta^t))}$$

Theorem: During the EM algorithm the marginal likelihood is not decreasing!

$$P(D|\theta^t) \leq P(D|\theta^{t+1})$$

Proof:

$$\begin{aligned}
\log P(D|\theta^t) &= F_{\theta^t}(P(y|D, \theta^t), D) \\
&\leq \int dy\, P(y|D, \theta^t) log P(y, D|\theta^{t+1}) - \int dy\, P(y|D, \theta^t) \log P(y|D, \theta^t) \\
&= F_{\theta^{t+1}}(P(y|D, \theta^t), D) \\
&= \log P(D|\theta^{t+1}) - KL(P(y|D, \theta^t) \| P(y|D, \theta^{t+1})) \\
&\leq \log P(D|\theta^{t+1})
\end{aligned}$$

General EM algorithm

Goal: $\arg\max_\theta \log P(D|\theta)$

E Step:

$$Q(\theta|\theta^{t-1}) = \mathbb{E}_y[\log P(y, D|\theta)|D, \theta^{t-1}]$$

$$= \int dy\, P(y|D, \theta^{t-1}) \log P(y, D|\theta)$$

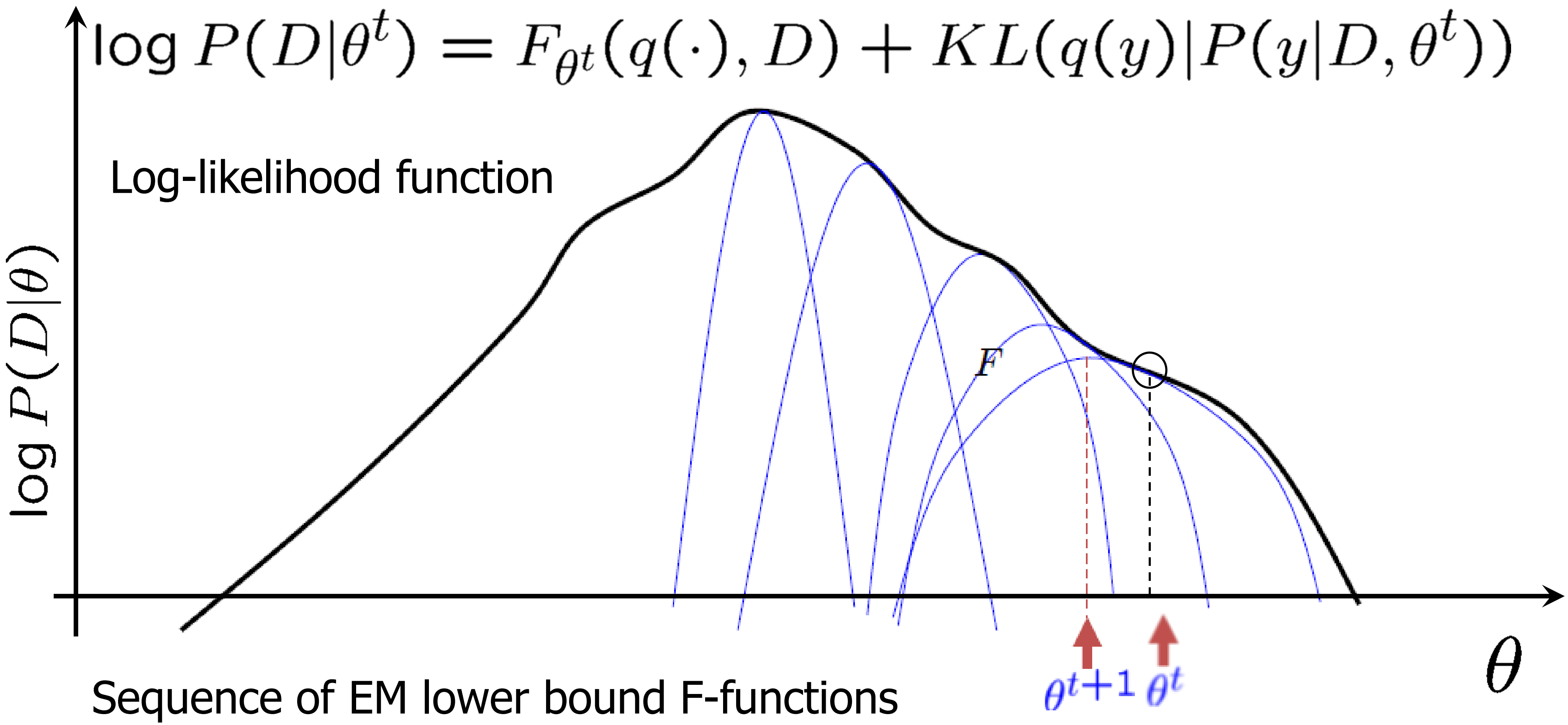
M Step:

$$\theta^t = \arg\max_\theta Q(\theta|\theta^{t-1})$$

During the EM algorithm the marginal likelihood is not decreasing!

$$P(D|\theta^t) \leq P(D|\theta^{t+1})$$

Convergence of EM

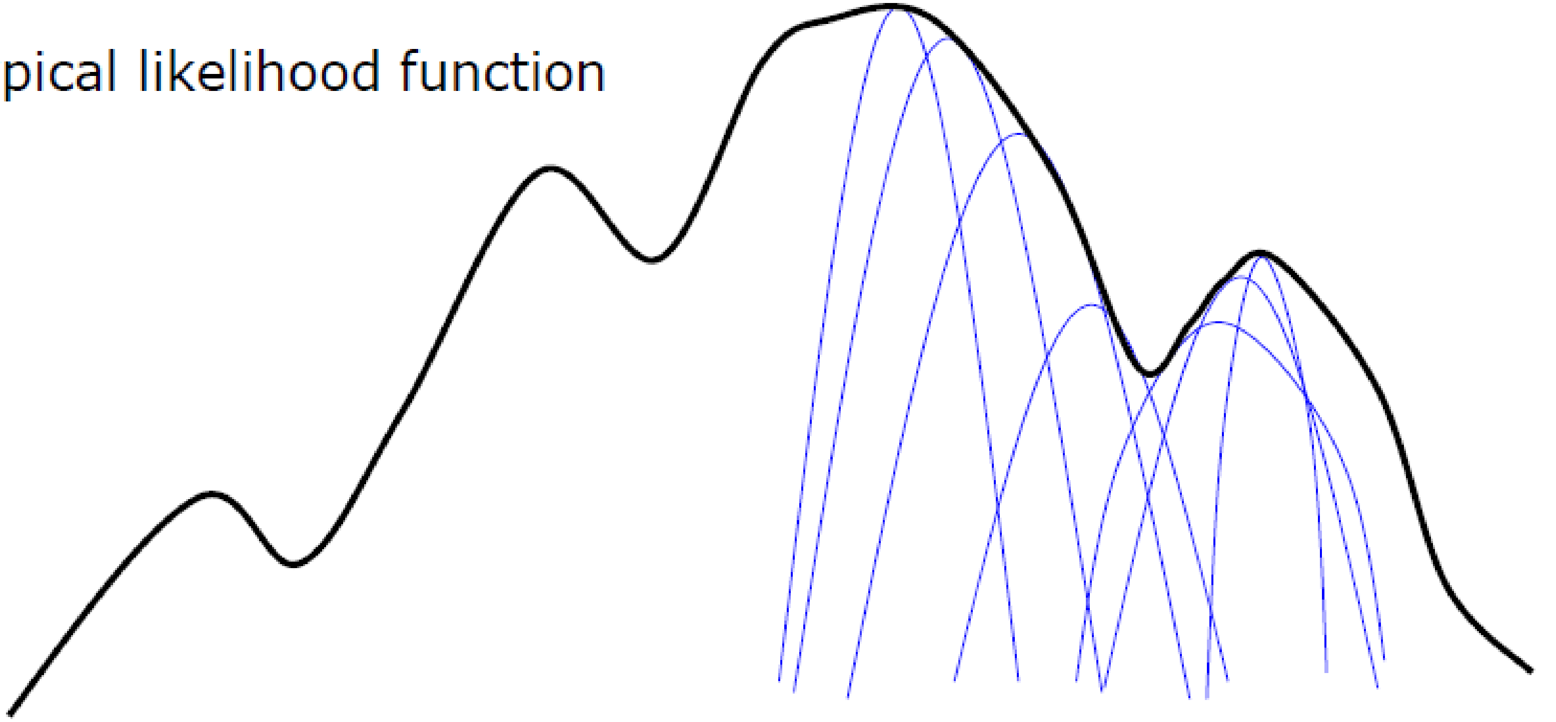


EM: (E) In a given θ_t set $q()$ such a way that the $KL = 0$ and F touches $\log P(D|\theta^t)$. (M) Maximise the lower bound F to get θ_{t+1}.

EM monotonically converges to a local maximum of likelihood !

Convergence of EM

Typical likelihood function



Different sequence of EM lower bound F-functions depending on initialization

Use multiple, randomized initializations in practice

Variational Methods

Variational methods

$$\log P(D|\theta^t) = \underbrace{\int dy\, q(y) logP(y, D|\theta^t) - \underbrace{\int dy\, q(y) \log q(y)}_{H(q)}}_{\text{Free energy: } F_{\theta^t}(q(\cdot), D)} + \underbrace{\int dy\, q(y) \log \frac{q(y)}{P(y|D, \theta^t)}}_{KL(q(y) \| P(y|D, \theta^t))}$$

$$\log P(D|\theta^t) \geq F_{\theta^t}(q(\cdot), D)$$

If $P(y|D, \theta^t))$ is complicated, then instead of setting

$$q(y) = P(y|D, \theta^t)),$$

try to find suboptimal maximum points of the free energy.

Variational methods might decrease the marginal likelihood!

Variational methods

$$\log P(D|\theta^t) = \underbrace{\int dy\, q(y) log P(y, D|\theta^t) - \underbrace{\int dy\, q(y) \log q(y)}_{H(q)}}_{\text{Free energy: } F_{\theta^t}(q(\cdot), D)} + \underbrace{\int dy\, q(y) \log \frac{q(y)}{P(y|D, \theta^t)}}_{KL(q(y) \| P(y|D, \theta^t))}$$

$$\log P(D|\theta^t) = F_{\theta^t}(q(\cdot), D) + KL(q(y) \| P(y|D, \theta^t)) \quad \log P(D|\theta^t) \geq F_{\theta^t}(q(\cdot), D)$$

Partial E Step:

θ^t is fixed

$$q^t(\cdot) = \arg\max_{q(\cdot)} F_{\theta^t}(q(\cdot), D) = \arg\min_{q(\cdot)} KL(q(y) \| P(y|D, \theta^t))$$

But **not** necessarily the best max/min which would be $P(y|D, \theta^t))$

Partial M Step:

q^t is fixed

$$\theta^{t+1} = \arg\max_{\theta} F_{\theta}(q^t(\cdot), D)$$

Variational methods might decrease the marginal likelihood!

Summary: EM Algorithm

A way of maximizing likelihood function for hidden variable models.

Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:

1. Estimate some “missing” or “unobserved” data from observed data and current parameters.
2. Using this “complete” data, find the MLE parameter estimates.

Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:

E Step: $q^t = \arg\max_q F_{\theta^t}(q(\cdot), D)$

M Step: $\theta^{t+1} = \arg\max_\theta F_\theta(q^t(\cdot), D)$

In the M-step we optimize a lower bound F on the log-likelihood L.

In the E-step we close the gap, making bound F =log-likelihood L.

EM performs coordinate ascent on F, can get stuck in local optima.

EM Examples

Expectation-Maximization (EM)

A simple case:

- We have unlabeled data $x_1, x_2, \ldots, x_n$
- We know there are K classes
- We know $P(y=1)=\pi_1$, $P(y=2)=\pi_2$, $P(y=3)=\pi_3 \ldots$, $P(y=K)=\pi_K$
- We know common variance σ^2
- We **don't** know $\mu_1, \mu_2, \ldots \mu_K$, and we want to learn them

We can write

$$p(x_1, \ldots, x_n | \mu_1, \ldots \mu_K) = \prod_{j=1}^{n} p(x_j | \mu_1, \ldots, \mu_K)$$ Independent data

$$= \prod_{j=1}^{n} \sum_{i=1}^{K} p(x_j, y_j = i | \mu_1, \ldots, \mu_K)$$ Marginalize over class

$$= \prod_{j=1}^{n} \sum_{i=1}^{K} p(x_j | y_j = i, \mu_1, \ldots, \mu_K) p(y_j = i)$$

$$\propto \prod_{j=1}^{n} \sum_{i=1}^{K} \exp\left(-\frac{1}{2\sigma^2} \|x_j - \mu_i\|^2\right) \pi_i$$ $\Rightarrow$ learn $\mu_1, \mu_2, \ldots \mu_K$

EXPECTATION (E) STEP

We want to learn: $\theta = [\mu_1, \ldots, \mu_K]$

Our estimator at the end of iteration t-1: $\theta^{t-1} = [\mu_1^{t-1}, \ldots, \mu_K^{t-1}]$

At iteration t, construct function Q:

$$Q(\theta^t|\theta^{t-1}) = \sum_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i|x_j, \theta^{t-1}) \log P(x_j, y_j = i|\theta^t)$$

E step

$$P(y_j = i|x_j, \theta^{t-1}) = P(y_j = i|x_j, \mu_1^{t-1}, \ldots, \mu_K^{t-1})$$

$$\propto P(x_j|y_j = i, \mu_1^{t-1}, \ldots, \mu_K^{t-1}) P(y_j = i)$$

$$\propto \exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^{t-1}\|^2)\pi_i$$

$$= \frac{\exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^{t-1}\|^2)\pi_i}{\sum_{i=1}^{K} \exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^{t-1}\|^2)\pi_i}$$

Equivalent to assigning clusters to each data point in K-means in a soft way

Maximization (M) step

$$Q(\theta^t|\theta^{t-1}) = \sum_{j=1}^{n}\sum_{i=1}^{K} P(y_j = i|x_j, \theta^{t-1}) \log P(x_j, y_j = i|\theta^t)$$

$$= \sum_{j=1}^{n}\sum_{i=1}^{K} P(y_j = i|x_j, \theta^{t-1}) \underbrace{[\log \underbrace{P(x_j|y_j = i, \theta^t)}_{\propto \exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^t\|^2)} + \log \underbrace{P(y_j = i|\theta^t)}_{\pi_i}]}_{\text{Joint distribution is simple}}$$

We calculated these weights in the E step

$$R_{i,j}^{t-1} = P(y_j = i|x_j, \theta^{t-1})$$

M step At iteration t, maximize function Q in θ^t:

$$Q(\mu_i^t|\theta^{t-1}) \propto \sum_{j=1}^{n} R_{i,j}^{t-1}(-\frac{1}{2\sigma^2}\|x_j - \mu_i^t\|^2)$$

$$\frac{\partial}{\partial \mu_i^t} Q(\mu_i^t|\theta^{t-1}) = 0 \Rightarrow \sum_{j=1}^{n} R_{i,j}^{t-1}(x_j - \mu_i^t) = 0$$

$$\boxed{\mu_i^t = \sum_{j=1}^{n} w_j x_j \text{ where } w_j = \frac{R_{i,j}^{t-1}}{\sum_{j=1}^{n} R_{i,j}^{t-1}} = \frac{P(y_j=i|x_j,\theta^{t-1})}{\sum_{l=1}^{n} P(y_l=i|x_l,\theta^{t-1})}}$$

Equivalent to updating cluster centers in K-means

EM for spherical, same variance GMMs

E-step

Compute "expected" classes of all datapoints for each class

$$P(y_j = i|x_j, \theta^{t-1}) = \frac{\exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^{t-1}\|^2)\pi_i^{t-1}}{\sum_{i=1}^{K}\exp(-\frac{1}{2\sigma^2}\|x_j - \mu_i^{t-1}\|^2)\pi_i^{t-1}}$$

In K-means "E-step" we do hard assignment. EM does soft assignment

M-step

Compute Max of function Q. [I.e. update $\boldsymbol{\mu}$ given our data's class membership distributions (weights)]

$$\mu_i^t = \sum_{j=1}^{n} w_j x_j \quad \text{where } w_j = \frac{P(y_j=i|x_j,\theta^{t-1})}{\sum_{l=1}^{n} P(y_l=i|x_l,\theta^{t-1})}$$

Iterate.

EM for general GMMs

The more general case:

- We have unlabeled data $x_1, x_2, \ldots, x_m$
- We know there are K classes
- We **don't** know $P(y=1)=\pi_1$, $P(y=2)=\pi_2$ $P(y=3)$ … $P(y=K)=\pi_K$
- We **don't** know $\Sigma_1, \ldots \Sigma_K$
- We **don't** know $\mu_1, \mu_2, \ldots \mu_K$

We want to learn: $\theta = [\mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, \Sigma_1, \ldots, \Sigma_K]$

Our estimator at the end of iteration t-1:

$$\theta^{t-1} = [\mu_1^{t-1}, \ldots, \mu_K^{t-1}, \pi_1^{t-1}, \ldots, \pi_K^{t-1}, \Sigma_1^{t-1}, \ldots, \Sigma_K^{t-1}]$$

The idea is the same:

At iteration t, construct function Q (E step) and maximize it in θ^t (M step)

$$Q(\theta^t|\theta^{t-1}) = \sum_{j=1}^{n} \sum_{i=1}^{K} P(y_j = i|x_j, \theta^{t-1}) \log P(x_j, y_j = i|\theta^t)$$

EM for general GMMs

At iteration t, construct function Q (E step) and maximize it in θ^t (M step)

$$Q(\theta^t|\theta^{t-1}) = \sum_{j=1}^{n}\sum_{i=1}^{K} P(y_j = i|x_j, \theta^{t-1}) \log P(x_j, y_j = i|\theta^t)$$

E-step

Compute "expected" classes of all datapoints for each class

$$R_{i,j}^{t-1} = P(y_j = i|x_j, \theta^{t-1}) = \frac{\exp(-\frac{1}{2}(x_j - \mu_i^{t-1})^T \Sigma^{-1}(x_j - \mu_i^{t-1}))\pi_i^{t-1}}{\sum_{i=1}^{K} \exp(-\frac{1}{2}(x_j - \mu_i^{t-1})^T \Sigma^{-1}(x_j - \mu_i^{t-1}))\pi_i^{t-1}}$$

M-step $\frac{\partial}{\partial\theta^t} Q(\theta^t|\theta^{t-1}) = 0$

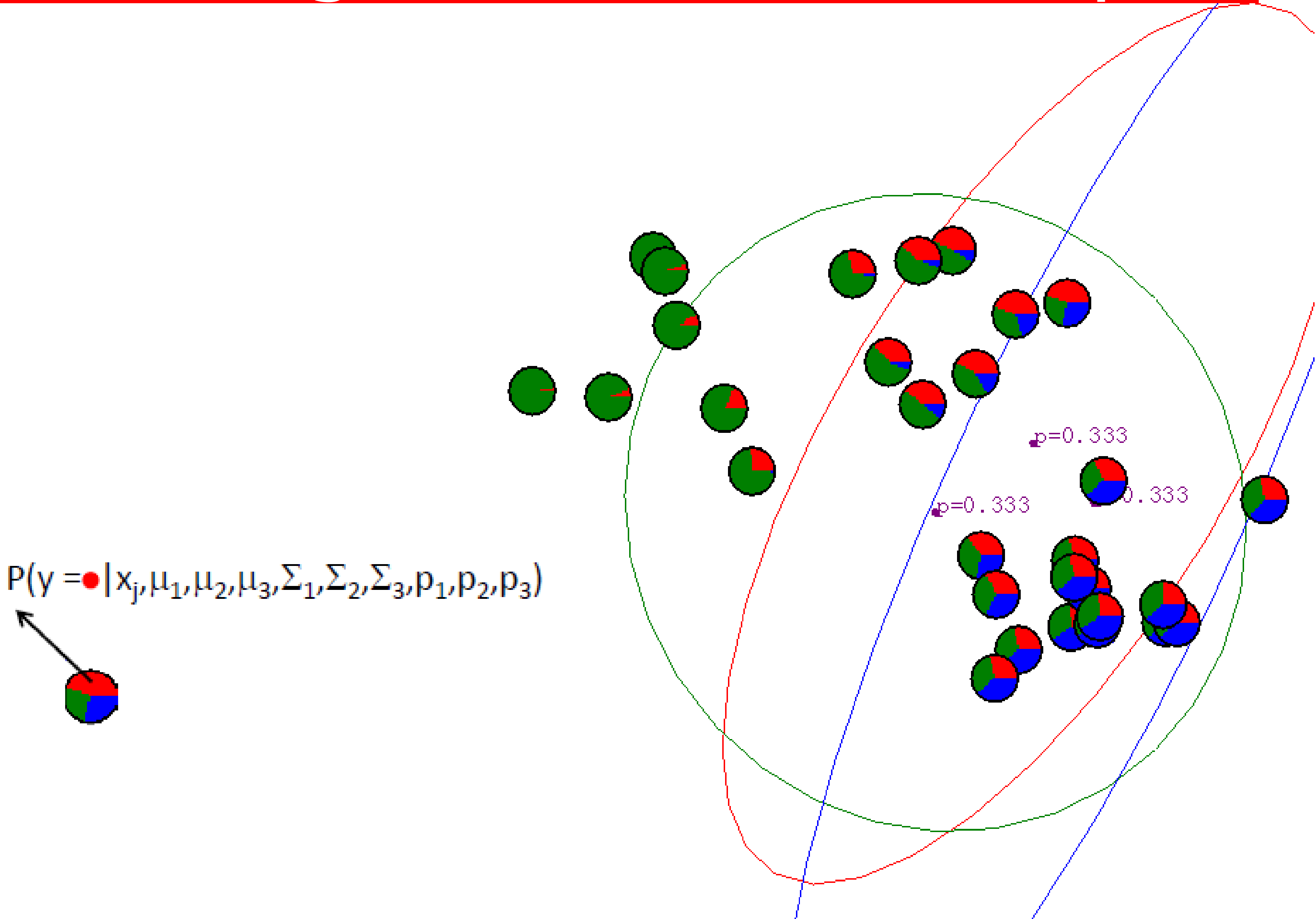
Compute MLEs given our data's class membership distributions (weights)

$$\mu_i^t = \sum_{j=1}^{n} w_j x_j \quad \text{where } w_j = \frac{R_{i,j}^{t-1}}{\sum_{j=1}^{n} R_{i,j}^{t-1}}$$

$$\Sigma_i^t = \sum_{j=1}^{n} w_j (x_j - \mu_i^t)^T (x_j - \mu_i^t)$$

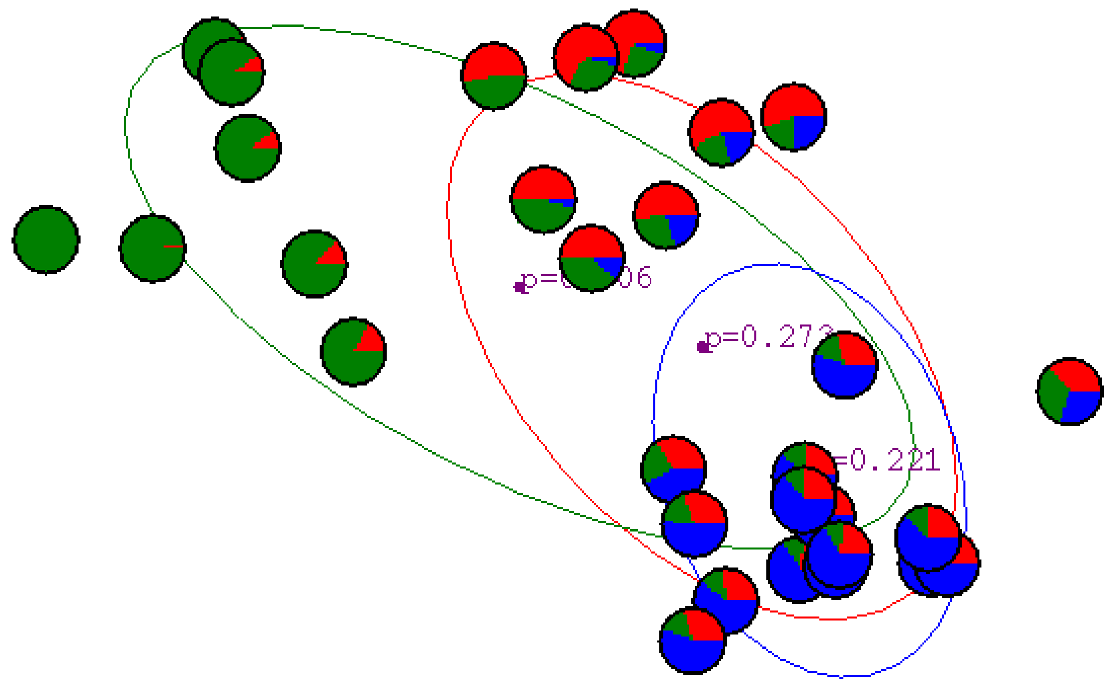
$$\pi_i^t = \frac{1}{n}\sum_{j=1}^{n} R_{i,j}^{t-1}$$

EM for general GMMs: Example



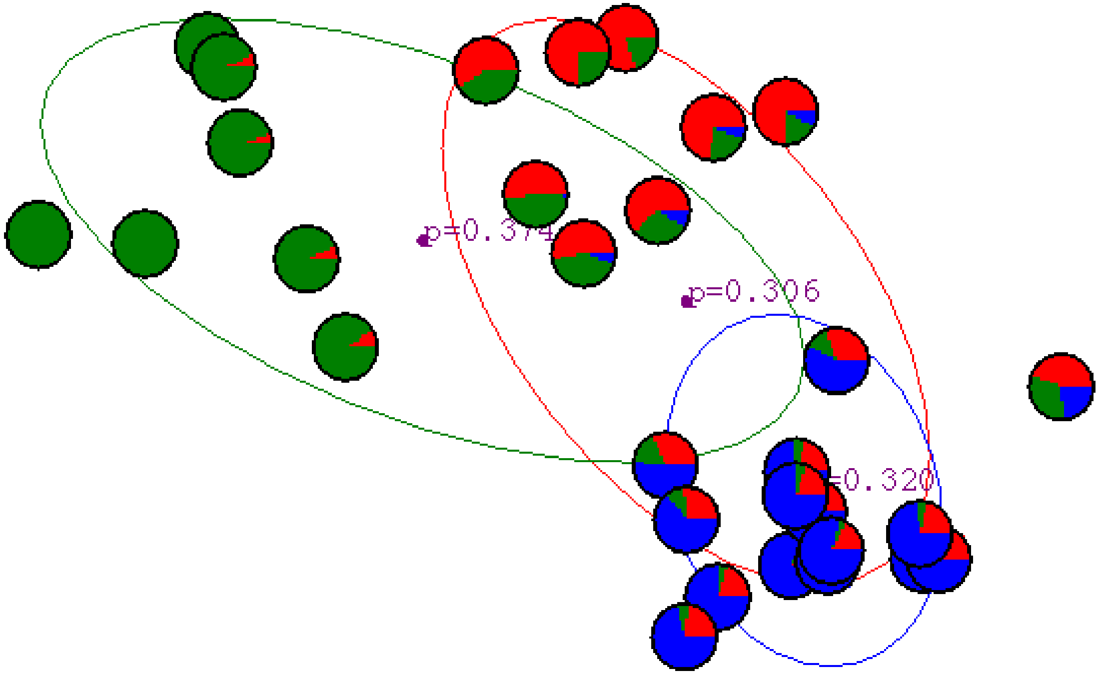
EM for general GMMs: Example

After 1st iteration



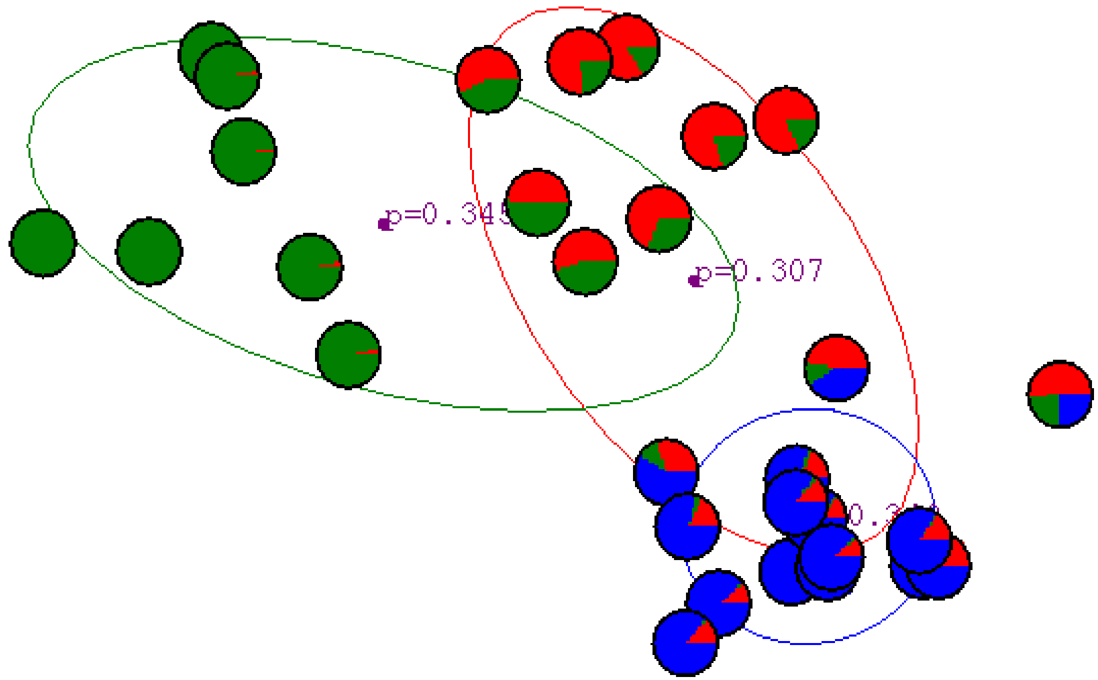
EM for general GMMs: Example

After 2nd iteration



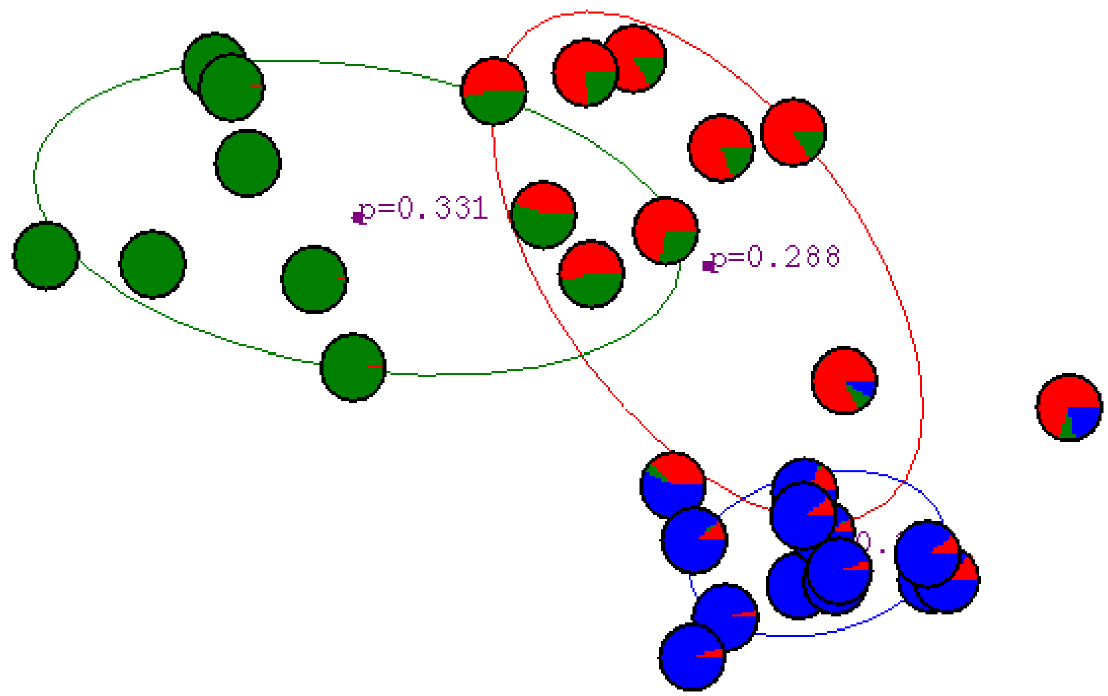
EM for general GMMs: Example

After 3rd iteration



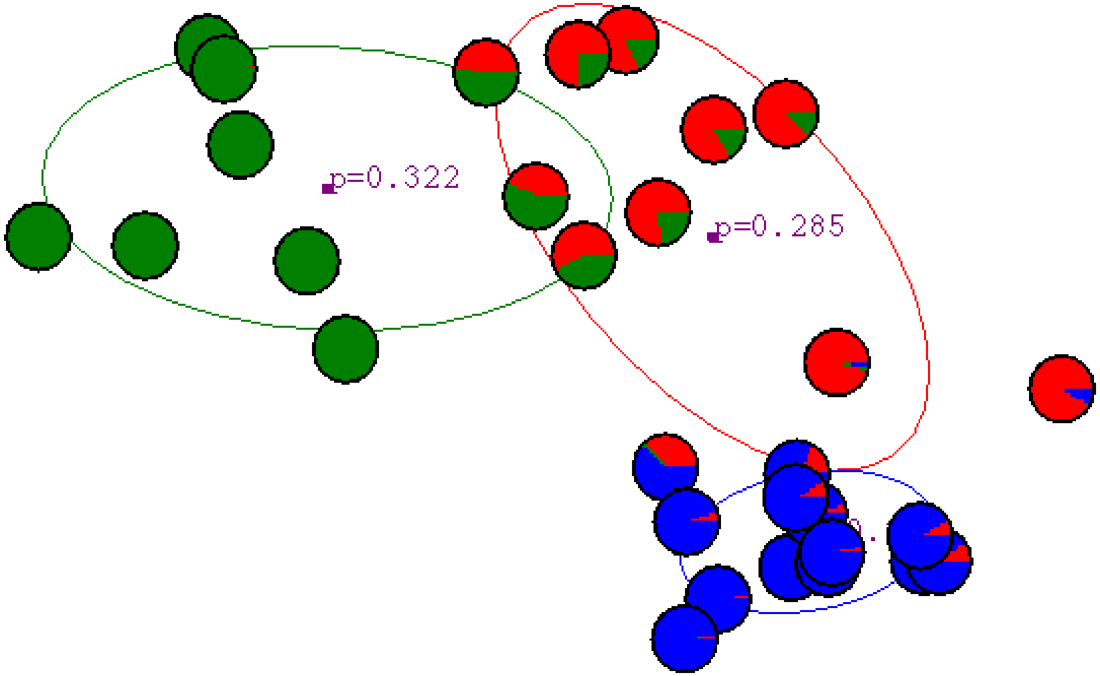
EM for general GMMs: Example

After 4th iteration



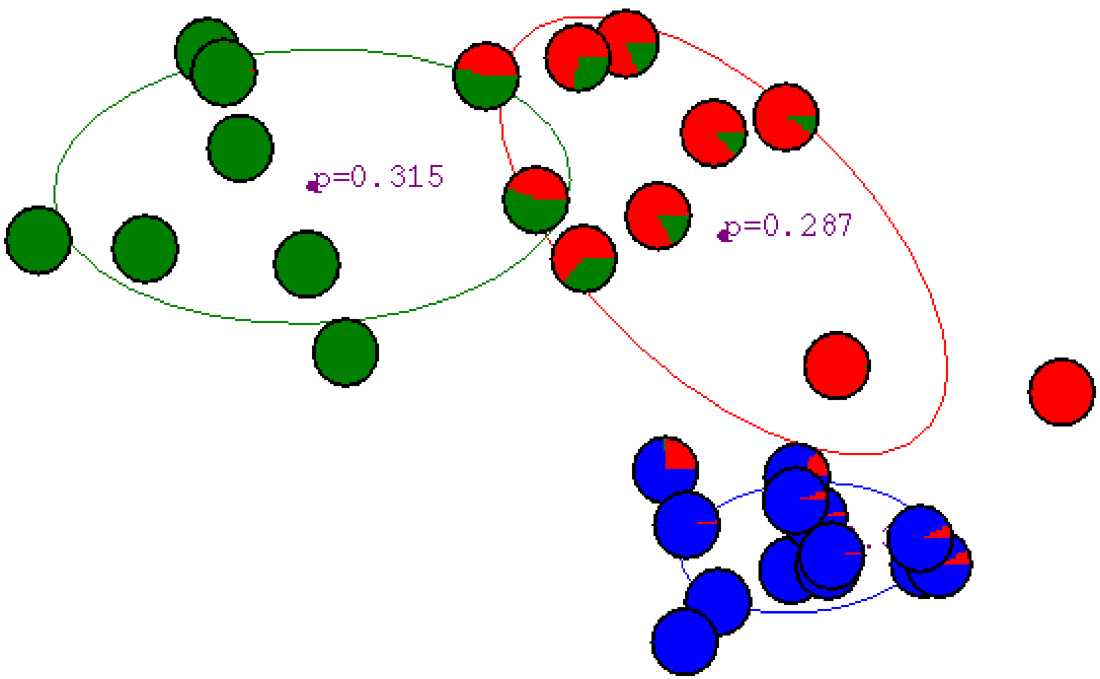
EM for general GMMs: Example

After 5th iteration



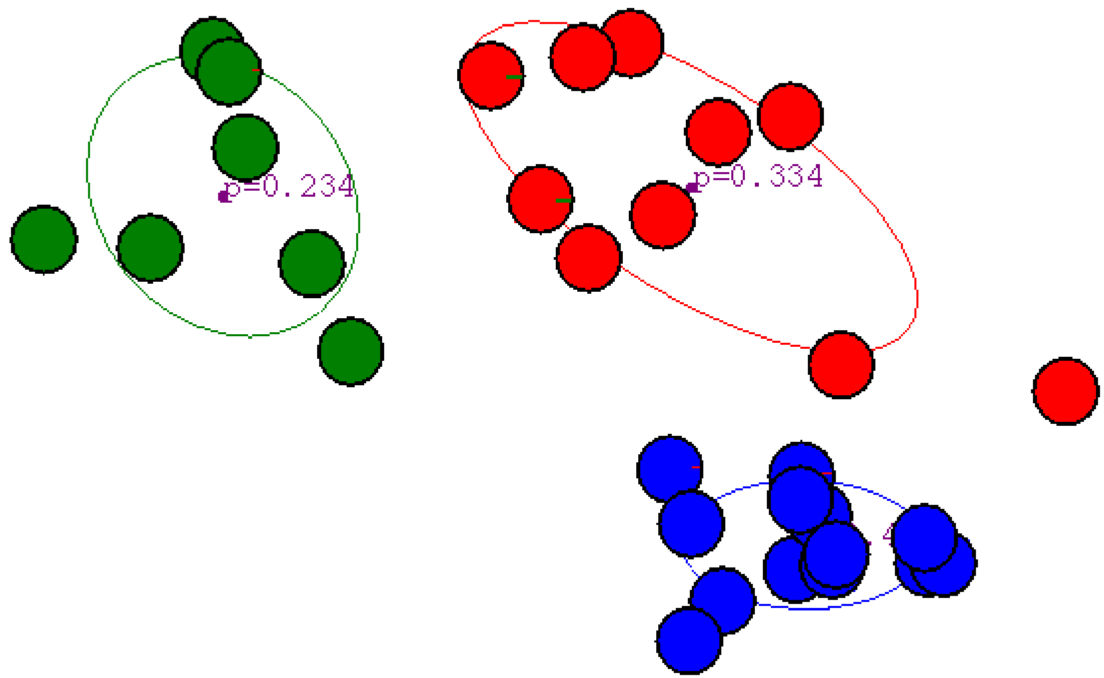
EM for general GMMs: Example

After 6th iteration

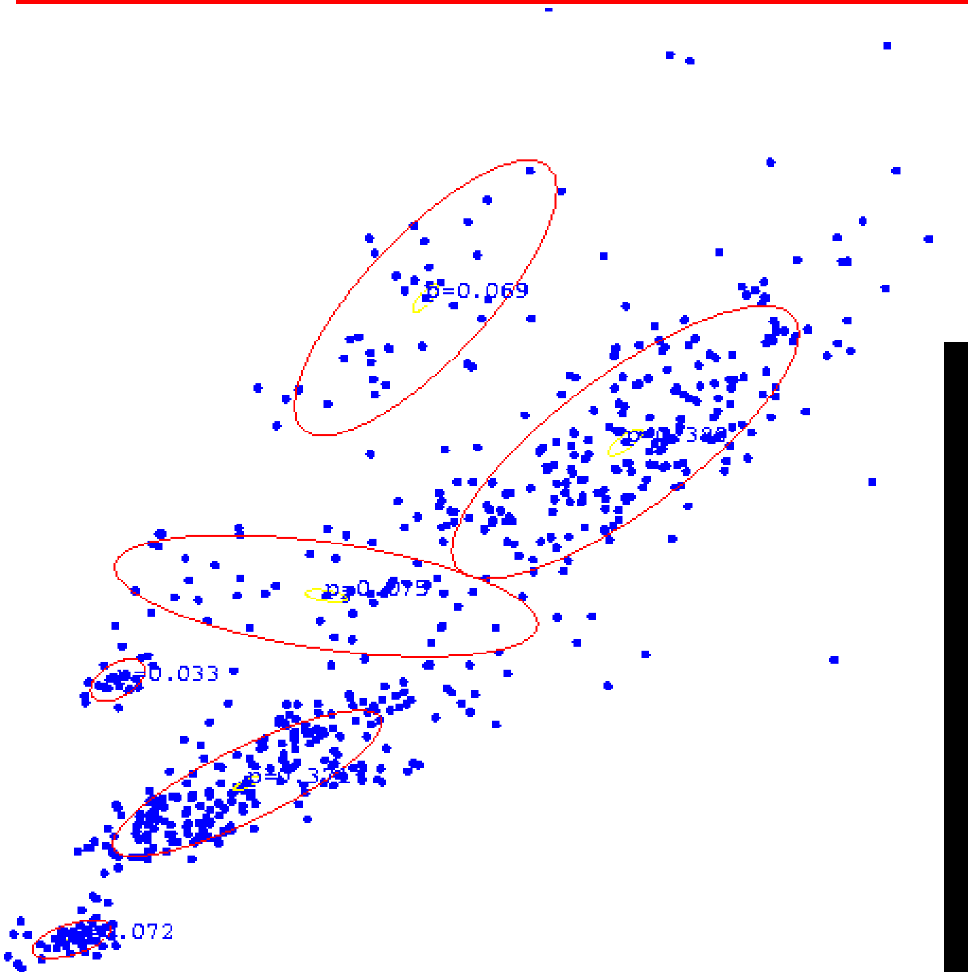


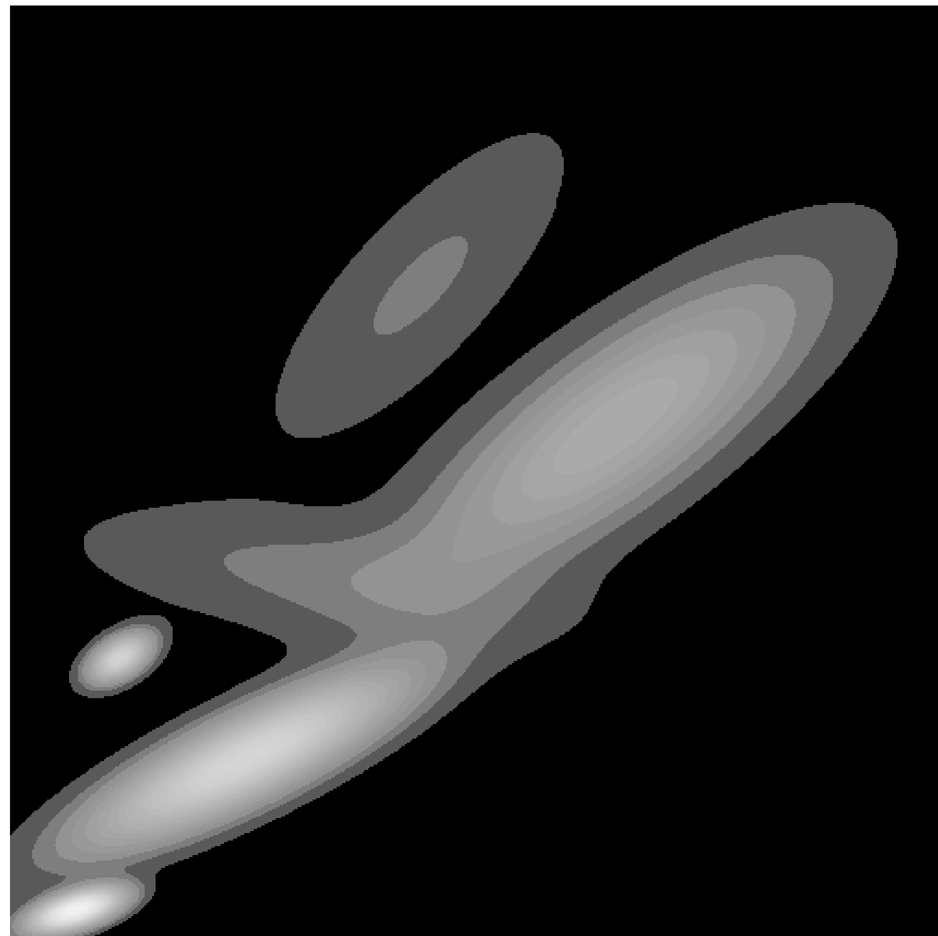
EM for general GMMs: Example

After 20th iteration



GMM for Density Estimation





WHAT YOU SHOULD KNOW

- K-means problem
- K-mean algorithm
- Mixture of Gaussians model
- Expectation Maximization Algorithm
- EM vs MLE

Thanks for your attention!