Lecture 18

Mixture Models & EM

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based on the slides of Nick Rouzzi and Vibhav Gogate

Previously…

- We looked at k-means and hierarchical clustering as mechanisms for unsupervised learning
  - k-means was simply a block coordinate descent scheme for a specific objective function

    ↑ Alt min

- Today: how to learn probabilistic models for unsupervised learning problems

  ↑ Probabilistic Clustering

EM: Soft Clustering

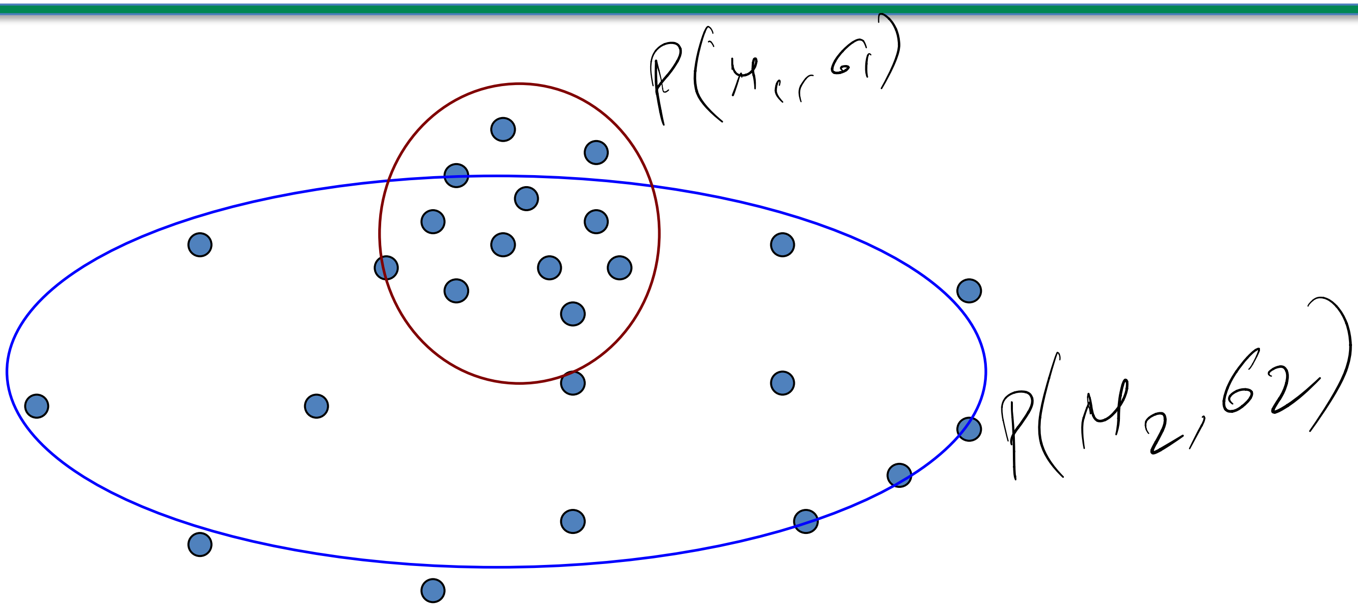
- Clustering (e.g., k-means) typically assumes that each instance is given a “hard” assignment to exactly one cluster
- Does not allow uncertainty in class membership or for an instance to belong to more than one cluster
  - Problematic because data points that lie roughly midway between cluster centers 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
  - $p(x|y)\, p(y)$
- Challenge: we need to estimate model parameters $\underbrace{\text{without labeled } y\text{'s}}$ (i.e., in the unsupervised setting)

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
…	…	…

Probabilistic Clustering



- Clusters of different shapes and sizes
- Clusters can overlap! (k-means doesn't allow this)

Finite Mixture Models

- Given a dataset: $x^{(1)}, \ldots, x^{(N)}$
- **Mixture model**: $\underline{\Theta} = \{\lambda_1, \ldots, \lambda_k, \overbrace{\theta_1, \ldots, \theta_k}\}$

$\theta_y = (\mu_y, \sigma_y)$ $\quad \lambda_y = p(y|\Theta)$

$$\underbrace{p(x|\Theta)} = \sum_{y=1}^{k} \boxed{\lambda_y p_y(x|\theta_y)}$$

$\sum_y p(x, y|\Theta)$

$= \underbrace{p(x|\Theta, y)\, p(y|\Theta)}$

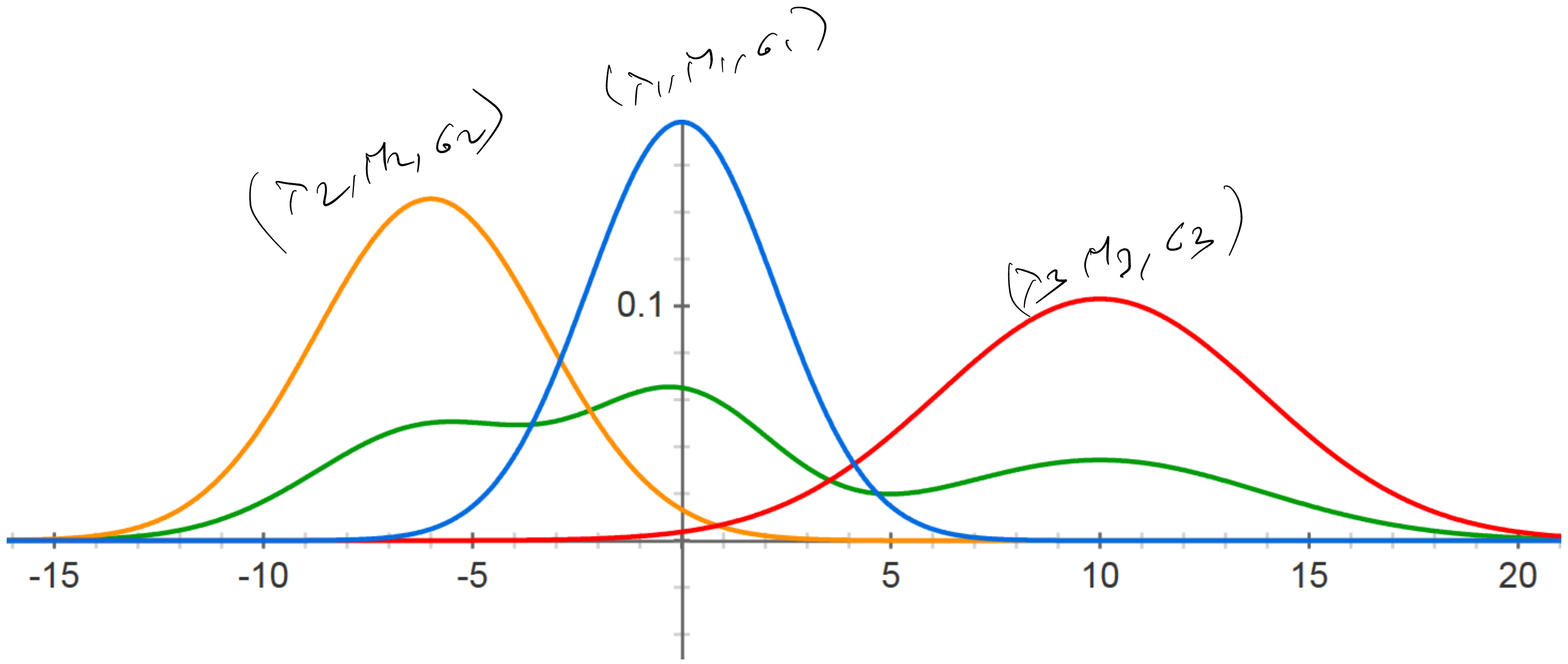
- $\underbrace{p_y(x|\theta_y)}$ is a mixture component from some family of probability distributions parameterized by θ_y and $\lambda \geq 0$ such that $\sum_y \lambda_y = 1$ are the mixture weights

- We can think of $\lambda_y = \underbrace{p(Y = y|\Theta)}$ for some random variable Y that takes values in $\{1, \ldots, k\}$

$p(x|\Theta, y) = p_y(x|\theta_y)$

$p(y|\Theta) = \lambda_y$

Finite Mixture Models



Uniform mixture of 3 Gaussians

Multivariate Gaussian

- A d-dimensional multivariate Gaussian distribution is defined by a $d \times d$ covariance matrix Σ and a mean vector μ

$$p(x|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^{\mathrm{d}}\det(\Sigma)}} \exp\left(-\frac{1}{2}(x-\mu)^T \underbrace{\Sigma^{-1}}(x-\mu) \right)$$

- The covariance matrix describes the degree to which pairs of variables vary together
  - The $\underline{\text{diagonal elements}}$ correspond to variances of the individual variables

$$\frac{(x-\mu)^2}{\sigma^2}$$

Multivariate Gaussian

- A d-dimensional multivariate Gaussian distribution is defined by a $d \times d$ covariance matrix Σ and a mean vector μ

$$p(x|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^{\mathrm{d}}\det(\Sigma)}} \exp\left(-\frac{1}{2}\underline{(x-\mu)^T\Sigma^{-1}(x-\mu)}\right)$$

- The covariance matrix must be a symmetric positive definite matrix in order for the above to make sense
  - Positive definite: all eigenvalues are positive & matrix is invertible
  - Ensures that the quadratic form is concave

Gaussian Mixture Models (GMMs)

- We can define a GMM by choosing the k^{th} component of the mixture to be a Gaussian density with parameters

$$\theta_k = \{\mu_k, \Sigma_k\}$$

$$\underbrace{\overset{\overset{p(x|\theta_k)}{\downarrow}}{p(x|\mu_k, \Sigma_\mathrm{k})}} = \frac{1}{\sqrt{(2\pi)^\mathrm{d}\det(\Sigma_\mathrm{k})}} \exp\left(\underbrace{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}\right)$$

We could cluster by fitting a mixture of k Gaussians to our data

How do we learn these kinds of models?

Learning Gaussian Parameters

- MLE for supervised univariate Gaussian

$$\left.\begin{aligned} \mu_{MLE} &= \frac{1}{N}\sum_{i=1}^{N} x^{(i)} \\ \sigma_{MLE}^2 &= \frac{1}{N}\sum_{i=1}^{N}\left(x^{(i)} - \mu_{MLE}\right)^2 \end{aligned}\right\} d=1$$

- MLE for supervised multivariate Gaussian

$$\underline{\mu_{MLE}} = \frac{1}{N}\sum_{i=1}^{N} x^{(i)}$$

$$\Sigma_{\mathrm{MLE}} = \frac{1}{N}\sum_{i=1}^{N}\left(x^{(i)} - \mu_{MLE}\right)\left(x^{(i)} - \mu_{MLE}\right)^T$$

Learning Gaussian Parameters

- MLE for supervised multivariate mixture of k Gaussian distributions

$$\mu_{MLE}^{k} = \frac{1}{|M_k|} \sum_{\boxed{i \in M_k}} x^{(i)}$$

$$\Sigma_{MLE}^{k} = \frac{1}{|M_k|} \sum_{i \in M_k} \left(x^{(i)} - \mu_{MLE}^{k}\right)\left(x^{(i)} - \mu_{MLE}^{k}\right)^T$$

Sums are over the observations that were generated by the k^{th} mixture component (this requires that we know which points were generated by which distribution!)

The Unsupervised Case

- What if our observations do not include information about which of the k mixture components generated them?

- Consider a joint probability distribution over data points, $x^{(i)}$, and mixture assignments, $\underbrace{y \in \{1, \dots, k\}}$

$x^{(1)}, \dots, x^{(N)}$

$$\arg\max_{\Theta} \prod_{i=1}^{N} \underbrace{p(x^{(i)}|\Theta)} = \arg\max_{\Theta} \prod_{i=1}^{N} \underbrace{\sum_{y=1}^{k} p(x^{(i)}, Y = y|\Theta)}$$

$p(x^{(i)}|\Theta)$

$$= \arg\max_{\underbrace{\Theta}} \prod_{i=1}^{N} \underbrace{\sum_{y=1}^{k}} p\left(x^{(i)}\middle|Y = y, \Theta\right) p(Y = y|\Theta)$$

The Unsupervised Case

- What if our observations do not include information about which of the k mixture components generated them?

- Consider a joint probability distribution over data points, $x^{(i)}$, and mixture assignments, $y \in \{1, \ldots, k\}$

$$\sum_{i=1}^{N} \log\left[\sum_{y} p(x^{(i)} | y, \Theta) p(y|\Theta)\right]$$

$$\arg\max_{\Theta} \prod_{i=1}^{N} p(x^{(i)}|\Theta) = \arg\max_{\Theta} \prod_{i=1}^{N} \sum_{y=1}^{k} p(x^{(i)}, Y = y|\Theta)$$

$$= \arg\max_{\Theta} \prod_{i=1}^{N} \sum_{y=1}^{k} \underbrace{p\big(x^{(i)}|Y = y, \Theta\big)}_{N(\mu_y, \Sigma_y)} \underbrace{p(Y = y|\Theta)}_{p_y}$$

We only know how to compute the probabilities for each mixture component

The Unsupervised Case

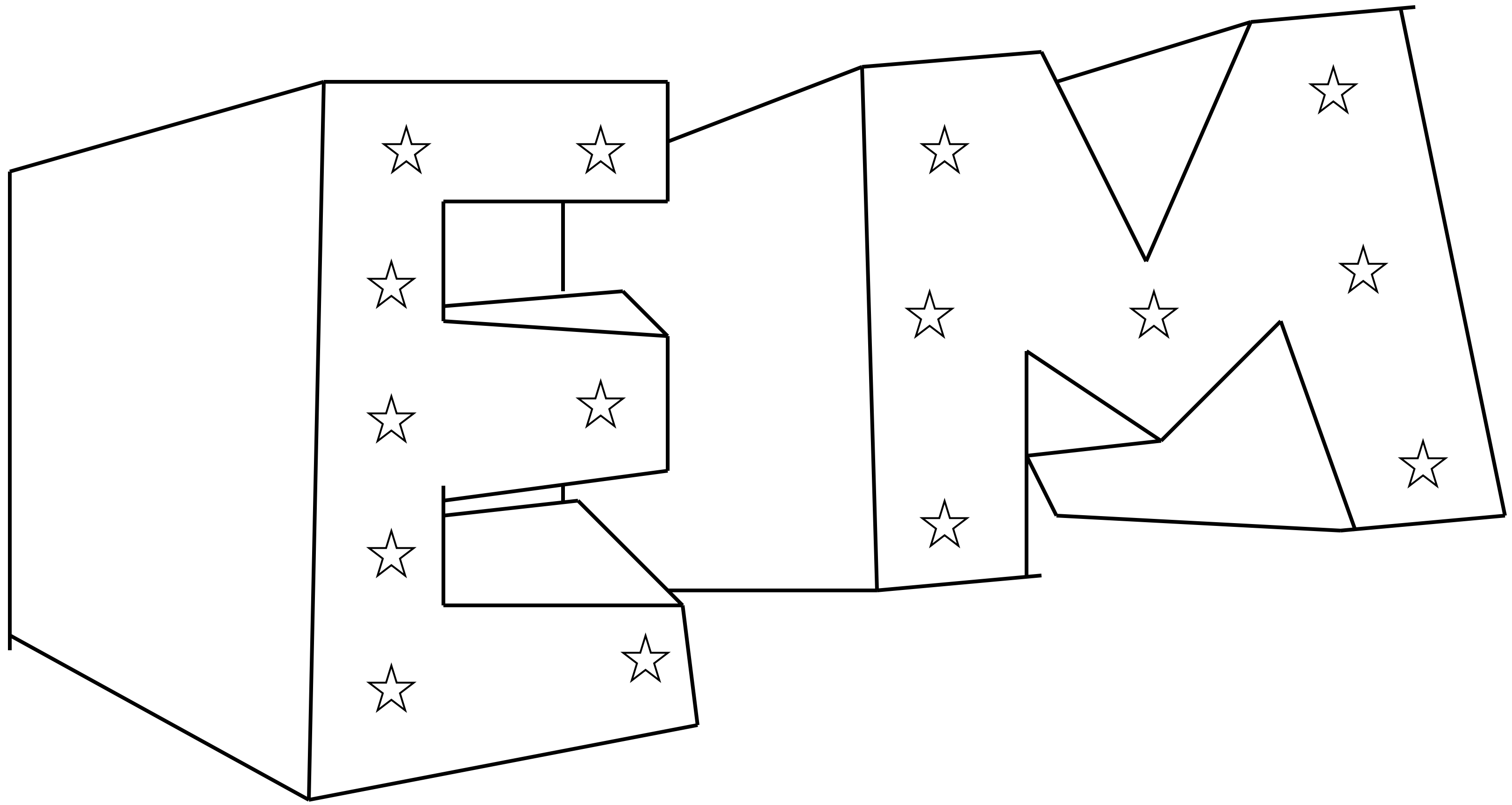
- In the case of a Gaussian mixture model

$$\underbrace{p\left(x^{(i)} \middle| Y = y, \Theta\right) = N(x^{(i)} | \mu_y, \Sigma_y)}$$

$$\underline{p(Y = y|\Theta)} = \underline{\lambda_y}$$

- Differentiating the MLE objective yields a system of equations that is difficult to solve in general
    - The solution: modify the objective to make the optimization easier

Expectation Maximization



Jensen's Inequality

For a convex function $f : \mathbb{R}^n \to \mathbb{R}$, any $a_1, \dots, a_k \in [0,1]$ such that $a_1 + \cdots + a_k = 1$, and any $x^{(1)}, \dots, x^{(k)} \in \mathbb{R}^n$,

$$\underbrace{a_1 f\left(x^{(1)}\right) + \cdots + a_k f\left(x^{(k)}\right)} \geq f\left(a_1 x^{(1)} + \cdots + a_k x^{(k)}\right)$$

Inequality is reversed for concave functions

$$a_1 \psi\left(x^{(1)}\right) + \cdots + a_k \psi\left(x^{(k)}\right) \leq \psi\left(a_1 x^{(1)} + \cdot\, a_k x^{(k)}\right)$$

EM Algorithm

$$p(x^{(i)} \mid Y=y, \Theta)\, p(Y=y \mid \Theta)$$

$$\underbrace{\log \ell(\Theta)} = \sum_{i=1}^{N} \log \sum_{y=1}^{k} \underbrace{p(x^{(i)}, Y = y|\Theta)}$$

$$= \sum_{i=1}^{N} \underbrace{\log \sum_{y=1}^{k} \frac{q_i(y)}{q_i(y)} p(x^{(i)}, Y = y|\Theta)}$$

$$\geq \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \underbrace{\log \frac{p(x^{(i)}, Y = y|\Theta)}{q_i(y)}}$$

$$\equiv \underbrace{F(\Theta, q)}$$

$$\log \ell(\Theta) \geq \max_{q} F(\Theta, q)$$

EM Algorithm

$$\log \ell(\Theta) = \sum_{i=1}^{N} \log \sum_{y=1}^{k} p\left(x^{(i)}, Y = y \middle| \Theta\right)$$

$$= \sum_{i=1}^{N} \log \sum_{y=1}^{k} \frac{q_i(y)}{q_i(y)} p\left(x^{(i)}, Y = y \middle| \Theta\right)$$

$q_i(y)$ is an arbitrary positive probability distribution

$$\geq \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \log \frac{p\left(x^{(i)}, Y = y \middle| \Theta\right)}{q_i(y)}$$

$$\equiv F(\Theta, q)$$

$$\max_{\Theta} \log \ell(\Theta) \geq \underbrace{\max_{\Theta, q} H(q, \Theta)}$$

EM Algorithm

$q_i(y) > 0$

$$\underbrace{\log \ell(\Theta)} = \sum_{i=1}^{N} \log \sum_{y=1}^{k} p\left(x^{(i)}, Y = y \middle| \Theta\right)$$

$$= \sum_{i=1}^{N} \log \sum_{y=1}^{k} \frac{q_i(y)}{q_i(y)} p\left(x^{(i)}, Y = y \middle| \Theta\right)$$

Jensen

$$\geq \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \log \frac{p\left(x^{(i)}, Y = y \middle| \Theta\right)}{q_i(y)}$$

Jensen's ineq.

$$\equiv F(\Theta, q)$$

log $\downarrow$ $\quad$ $q_i(y)$ $\downarrow$

$$\psi\left(\sum_{y} a_{iy} x_{iy}\right) \geq \sum_{i} a_{iy} \psi(x_{iy}) \leftarrow \text{Jensen's Ineq.}$$

EM Algorithm

$$\arg \underbrace{\max_{\Theta, q_1, \ldots, q_N}} \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \log \frac{p(x^{(i)}, Y = y | \Theta)}{q_i(y)}$$

- This objective is not jointly concave in Θ and $q_1, \ldots, q_N$
  - Best we can hope for is a local maxima (and there could be **A LOT** of them)
- The EM algorithm is a block coordinate ascent scheme that finds a local optimum of this objective $\leftarrow$ Alternating Max Scheme
  - Start from an initialization Θ^0 and $q_1^0, \ldots, q_N^0$

EM Algorithm

- E step: with the θ's fixed, maximize the objective over q

known

$$\underbrace{q^{t+1}} \in \arg\max_{q_1,\dots,q_N} \sum_{i=1}^{N} \sum_{y=1}^{k} \underbrace{q_i(y)} \log \frac{\boxed{p(x^{(i)}, Y = y | \Theta^t)}}{q_i(y)}$$

- Using the method of Lagrange multipliers for the constraint that $\sum_y q_i(y) = 1$ gives

$$\boxed{q_i^{t+1}(y) = p(Y = y | X = x^{(i)}, \Theta^t)}$$

$$q^{t+1} \in \underset{\underline{q_1}, \dots q_N}{\operatorname{argmax}} \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \log \frac{P}{q_i(y)}$$

$$\text{s.t} \quad \forall\ i = 1:N, \quad \sum_{y=1}^{k} q_i(y) = 1$$

$$L(q, \mu) = \sum_{i=1}^{N} \sum_{y=1}^{k} q_i(y) \log \frac{P}{q_i(y)} + \sum_{i=1}^{N} \mu_i \left(\sum_{y=1}^{k} q_i(y) - 1 \right)$$

EM Algorithm

$= \pi_y (x^{(i)} - \mu_y)^T \Sigma^{-1} (x^{(i)} - \mu_y))$

- M step: with the q's fixed, maximize the objective over Θ

$$\theta^{t+1} \in \arg\max_{\Theta} \sum_{i=1}^{N} \sum_{y=1}^{k} \underbrace{q_i^{t+1}(y)}\log \frac{\boxed{p}(x^{(i)}, Y = y|\theta)}{q_i^{t+1}(y)}$$

$p(x^{(i)}, Y=y|\Theta) = p(Y|\Theta)\, p(x^{(i)}|Y, \Theta)$

- For the case of GMM, we can compute this update in closed form
  - This is not necessarily the case for every model
  - May require gradient ascent

$$\sum \sum_{y=1}^{k} \underbrace{q_i^{t+1}(y)} (x^{(i)} - \mu_y)^T \Sigma^{-1} \cdots$$

EM Algorithm

- Start with random parameters $(q^0, \mu^0, \Sigma^0, \lambda^0)$
- E-step maximizes a lower bound on the log-sum for fixed parameters q^{t+1}
- M-step solves a MLE estimation problem for fixed probabilities
- Iterate between the E-step and M-step until convergence

$$\downarrow$$

$$\mu^{t+1}, \Sigma^{t+1}, \lambda^{t+1}$$

EM for Gaussian Mixtures

- E-step:

Assign

$$\underbrace{q_i^t(y)} = \frac{\lambda_y^t \cdot p\left(x^{(i)} \middle| \mu_y^t, \Sigma_y^t\right)}{\sum_{y'} \lambda_{y'}^t \cdot p\left(x^{(i)} \middle| \mu_{y'}^t, \Sigma_{y'}^t\right)}$$

Probability of $x^{(i)}$ under the appropriate multivariate normal distribution

- M-step:

Parameter learning given Assignment.

$$\rightarrow \mu_y^{t+1} = \frac{\sum_{i=1}^N q_i^t(y) x^{(i)}}{\underbrace{\sum_{i=1}^N q_i^t(y)}} \leftarrow$$

$$\Sigma_y^{t+1} = \frac{\sum_{i=1}^N q_i^t(y)\left(x^{(i)} - \mu_y^{t+1}\right)\left(x^{(i)} - \mu_y^{t+1}\right)^T}{\sum_{i=1}^N q_i^t(y)} \checkmark$$

$$\lambda_y^{t+1} = \frac{1}{N} \sum_{i=1}^N q_i^t(y)$$

EM for Gaussian Mixtures

- E-step:

$$q_i^t(y) = \frac{\lambda_y^t \cdot p\left(x^{(i)} \middle| \mu_y^t, \Sigma_y^t\right)}{\sum_{y'} \lambda_{y'}^t \cdot p\left(x^{(i)} \middle| \mu_{y'}^t, \Sigma_{y'}^t\right)}$$

Probability of $x^{(i)}$ under the mixture model

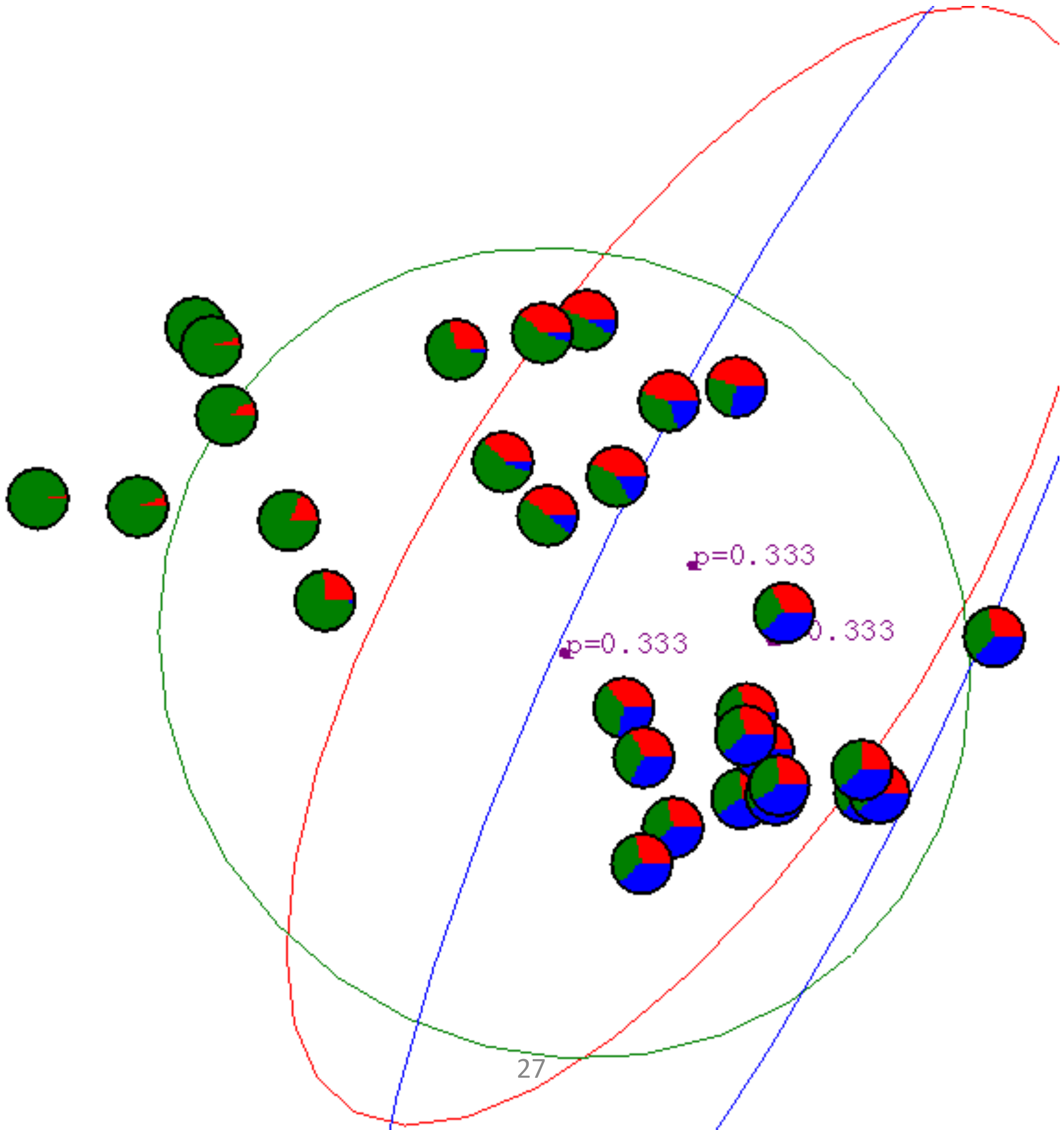
- M-step:

$$\mu_y^{t+1} = \frac{\sum_{i=1}^N q_i^t(y) x^{(i)}}{\sum_{i=1}^N q_i^t(y)}$$

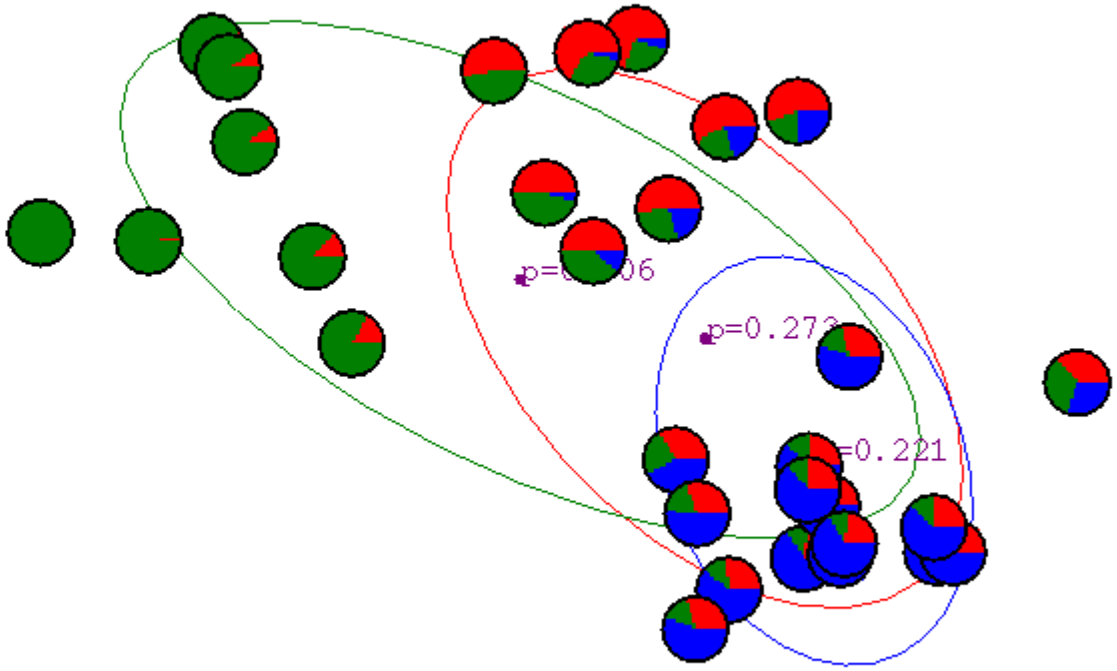
$$\Sigma_y^{t+1} = \frac{\sum_{i=1}^N q_i^t(y)\left(x^{(i)} - \mu_y^{t+1}\right)\left(x^{(i)} - \mu_y^{t+1}\right)^T}{\sum_{i=1}^N q_i^t(y)}$$

$$\lambda_y^{t+1} = \frac{1}{N} \sum_{i=1}^N q_i^t(y)$$

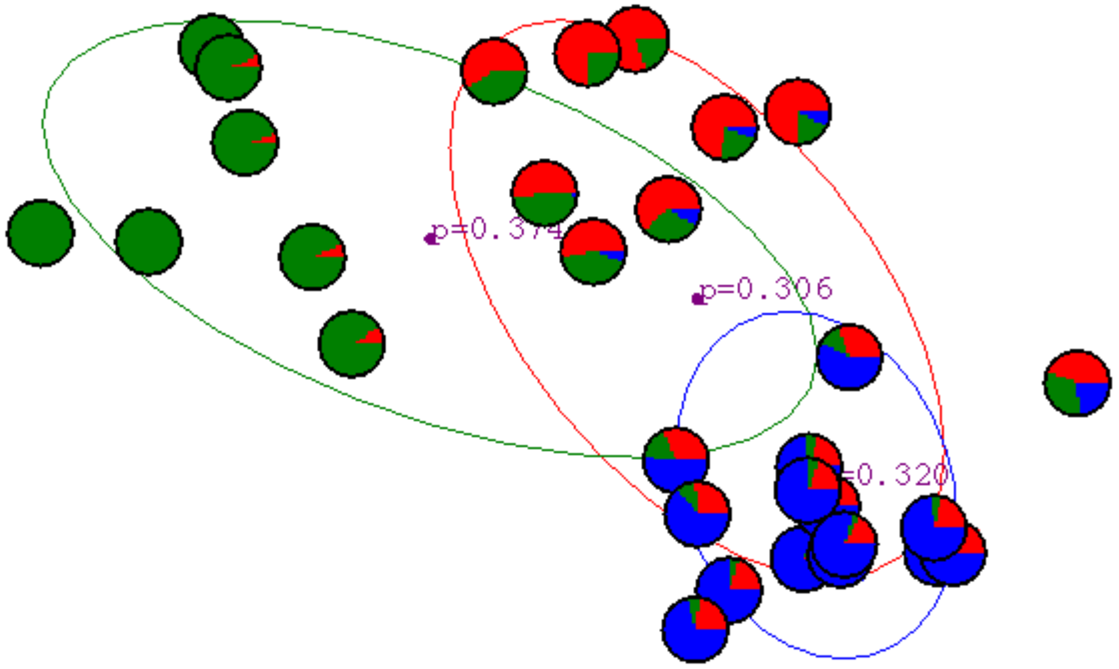
Gaussian Mixture Example: Start



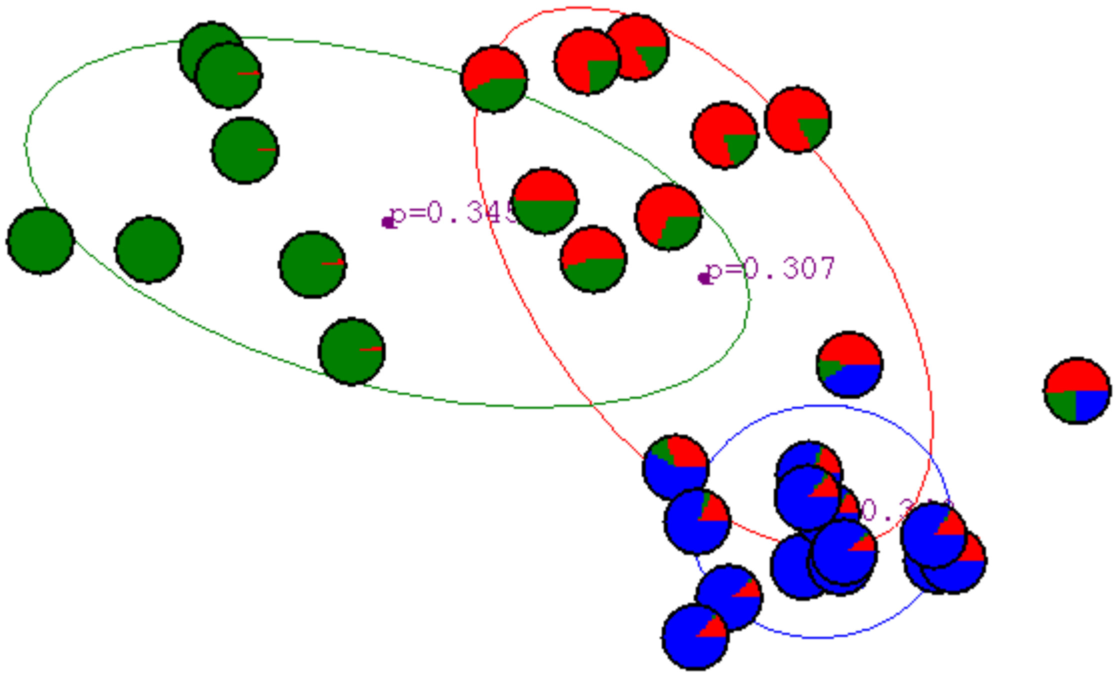
After first iteration



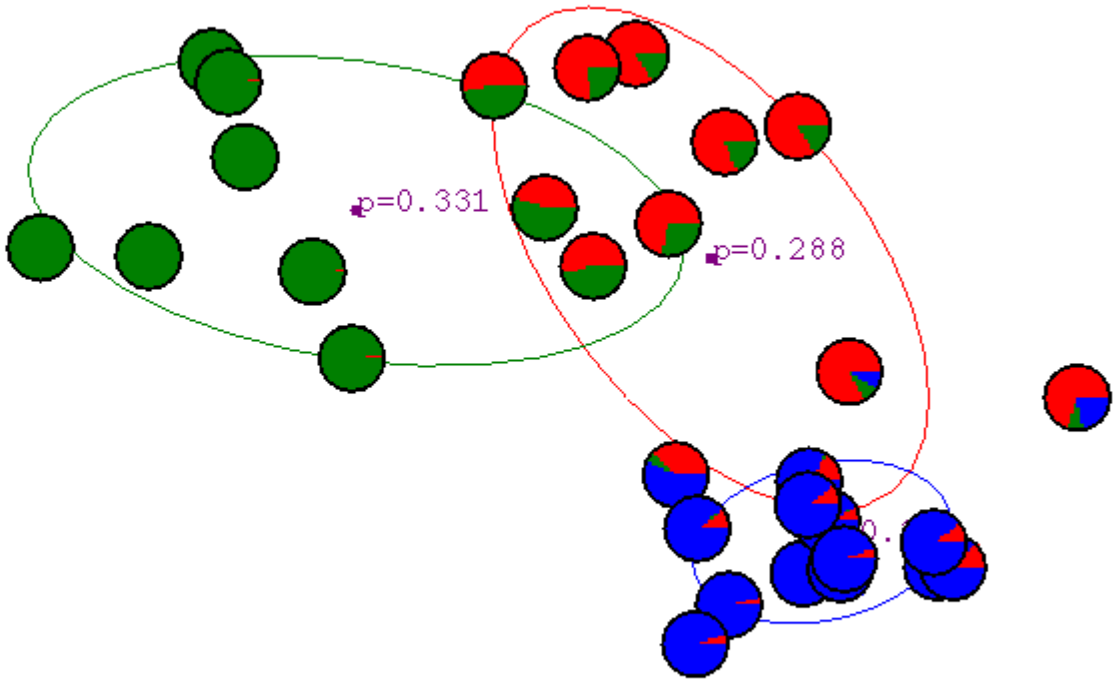
After 2nd iteration



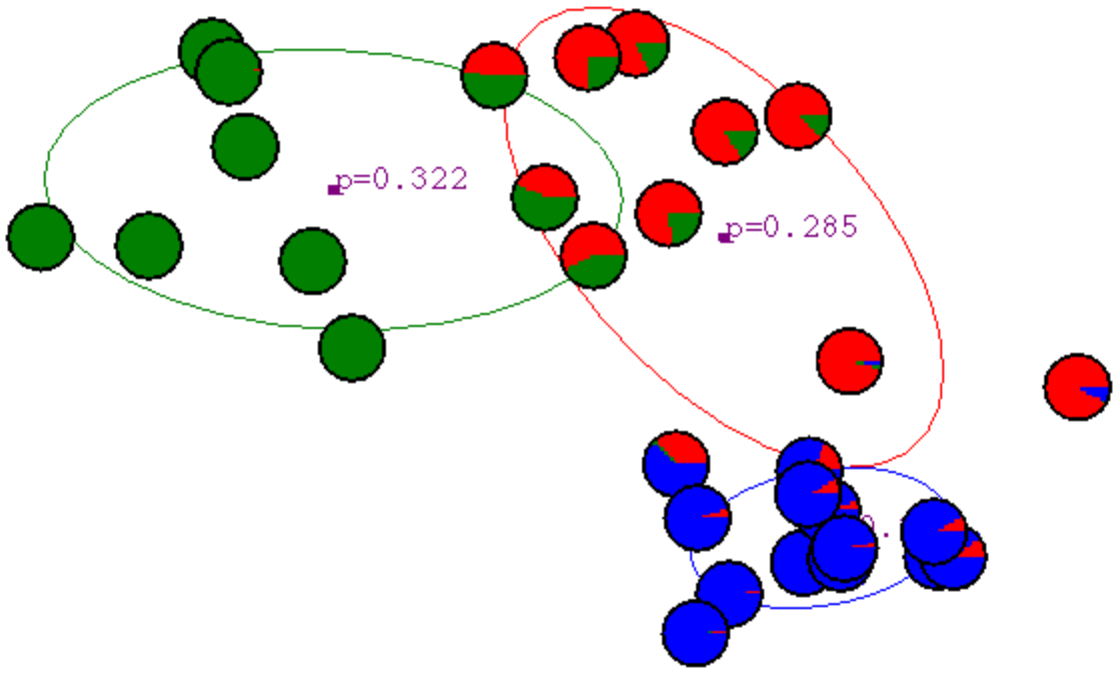
After 3rd iteration



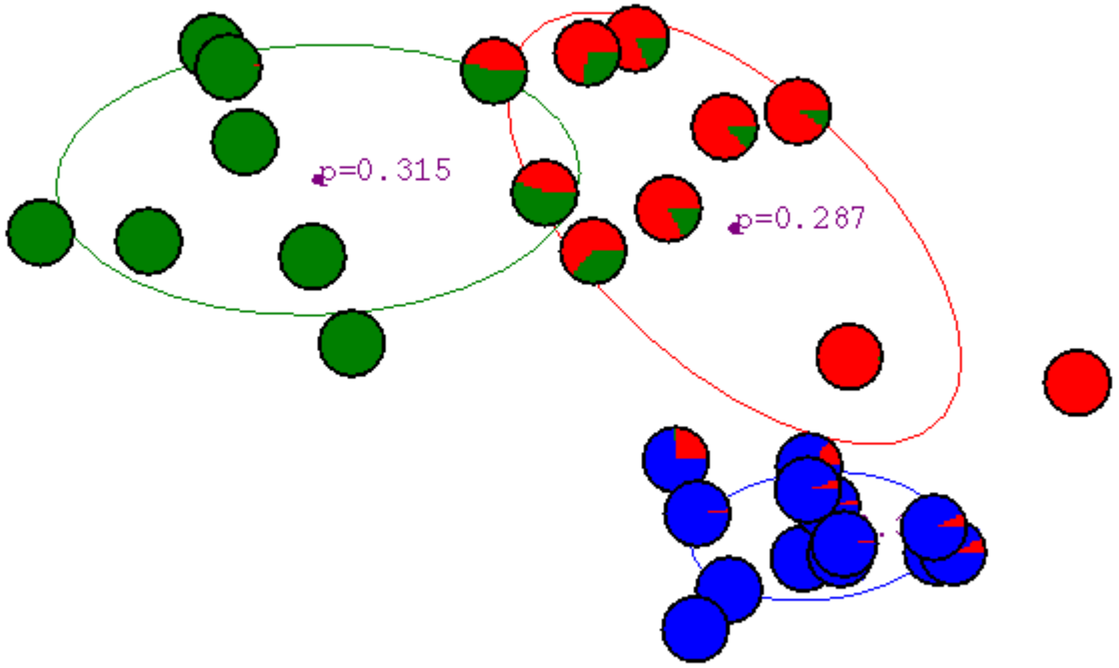
After 4th iteration



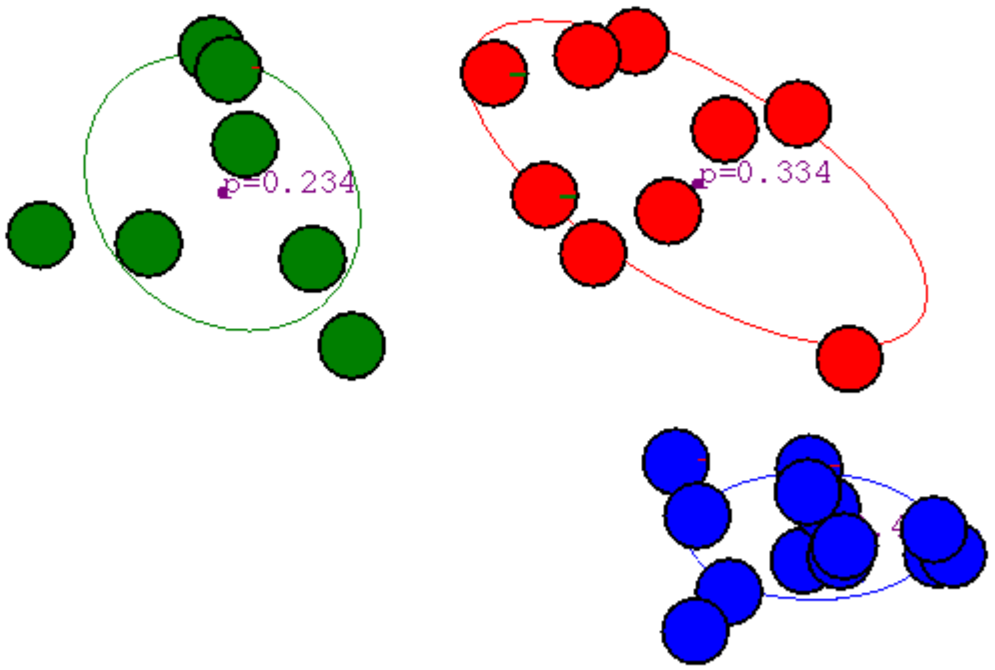
After 5th iteration



After 6th iteration



After 20th iteration



Properties of EM

- EM converges to a local optimum
  - This is because each iteration improves the log-likelihood
  - Proof same as k-means (just block coordinate ascent)
    - E-step can never decrease likelihood
    - M-step can never decrease likelihood

$\Big\}$ Improve likelihood function

- If we make hard assignments instead of soft ones, algorithm is equivalent to k-means!

Properties of EM

- EM converges to a local optimum
  - This is because each iteration improves the log-likelihood
  - Proof same as k-means (just block coordinate ascent)
    - 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!