# Mixture Models & EM

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based on the slides of 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
- Today: how to learn probabilistic models for unsupervised learning problems

# EM: Soft Clustering

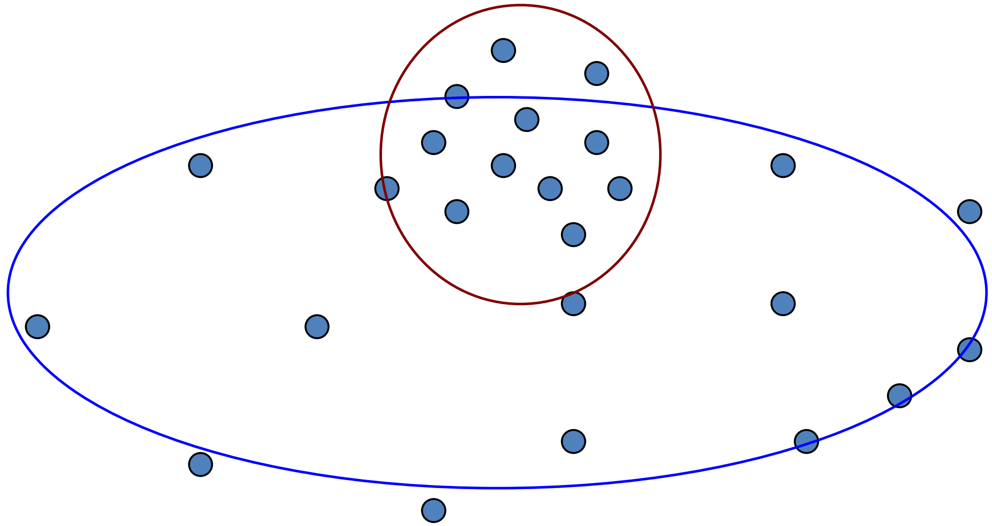
- Clustering (e.g., k-means) typically assumes that each instance is given a "hard" assignment to exactly one cluster
- Does not allow uncertainty in class membership or for an instance to belong to more than one cluster
  - Problematic because data points that lie roughly midway between cluster centers 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 without labeled $y$'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)

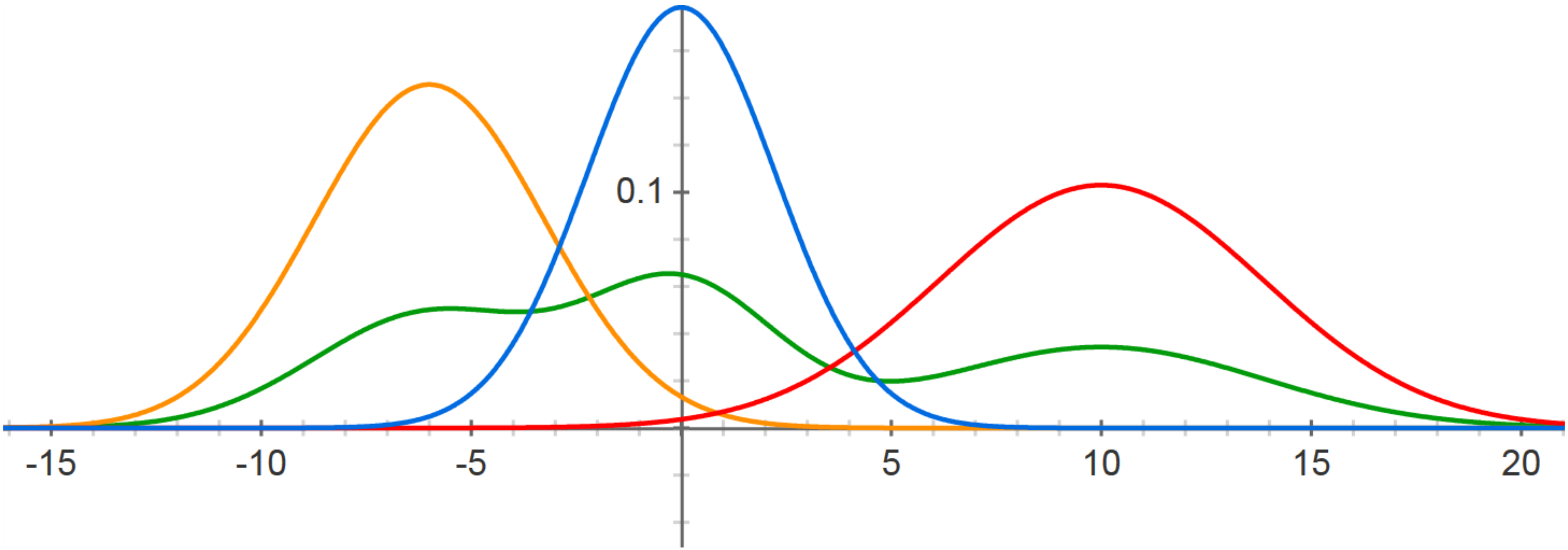
# Finite Mixture Models

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

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

  - $p_y(x|\theta_y)$ is a mixture component from some family of probability distributions parameterized by $\theta_y$ and $\lambda \geq 0$ such that $\sum_y \lambda_y = 1$ are the mixture weights
  - We can think of $\lambda_y = p(Y = y|\Theta)$ for some random variable $Y$ that takes values in $\{1, \dots, k\}$

# 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 $\Sigma$ and a mean vector $\mu$

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

- The covariance matrix describes the degree to which pairs of variables vary together
  - The diagonal elements correspond to variances of the individual variables

# Multivariate Gaussian

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- 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

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

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

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

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

$$\sigma_{MLE}^2 = \frac{1}{N}\sum_{i=1}^{N} \left(x^{(i)} - \mu_{MLE}\right)^2$$

- MLE for supervised multivariate Gaussian

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

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

# Learning Gaussian Parameters

- MLE for supervised multivariate mixture of $k$ Gaussian distributions

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

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

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, $y \in \{1, \dots, k\}$

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

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

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

# The Unsupervised Case

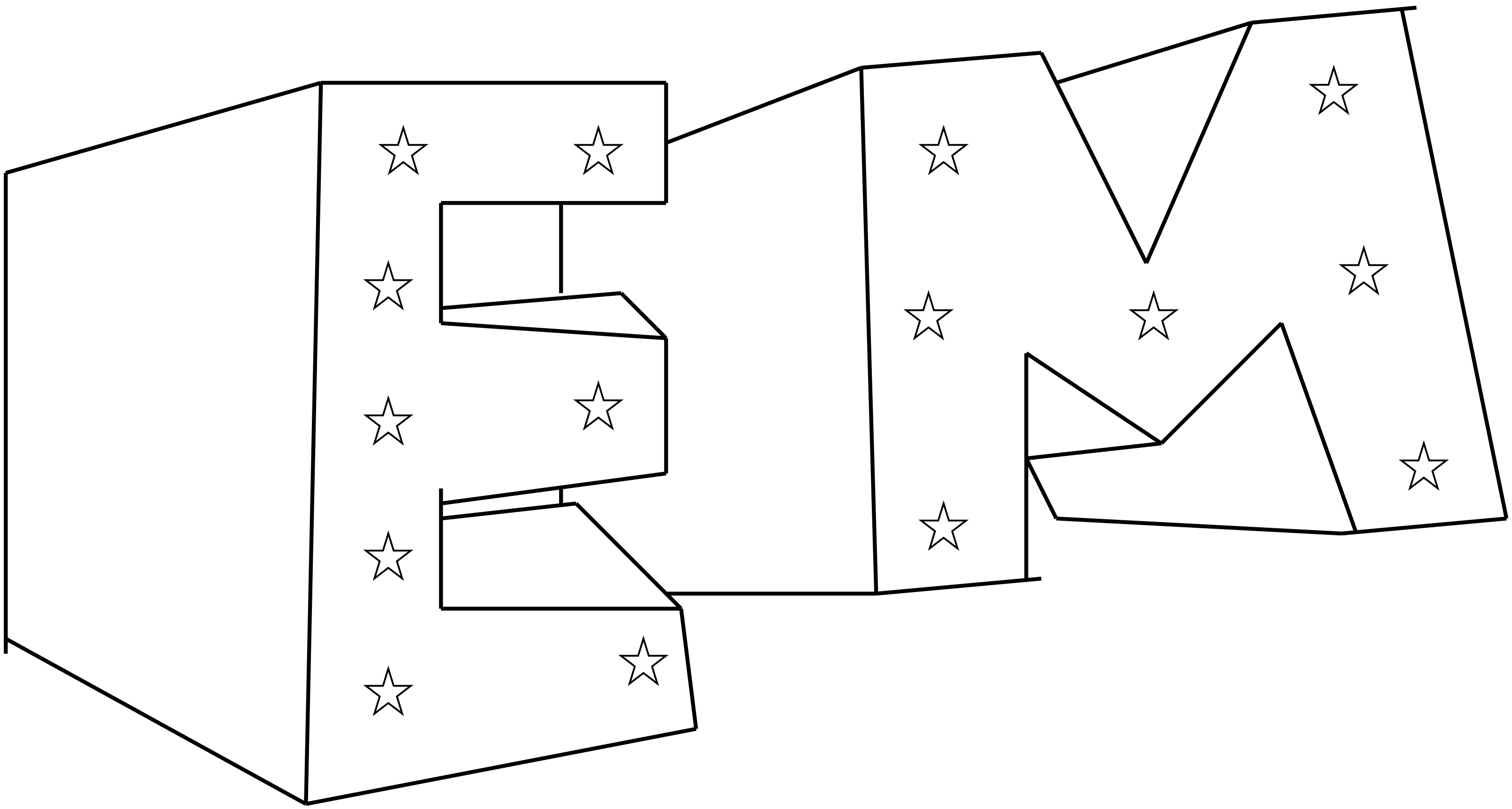
- In the case of a Gaussian mixture model

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

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

- 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 $x^{(1)}, \dots, x^{(k)} \in \mathbb{R}^n$,

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

Inequality is reversed for concave functions

# EM Algorithm

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

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

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

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

# EM Algorithm

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

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

# EM Algorithm

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

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Jensen's ineq.

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

# EM Algorithm

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

- This objective is not jointly concave in $\Theta$ 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
  - Start from an initialization $\Theta^0$ and $q_1^0, \ldots, q_N^0$

# EM Algorithm

- E step: with the $\theta$'s fixed, maximize the objective over $q$

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

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

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

# EM Algorithm

- M step: with the $q$'s fixed, maximize the objective over $\Theta$

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

- 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

# EM Algorithm

- Start with random parameters
- E-step maximizes a lower bound on the log-sum for fixed parameters
- M-step solves a MLE estimation problem for fixed probabilities
- Iterate between the E-step and M-step until convergence

# 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 appropriate multivariate normal distribution

- M-step:

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

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

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

# 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

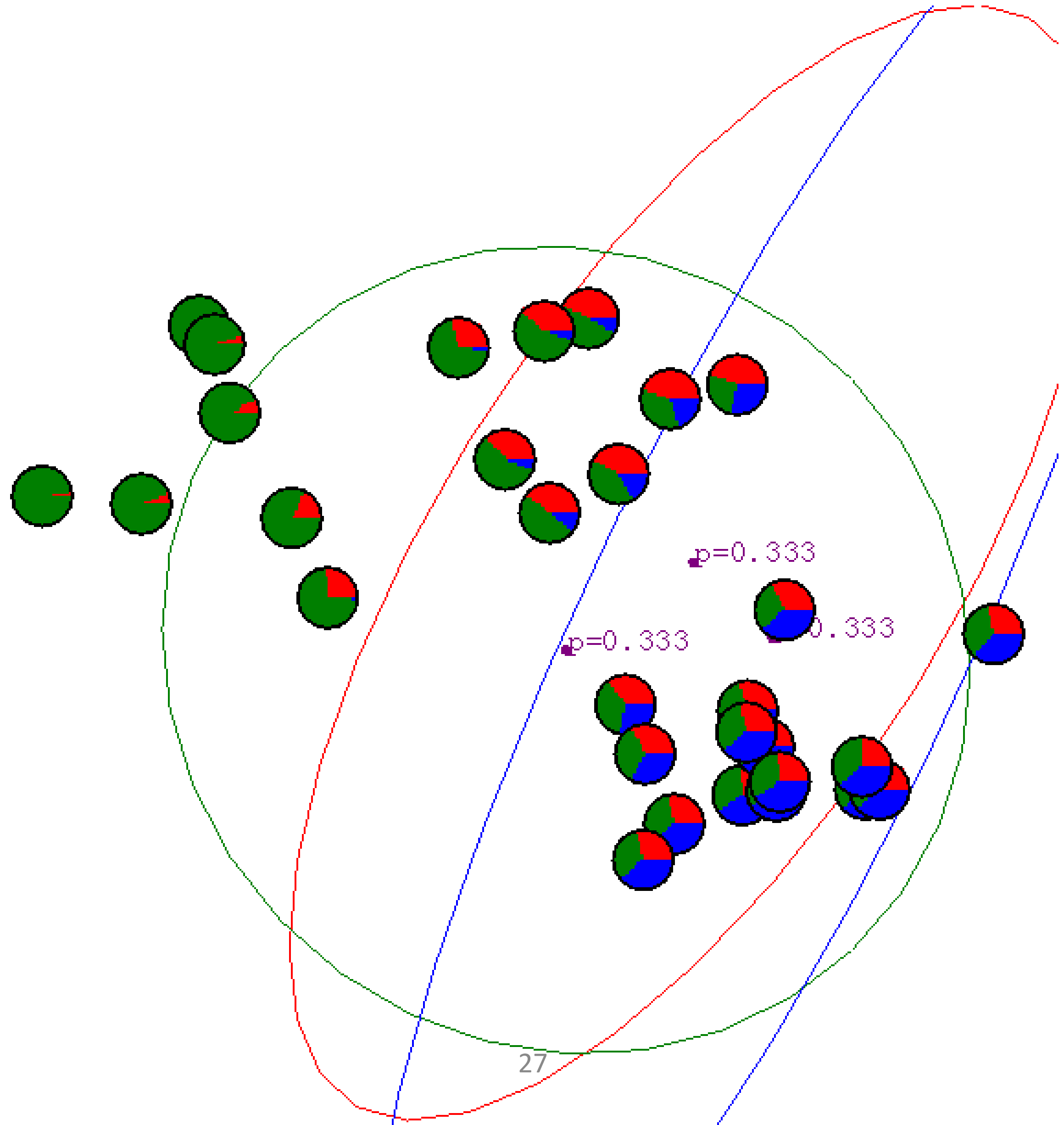
- M-step:

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

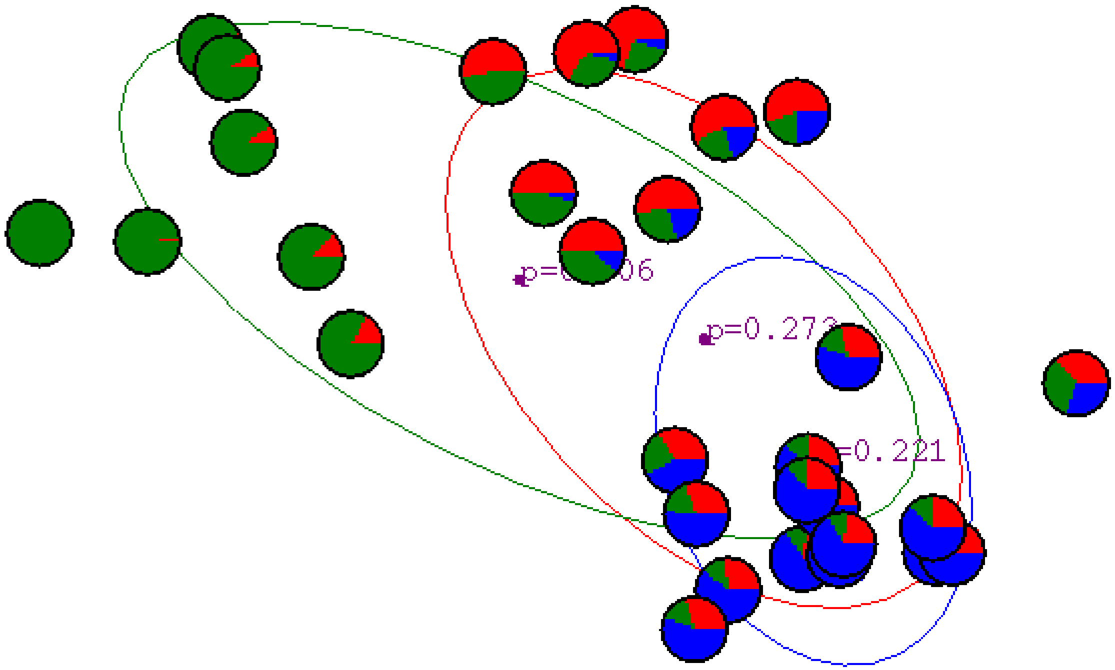
$$\Sigma_y^{t+1} = \frac{\sum_{i=1}^N q_i^t(y)\left(x^{(i)} - \mu_y^{t+1}\right)\left(x^{(i)} - \mu_y^{t+1}\right)^T}{\sum_{i=1}^N q_i^t(y)}$$

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

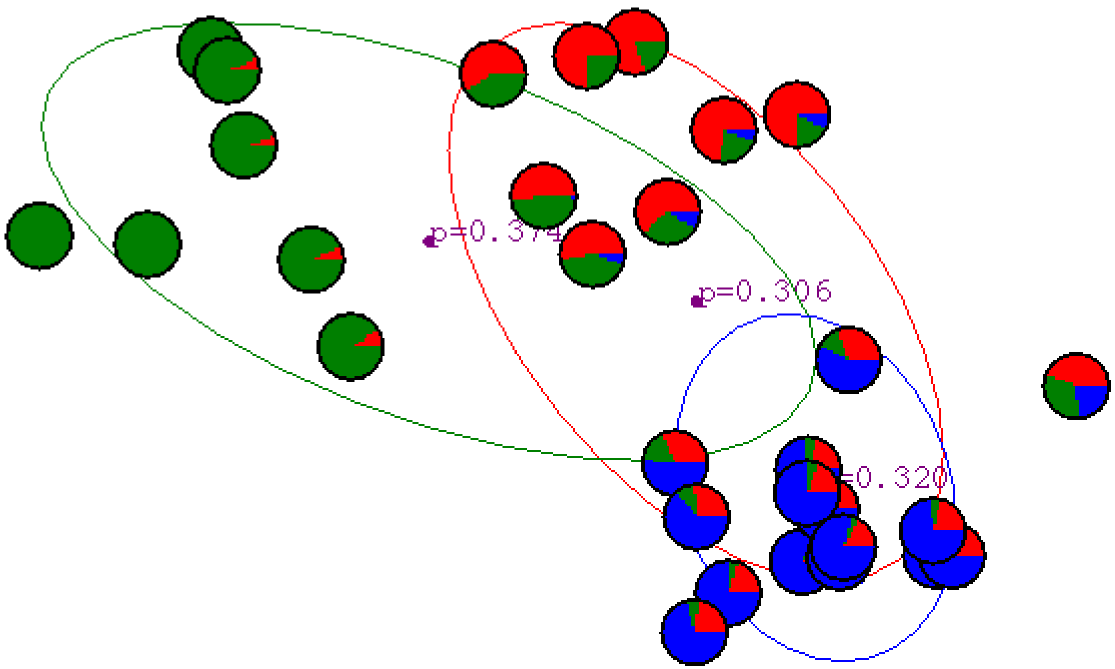
# Gaussian Mixture Example: Start



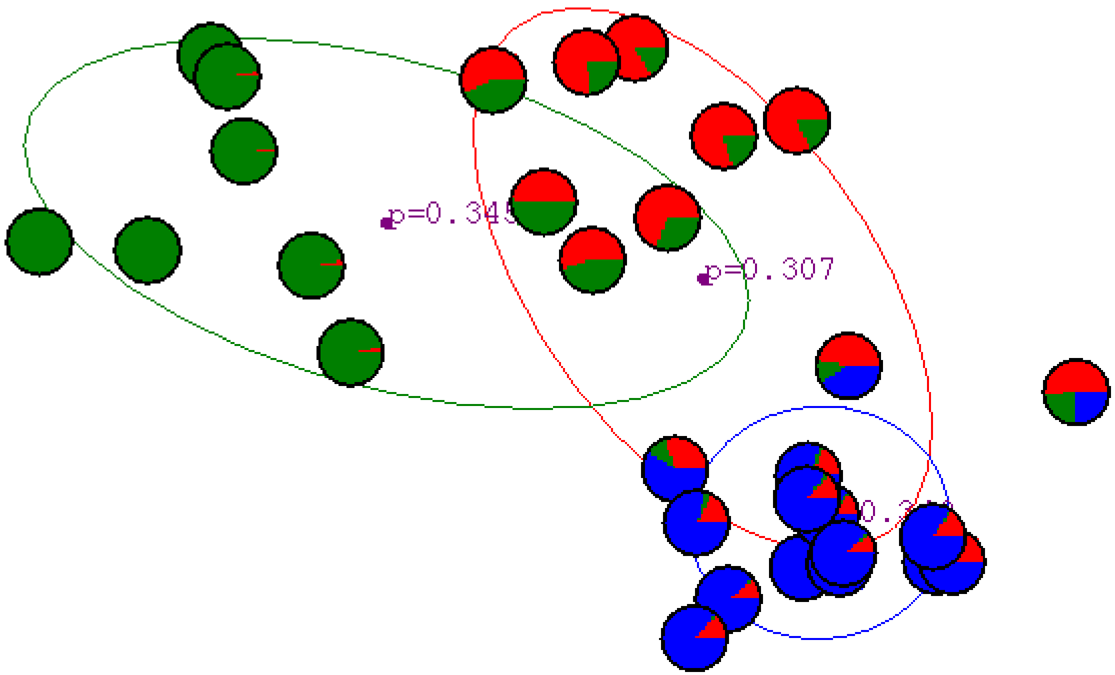
# After first iteration



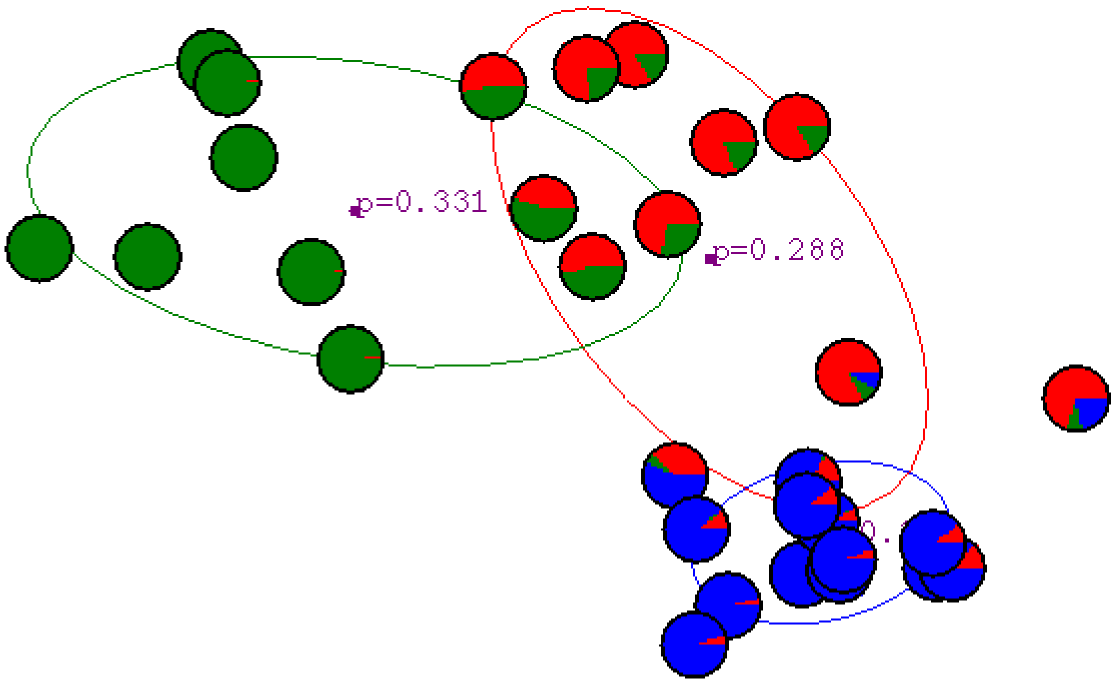
# After 2nd iteration



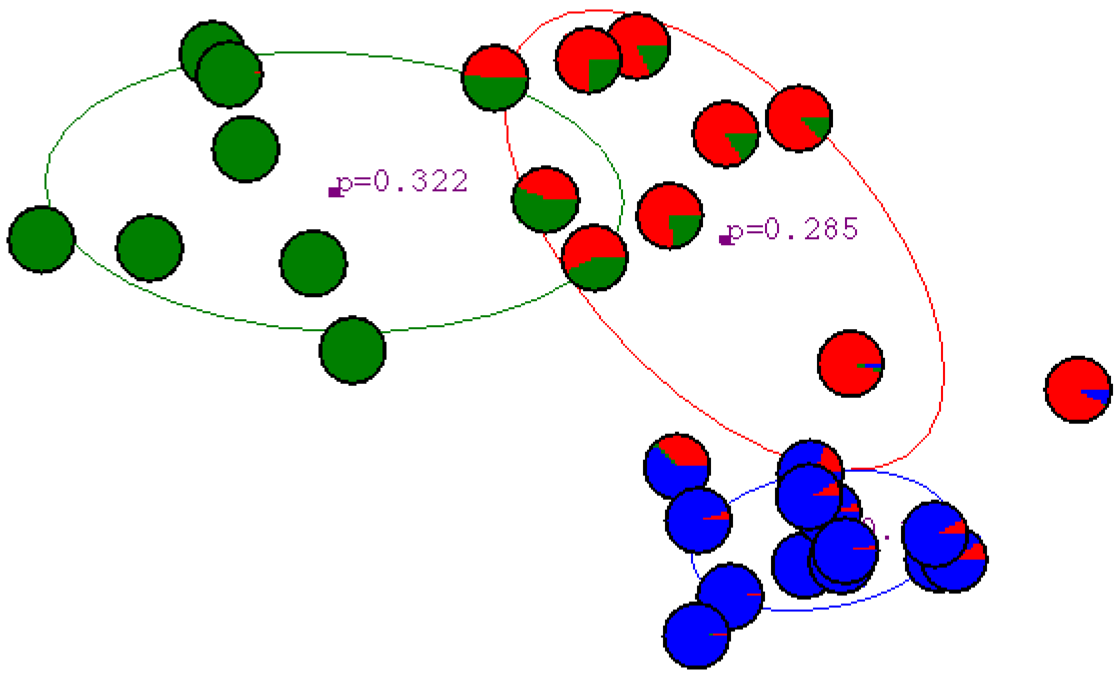
# After 3rd iteration



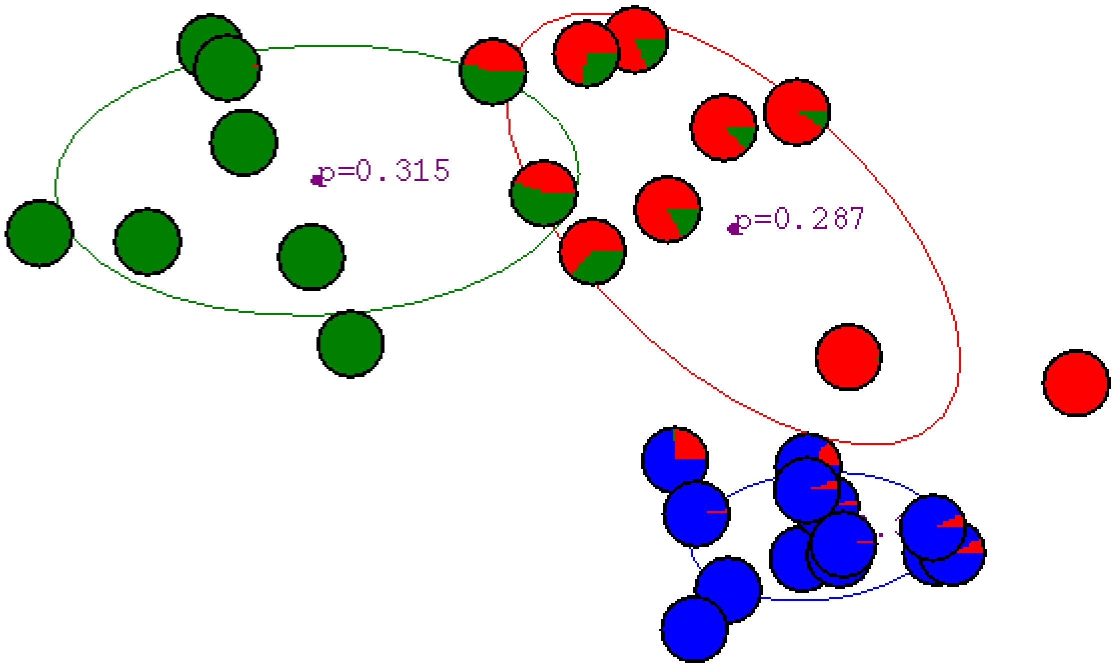
# After 4th iteration



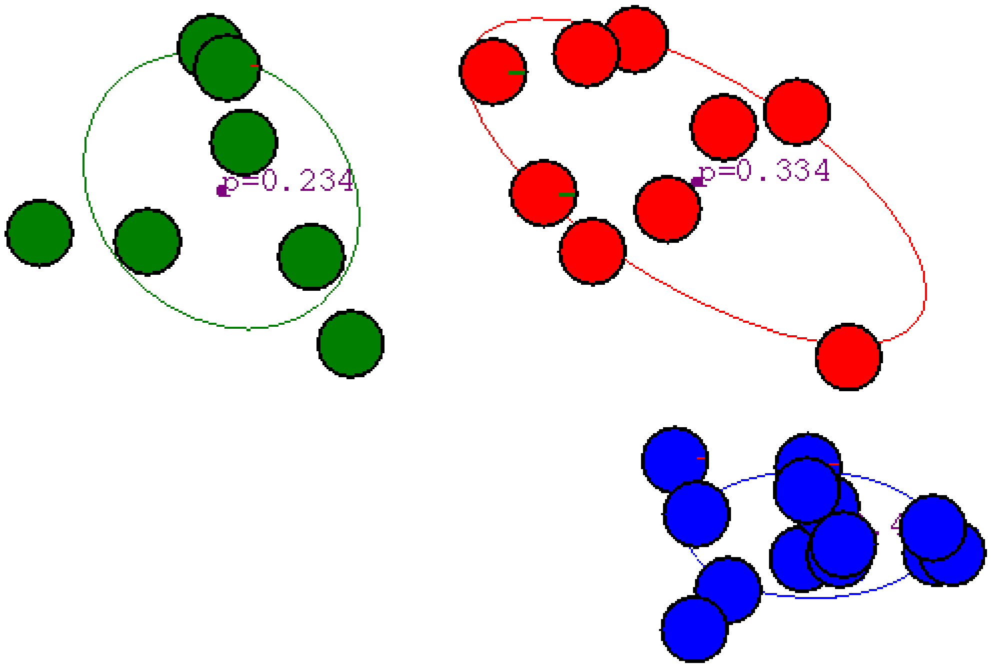
# After 5th iteration



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