Machine Learning

Gaussian Mixture Models

Discriminative vs Generative Models

- Discriminative: Just learn a decision boundary between your sets.

  Support Vector Machines

- Generative: Learn enough about your sets to be able to make new examples that would be set members

  Gaussian Mixture Models

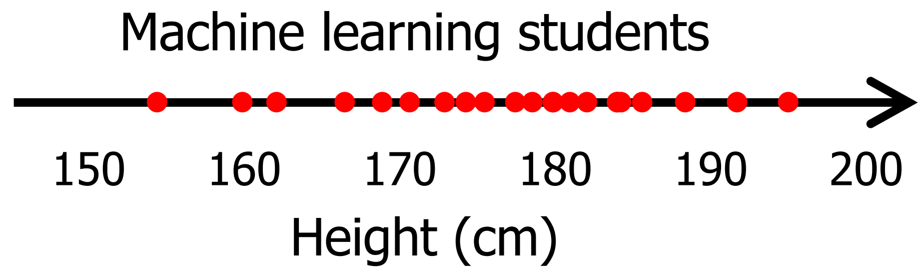
The Generative Model POV

- Assume the data was generated from a process we can model as a probability distribution

- Learn that probability distribution

- Once learned, use the probability distribution to
  - "Make" new examples
  - Classify data we haven't seen before.

Non-parametric distribution not feasible

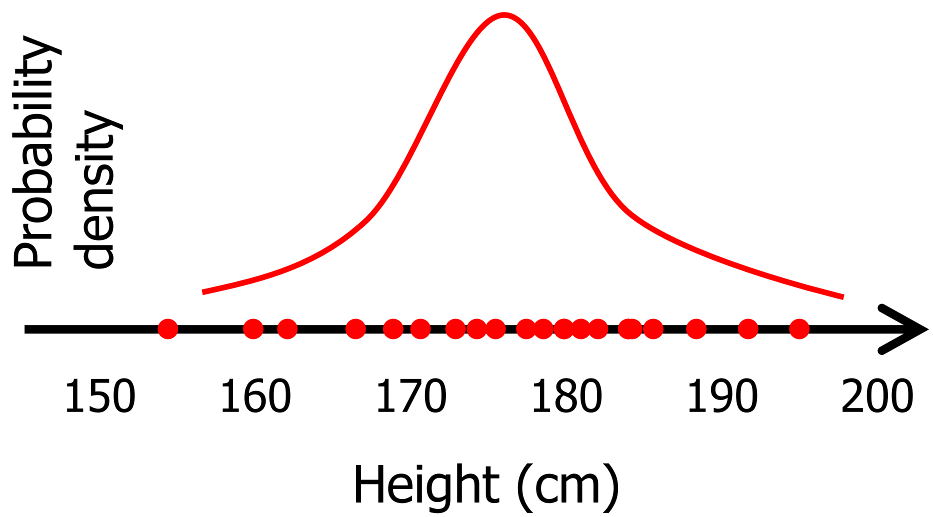


- Let’s probabilistically model ML student heights.
- Ruler has 200 marks (100 to 300 cm)
- How many probabilities to learn?
- How many students in the class?
- What if the ruler is continuous?

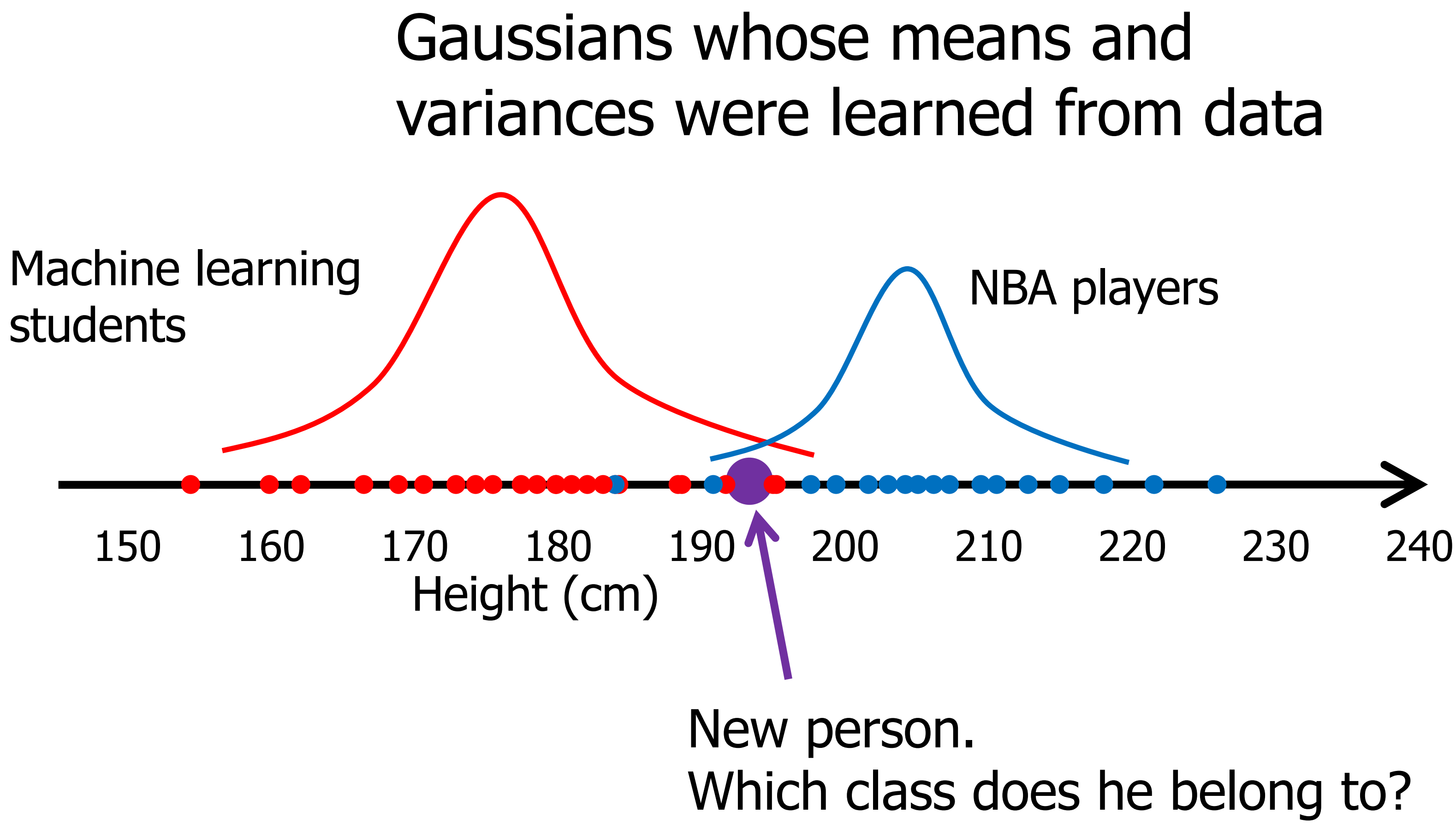
Learning a Parametric Distribution

- Pick a parametric model (e.g. Gaussian)
- Learn just a few parameter values

$$p(x \mid \Theta) \equiv \text{ prob. of x, given parameters } \Theta$$
$$\text{of a model, M}$$



Using Generative Models for Classification



Answer: the class that calls him most probable.

Learning a Gaussian Distribution

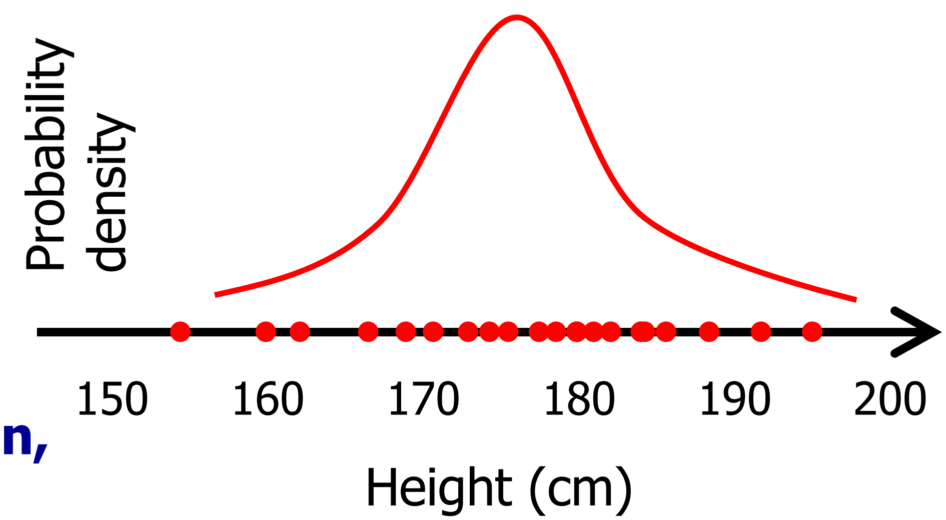
$$p(x \mid \Theta) \equiv \text{ prob. of x, given parameters } \Theta \text{ of a model, M}$$

$$\Theta \equiv \{\mu, \sigma\}$$

The parameters we must learn

$$M \equiv \frac{1}{(2\pi)^{1/2}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

The "normal" Gaussian distribution, often denoted N, for "normal"



Goal: Find the best Gaussian

- Hypothesis space is Gaussian distributions.
- Find parameters Θ^* that maximize the prob. of observing data $X \equiv \{x_1, \ldots x_n\}$

$$\Theta^* = \underset{\Theta}{\operatorname{argmax}}\, p(X \mid \Theta)$$

$$\text{where each } \Theta \equiv \{\mu, \sigma\}$$

Some math

$$\Theta^* = \underset{\Theta}{\operatorname{argmax}}\, p(X \mid \Theta), \text{where each } \Theta \equiv \{\mu, \sigma\}$$

$$p(X \mid \Theta) = \prod_{i=1}^{n} p(x_i \mid \Theta)$$

...if can we assume all x_i are i.i.d.

Numbers getting smaller

$$p(X \mid \Theta) = \prod_{i=1}^{n} p(x_i \mid \Theta)$$

What happens as n grows? Problem?

We get underflow if n is, say, 500

$$p(X \mid \Theta) \propto \sum_{i=1}^{n} \log(p(x_i \mid \Theta)) \text{ solves underflow.}$$

Remember what we're maximizing

$$\Theta^* \equiv \underset{\text{argmax}\,\Theta}{p(X \mid \Theta)} = \underset{\text{argmax}\,\Theta}{\sum_{i=1}^{n} \log(p(x_i \mid \Theta))}$$

fitting the Gaussian into this...

$$\log(p(x \mid \Theta)) = \log\left(\frac{e^{\frac{-(x-\mu)^2}{2\sigma^2}}}{(2\pi)^{1/2}\sigma} \right)$$

Some math gets you…

$$\log\left(\frac{e^{\frac{-(x-\mu)^2}{2\sigma^2}}}{(2\pi)^{1/2}\sigma}\right) = \log\left(e^{\frac{-(x-\mu)^2}{2\sigma^2}}\right) - \log((2\pi)^{1/2}\sigma)$$

$$= \boxed{\frac{-(x-\mu)^2}{2\sigma^2} - \log\sigma} - \log(2\pi)^{1/2}$$

Plug back into equation from slide 11

..which gives us

$$\Theta^* \equiv \underset{\Theta}{\operatorname{argmax}}\; p(X \mid \Theta)$$

$$= \underset{\Theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log(p(x_i \mid \Theta))$$

$$= \underset{\Theta}{\operatorname{argmax}} \sum_{i=1}^{n} \left(\frac{-(x_i - \mu)^2}{2\sigma^2} - \log \sigma \right)$$

Maximizing Log-likelihood

- To find best parameters, take the partial derivative with respect to parameters $\{\sigma, \mu\}$ and set to 0.

$$\Theta^* = \sum_{i=1}^{n} \left(\frac{-(x_i - \mu)^2}{2\sigma^2} - \log \sigma \right)$$

$$\operatorname{argmax} \Theta$$

- The result is a closed-form solution

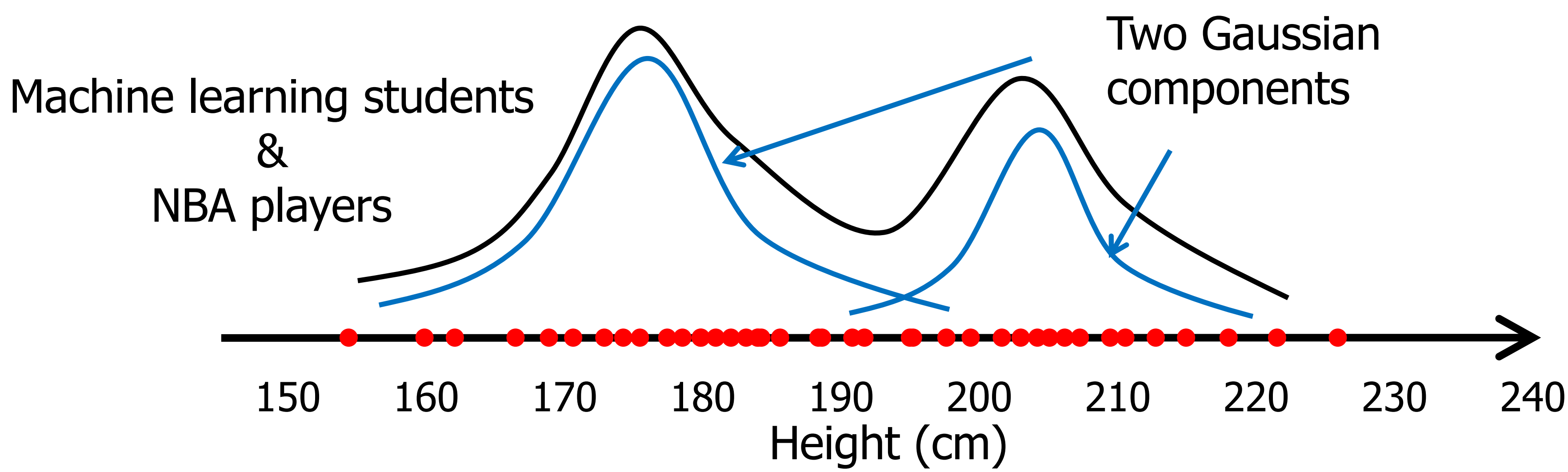
$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i \qquad \sigma^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu)^2$$

What if…

- …the data distribution can't be well represented by a single Gaussian?

- Can we model more complex distributions using multiple Gaussians?

Gaussian Mixture Model (GMM)



Model the distribution as a mix of Gaussians

$$P(x) = \sum_{j=1}^{K} P(z_j) P(x \mid z_j)$$

x is the observed value

z_j is a Boolean saying whether Gaussian j "made" x

What are we optimizing?

$$P(x) = \sum_{j=1}^{K} P(z_j) P(x \mid z_j)$$

Notating $P(z_j)$ as weight w_j and using the Normal (a.k.a. Gaussian) distribution $N(\mu_j, \sigma_j^2)$ gives us...

$$= \sum_{j=1}^{K} w_j N(x \mid \mu_j, \sigma_j^2) \quad \text{such that } 1 = \sum_{j=1}^{K} w_j$$

This gives 3 variables per Gaussian to optimize:

w_j, μ_j, σ_j

Bad news: No closed form solution.

$$\Theta^* \equiv \underset{\Theta}{\operatorname{argmax}}\, p(X \mid \Theta) = \underset{\Theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log(p(x_i \mid \Theta)\ )$$

$$= \underset{\Theta}{\operatorname{argmax}} \sum_{i=1}^{n} \log\left(\sum_{j=1}^{K} w_j\, p(x_i \mid N(\mu_j, \sigma_j^2)) \right)$$

Expectation Maximization (EM)

- Solution: The EM algorithm
- EM updates model parameters iteratively.
- After each iteration, the likelihood the model would generate the observed data increases (or at least it doesn't decrease).
- EM algorithm always converges to a local optimum.

EM Algorithm Summary

- Initialize the parameters
- E step: calculate the likelihood a model with these parameters generated the data
- M step: Update parameters to increase the likelihood from E step
- Repeat E & M steps until convergence to a local optimum.

EM for GMM - Initialization

- Choose the number of Gaussian components K

  K should be much less than the number of data points to avoid overfitting.

- (Randomly) select parameters for each Gaussian j: w_j, μ_j, σ_j

$$\text{...such that } 1 = \sum_{j=1}^{K} w_j$$

EM for GMM – Expectation step

The responsibility $\gamma_{j,n}$ of Gaussian j for observation x_n is defined as...

$$\gamma_{j,n} \equiv p(z_j \mid x_n) = \frac{p(x_n \mid z_j)p(z_j)}{p(x_n)}$$

$$= \frac{p(x_n \mid z_j)p(z_j)}{\sum_{k=1}^{K} p(z_k)p(x_n \mid z_k)} = \frac{w_j N(x_n \mid \mu_j, \sigma_j^2)}{\sum_{k=1}^{K} w_k N(x_n \mid \mu_k, \sigma_k^2)}$$

EM for GMM – Expectation step

Define the responsibility Γ_j of Gaussian j for all the observed data as...

$$\Gamma_j \equiv \sum_{n=1}^{N} \gamma_{j,n}$$

You can think of this as the proportion of the data explained by Gaussian j.

EM for GMM – Maximization step

Update our parameters as follows...

$$\text{new } w_j = \frac{\Gamma_j}{N}$$

$$\text{new } \mu_j = \frac{\sum_{i=1}^{N} \gamma_{j,i} x_i}{\Gamma_j}$$

$$\text{new } \sigma_j^2 = \frac{\sum_{i=1}^{N} \gamma_{j,i} (x_i - \mu_j)^2}{\Gamma_j}$$

Why does this work?

- We need to prove that, as our model parameters are adjusted, likelihood of the data never goes down (monotonically non-decreasing)

- This is the part where I point you to the textbook

What happens if…

- If I initialize each Gaussian distribution to have a mean = to the location of a data point…
- …And I allow sigma to go to 0 for any Gaussian?
- What is one (probably bad) solution for the local optimization algorithm?

What if…

- …our data isn't just scalars, but each data point has multiple dimensions?
- Can we generalize to multiple dimensions?
- We need to define a covariance matrix.

Covariance Matrix

Given d-dimensional random variable vector $\vec{\mathbf{X}} = \left[X_1, ..., X_d \right]$

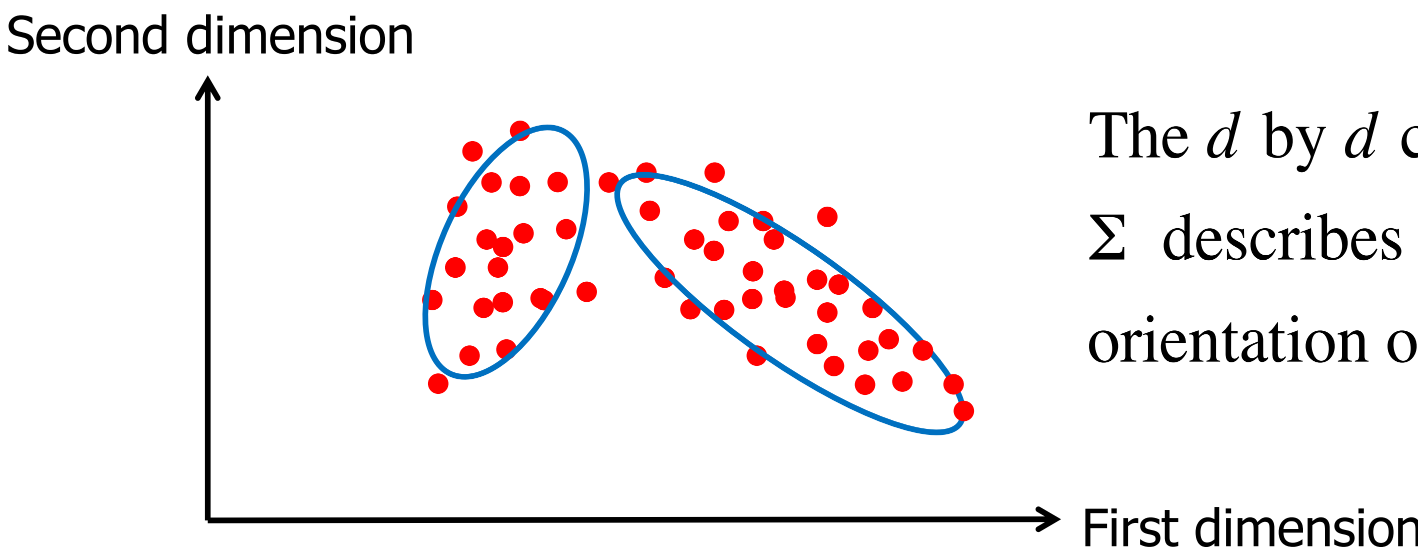
the covariance matrix denoted Σ (confusing, eh?) is defined as...

$$\Sigma \equiv \begin{bmatrix} \mathbf{E}\left[(X_1-\mu_1)(X_1-\mu_1)\right] & \mathbf{E}\left[(X_1-\mu_1)(X_2-\mu_2)\right] & ... & \mathbf{E}\left[(X_1-\mu_1)(X_d-\mu_d)\right] \\ \mathbf{E}\left[(X_2-\mu_2)(X_1-\mu_1)\right] & \mathbf{E}\left[(X_2-\mu_2)(X_2-\mu_2)\right] & \cdots & \mathbf{E}\left[(X_2-\mu_2)(X_d-\mu_d)\right] \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{E}\left[(X_d-\mu_d)(X_1-\mu_1)\right] & \mathbf{E}\left[(X_d-\mu_d)(X_2-\mu_2)\right] & \cdots & \mathbf{E}\left[(X_d-\mu_d)(X_d-\mu_d)\right] \end{bmatrix}$$

This is a generalization of one-dimensional variance for a scalar random variable X

$$\sigma^2 = \mathrm{var}(X) = E\left[\left(X-\mu\right)^2\right]$$

Multivariate Gaussian Mixture

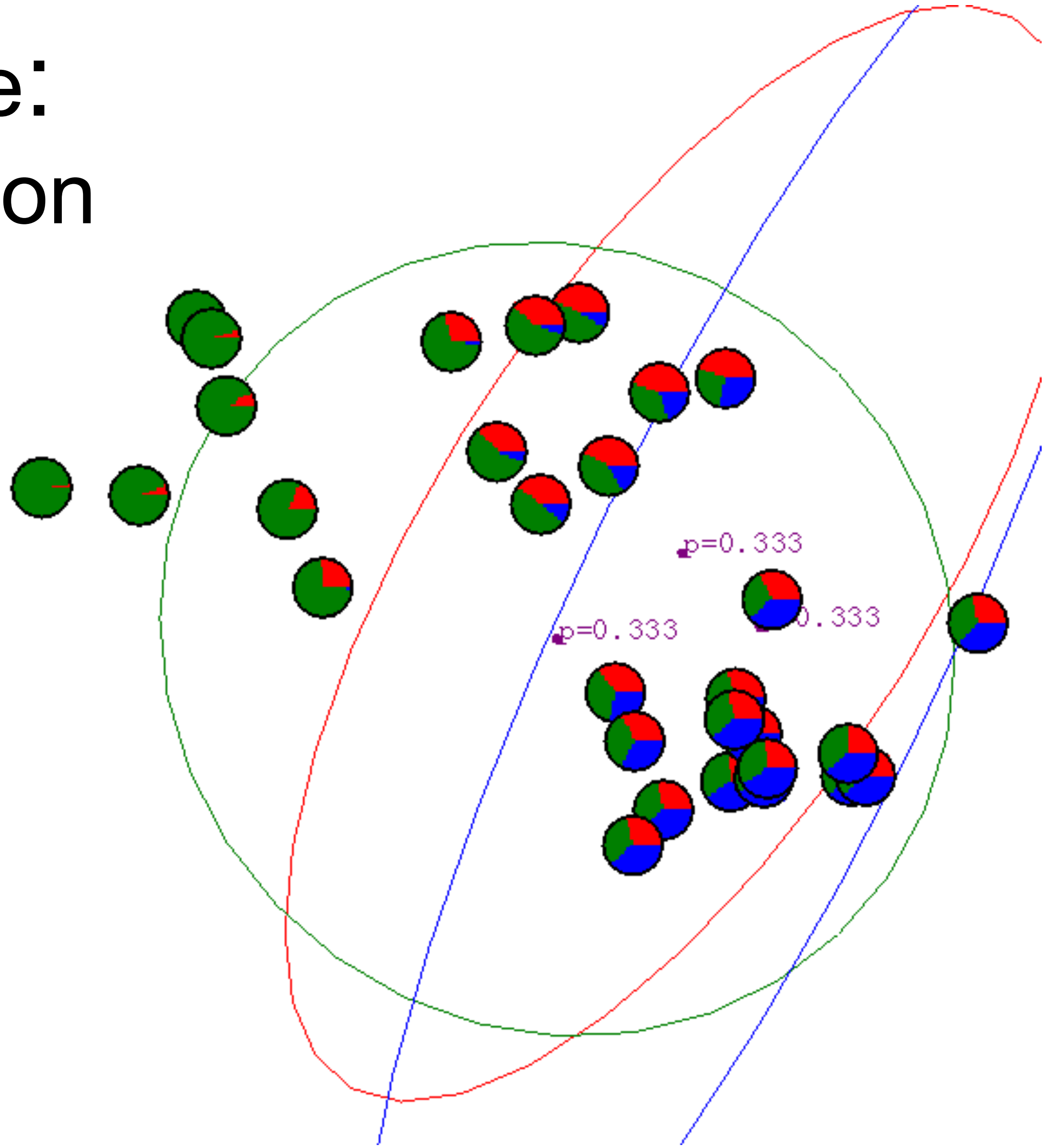


The d by d covariance matrix Σ describes the shape and orientation of an elipse.

$$P(\vec{\mathbf{X}}) = \sum_{j=1}^{K} w_j \, p(\vec{\mathbf{X}} \mid N(\vec{\mu}, \Sigma_j))$$

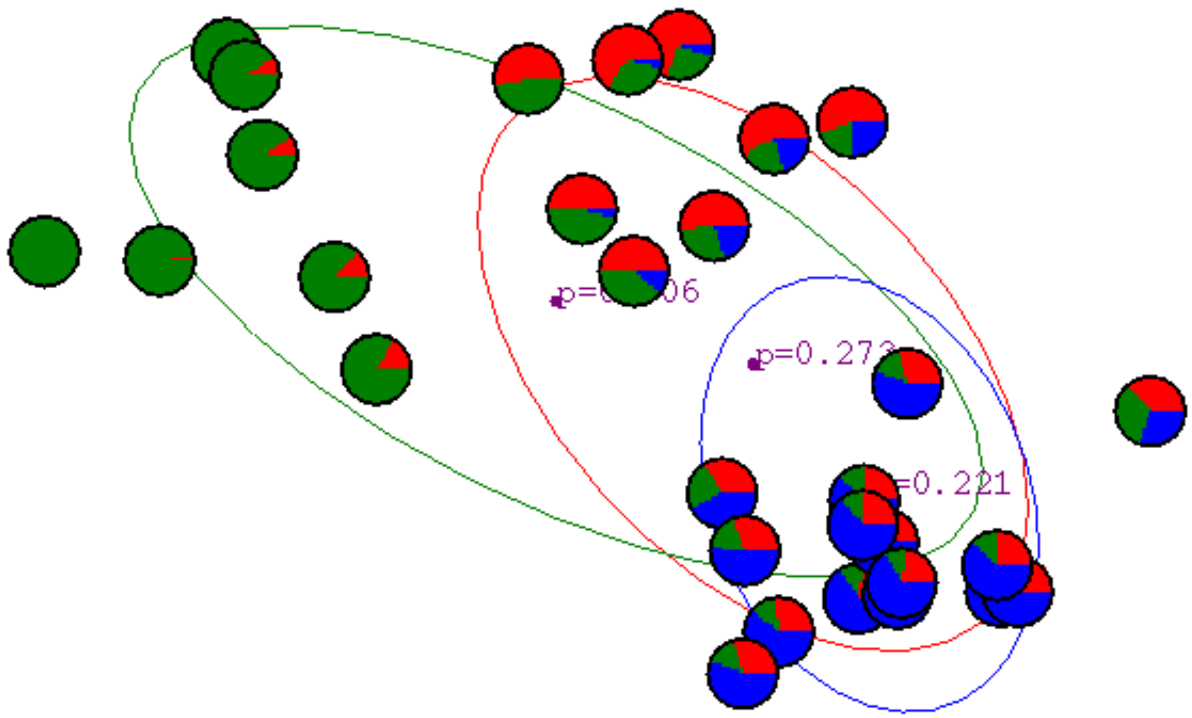
Given d dimensions and K Gaussians, how many parameters?

Example: Initialization



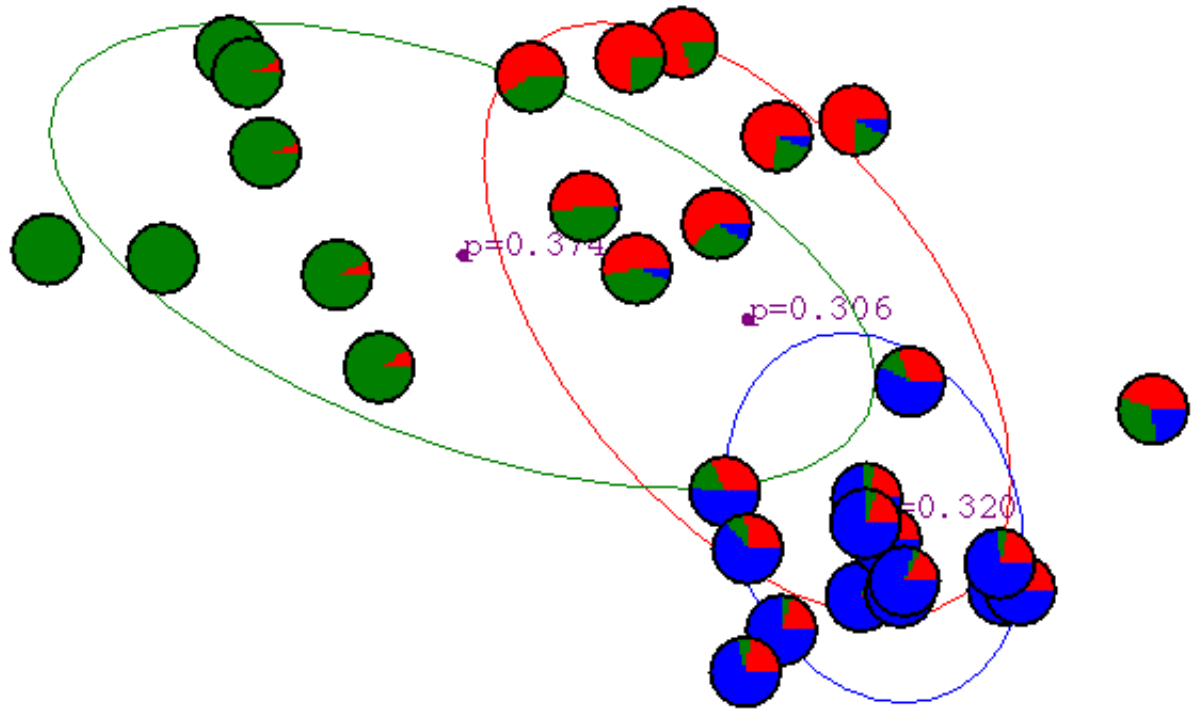
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #1



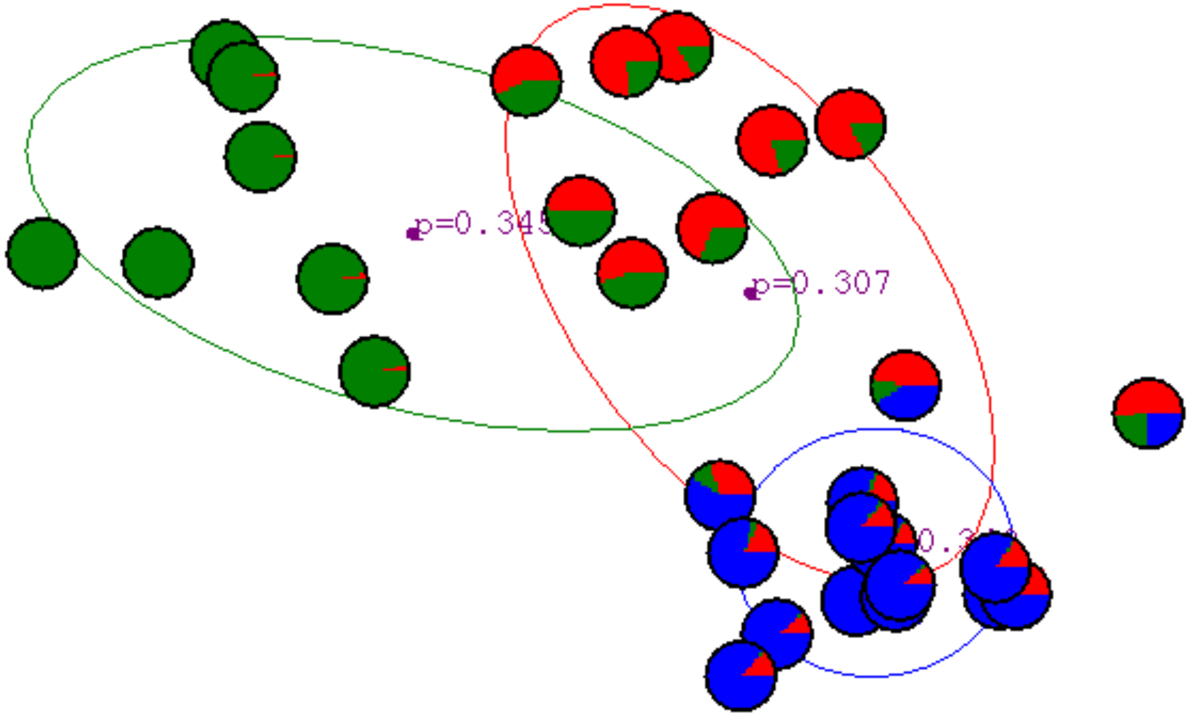
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #2



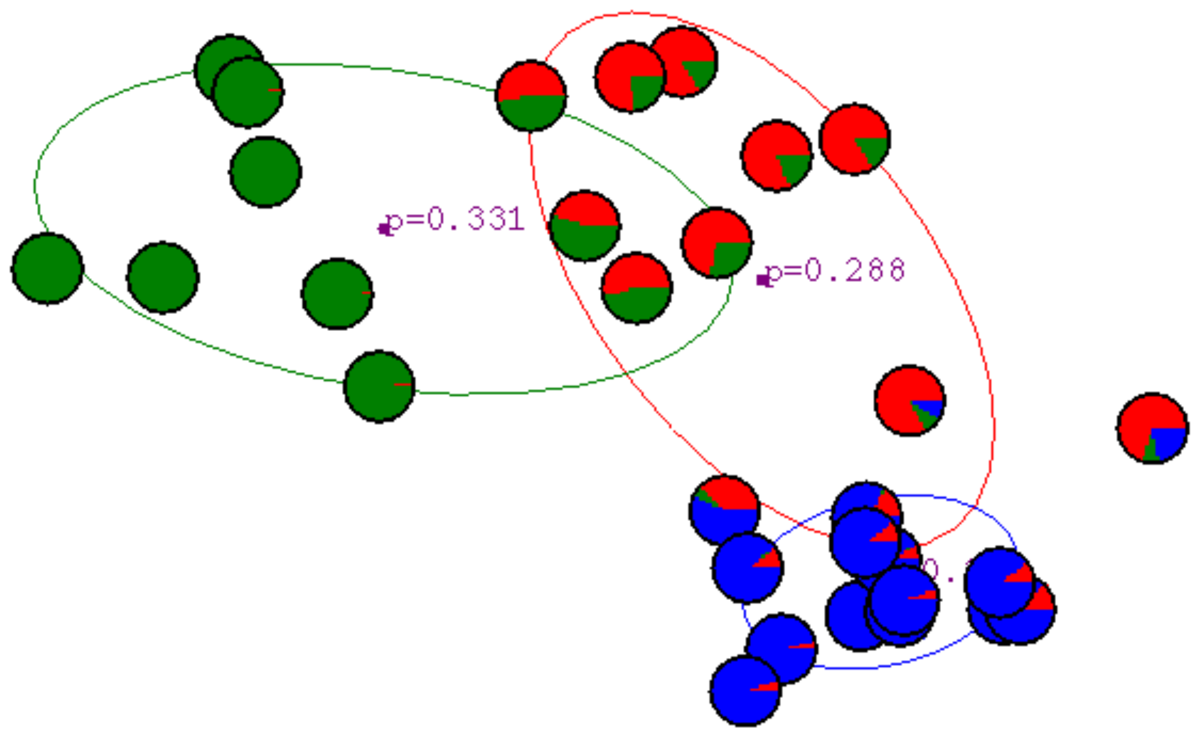
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #3



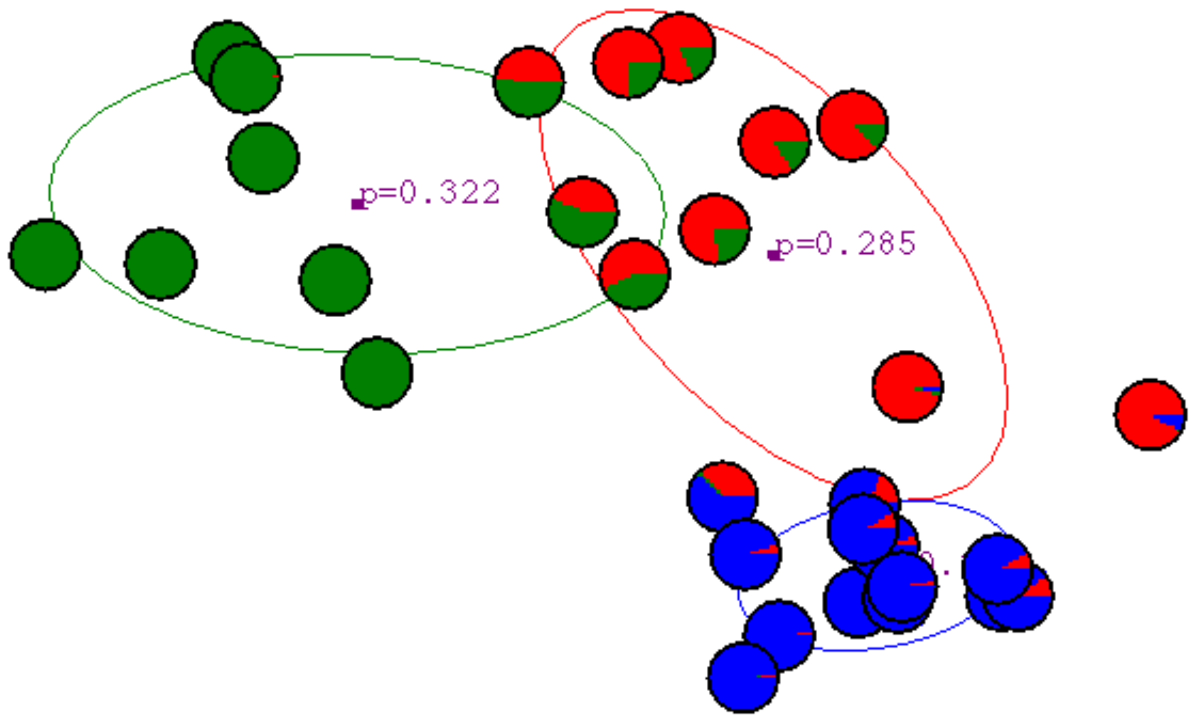
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #4



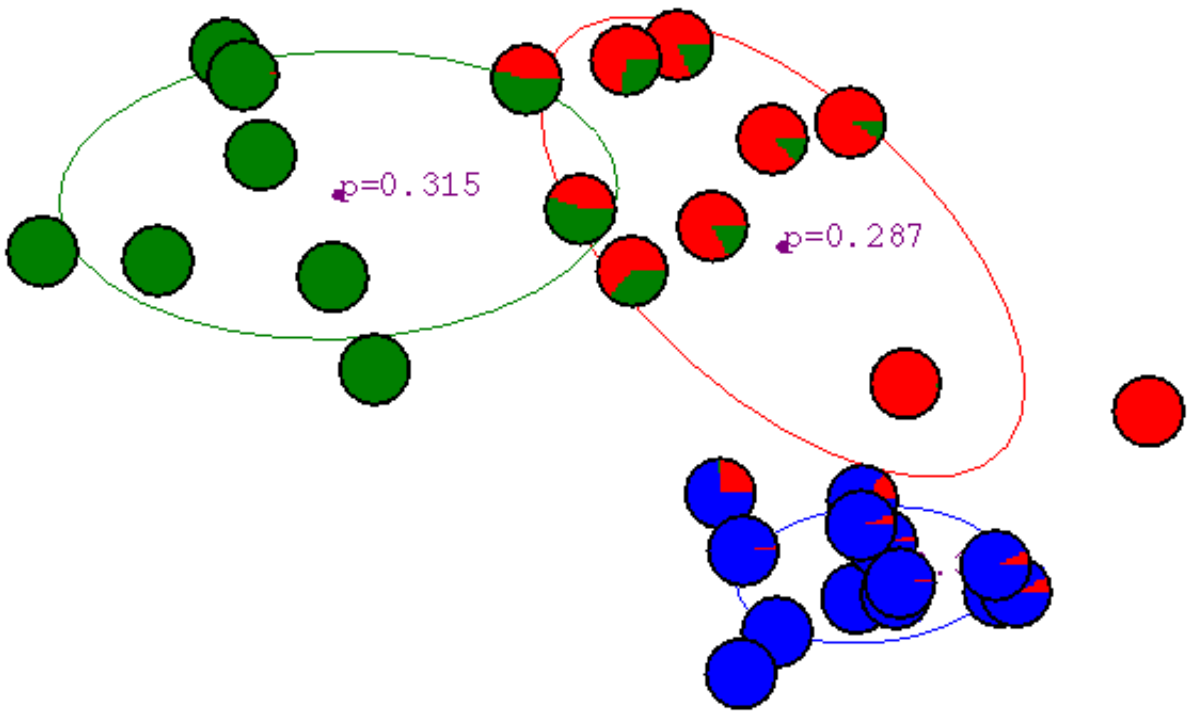
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #5



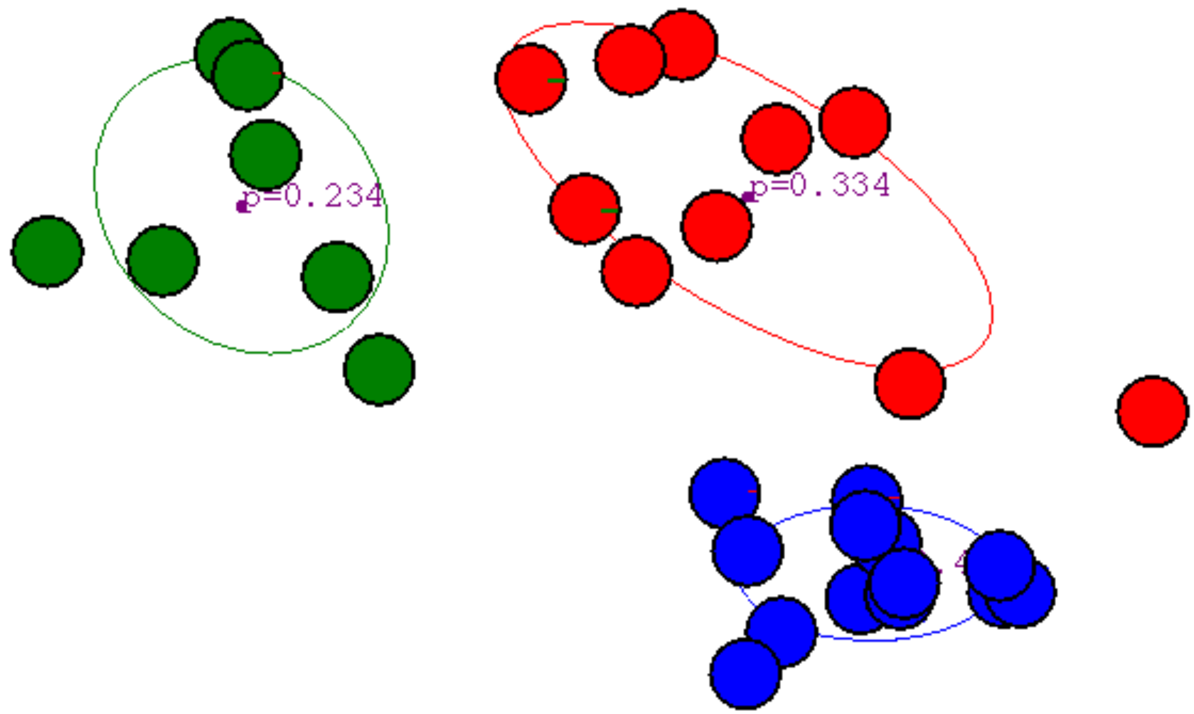
(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #6



(Illustration from Andrew Moore's tutorial slides on GMM)

After Iteration #20



(Illustration from Andrew Moore's tutorial slides on GMM)

GMM Remarks

- GMM is powerful: any density function can be arbitrarily-well approximated by a GMM with enough components.
- If the number of components K is too large, data will be overfitted.
  - Likelihood increases with K.
  - Extreme case: N Gaussians for N data points, with variances $\rightarrow 0$, then likelihood $\rightarrow \infty$.
- How to choose K?
  - Use domain knowledge.
  - Validate through visualization.

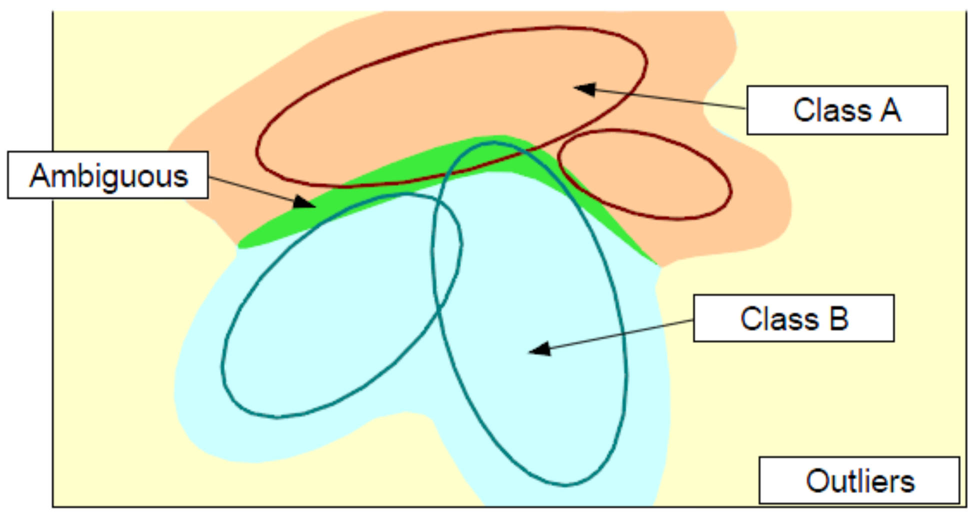
GMM is a "soft" version of K-means

- Similarity
  - K needs to be specified.
  - Converges to some local optima.
  - Initialization matters final results.
  - One would want to try different initializations.

- Differences
  - GMM Assigns "soft" labels to instances.
  - GMM Considers variances in addition to means.

GMM for Classification

- Given training data with multiple classes…
  1) Model the training data for each class with a GMM
  2) Classify a new point by estimating the probability each class generated the point
  3) Pick the class with the highest probability as the label.



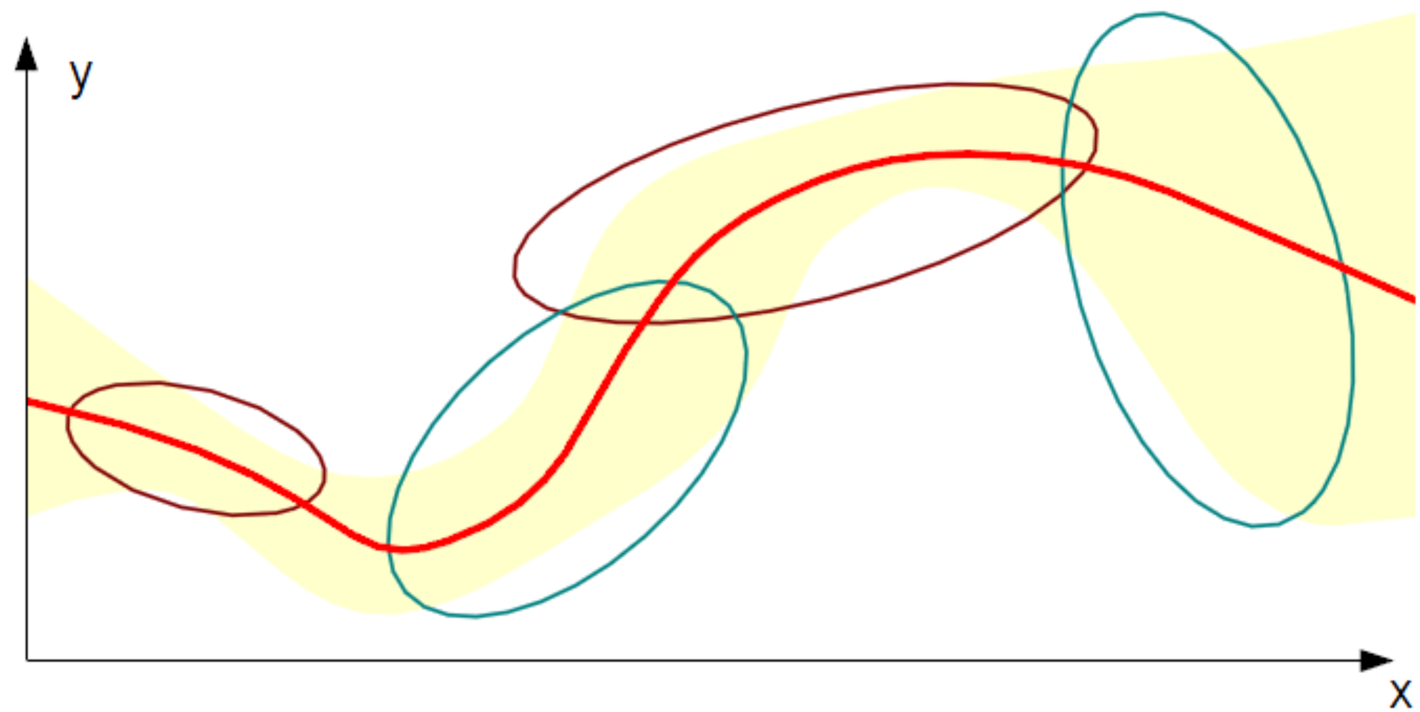
(illustration from Leon Bottou's slides on EM)

GMM for Regression

Given dataset $D=\{<\mathrm{x}_1, y_1>, \ldots, <\mathrm{x}_n, y_n>\}$, where $y_i \in \Re$ and x_i is a vector of d dimensions...

Learn a $d+1$ dimensional GMM.

Then, compute $f(x) = \mathbf{E}[y \mid x]$



(illustration from Leon Bottou's slides on EM)