K-Means and Gaussian Mixture Models

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April 25, 2017

Intro Question

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Consider the following probability model for generating data.

1. Roll a weighted k-sided die to choose a label $z \in \{1, \ldots, k\}$. Let π denote the PMF for the die.
2. Draw $x \in \mathbf{R}^d$ randomly from the multivariate normal distribution $\mathcal{N}(\mu_z, \Sigma_z)$.

Solve the following questions.

1. What is the joint distribution of x, z given π and the μ_z, Σ_z values?
2. Suppose you were given the dataset $\mathcal{D} = \{(x_1, z_1), \ldots, (x_n, z_n)\}$. How would you estimate the die weightings, and the μ_z, Σ_z values?
3. How would you determine the label for a new datapoint x?

Intro Solution

1. The joint PDF/PMF is given by

$$p(x,z) = \pi(z) f(x; \mu_z, \Sigma_z)$$

where

$$f(x;\mu_z,\Sigma_z) = \frac{1}{\sqrt{|2\pi\Sigma_z|}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right).$$

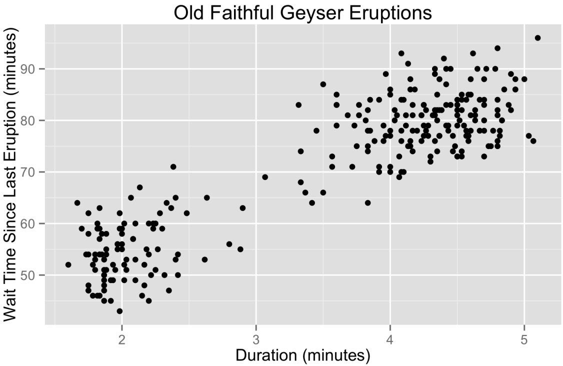
2. We could use maximum likelihood estimation. Our estimates are

$$\begin{aligned} n_z &= \textstyle\sum_{i=1}^n \mathbf{1}(z_i = z) \\ \hat{\pi}(z) &= \tfrac{n_z}{n} \\ \hat{\mu}_z &= \tfrac{1}{n_z} \textstyle\sum_{i:z_i=z} x_i \\ \hat{\Sigma}_z &= \tfrac{1}{n_z} \textstyle\sum_{i:z_i=z} (x_i - \hat{\mu}_z)(x_i - \hat{\mu}_z)^T. \end{aligned}$$

3. $\arg\max_z p(x,z)$

K-Means Clustering

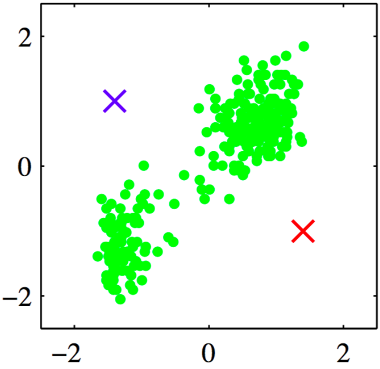
Example: Old Faithful Geyser



- Looks like two clusters.
- How to find these clusters algorithmically?

k-Means: By Example

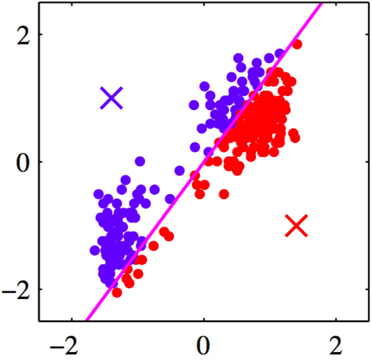
- Standardize the data.
- Choose two cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(a).

k-means: by example

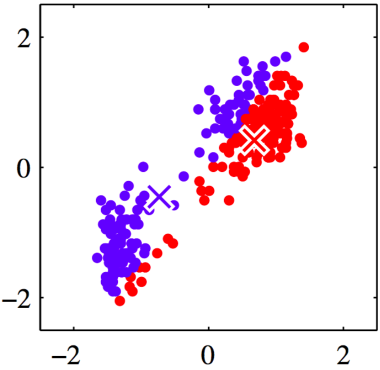
- Assign each point to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(b).

k-means: by example

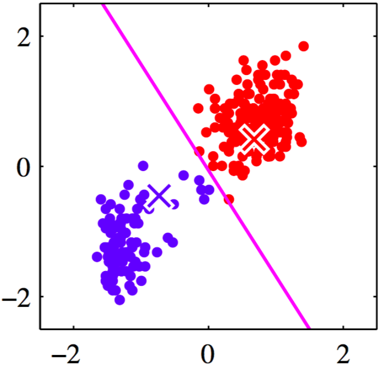
- Compute new class centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(c).

k-means: by example

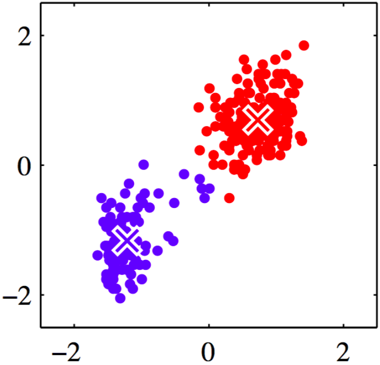
- Assign points to closest center.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(d).

k-means: by example

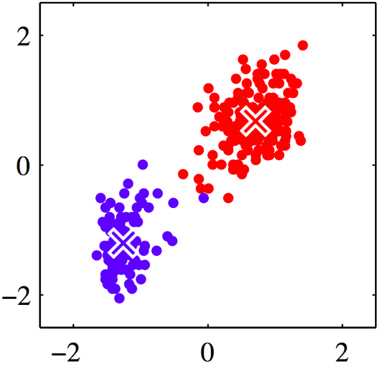
- Compute cluster centers.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(e).

k-means: by example

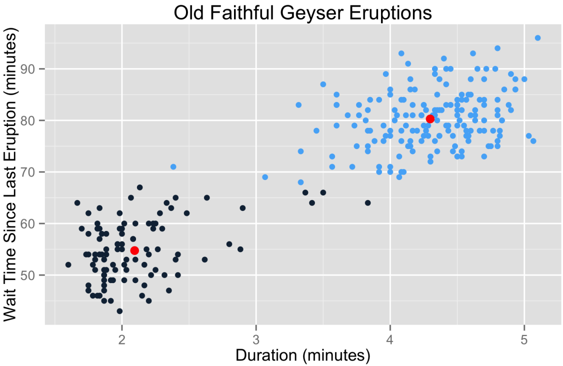
- Iterate until convergence.



From Bishop's *Pattern recognition and machine learning*, Figure 9.1(i).

k-Means Algorithm: Standardizing the data

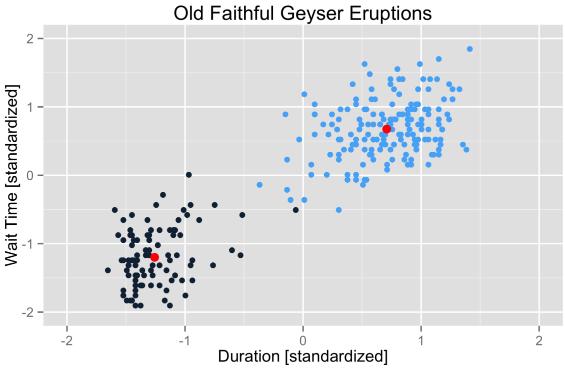
- Without standardizing:



- Blue and black show results of k-means clustering
- Wait time dominates the distance metric

k-Means Algorithm: Standardizing the data

- With standardizing:



- Note several points have been reassigned from black to blue cluster.

k-Means: Objective

- Let $x_1, \ldots, x_n$ denote the data points and $\mu_1, \ldots, \mu_k$ the cluster points.
- Define the objective ϕ by

$$\phi(x, \mu) = \sum_{i=1}^{n} \|x_i - \mu_{c(x_i)}\|_2^2,$$

  where $\mu_{c(x_i)}$ is the cluster point associated to x_i.
- Then ϕ decreases at every round of k-means. Why?

k-Means: Objective

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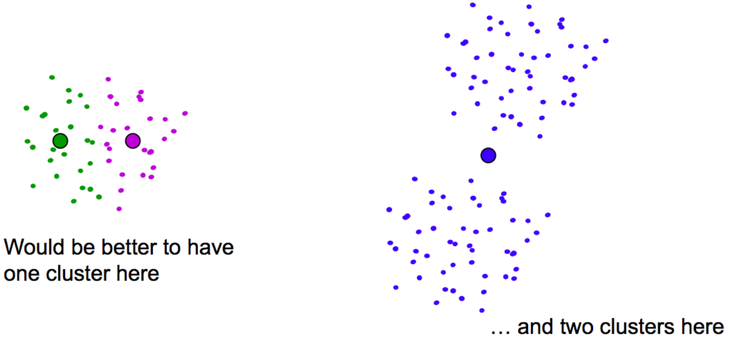
where $\mu_{c(x_i)}$ is the cluster point associated to x_i.
- Then ϕ decreases at every round of k-means. Why?
- Selecting mean of all associated data points improves objective.
- Selecting closest cluster point for each data points improves objective.

k-Means: Failure Cases

k-Means: Suboptimal Local Minimum

- The clustering for $k = 3$ below is a local minimum, but suboptimal:



From Sontag's DS-GA 1003, 2014, Lecture 8.

k-Means++

- Improvement on k-means by controlling the random initialization of the cluster centers.
- Randomly choose first center amongst the data points.
- For each of the remaining $k-1$ centers:
  - Compute the distance from each data point to the closest already chosen center.
  - Randomly choose a point as the new center with probability proportional to its computed distance squared.
- If we let ϕ denote the total sum of squares distances from each point to the closest cluster, then k-means++ has

$$E[\phi] \leqslant 8(\log k + 2)\phi_{\mathrm{OPT}},$$

where ϕ_{OPT} is from the optimal k-cluster assignment.

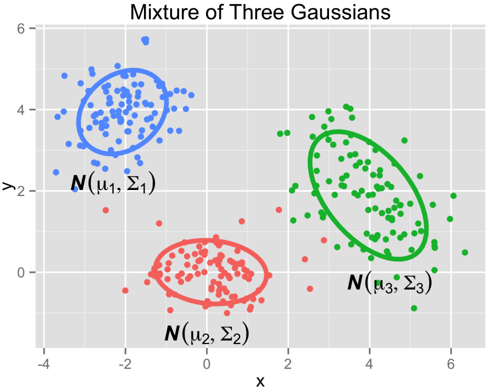
Gaussian Mixture Models

Probabilistic Model for Clustering

- Let's consider a **generative model** for the data.
- Suppose
  1. There are k clusters.
  2. We have a probability density for each cluster.
- Generate a point as follows
  1. Choose a random cluster $z \in \{1, 2, \ldots, k\}$.
  2. Choose a point from the distribution for cluster Z.

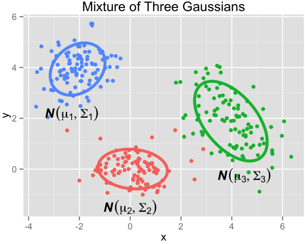
Gaussian Mixture Model ($k = 3$)

1. Choose $z \in \{1, 2, 3\}$ with $p(1) = p(2) = p(3) = \frac{1}{3}$.
2. Choose $x \mid z \sim \mathcal{N}(X \mid \mu_z, \Sigma_z)$.



Gaussian Mixture Model Parameters (k Components)

$$\begin{aligned} \text{Cluster probabilities :} \quad & \pi = (\pi_1, \ldots, \pi_k) \\ \text{Cluster means :} \quad & \mu = (\mu_1, \ldots, \mu_k) \\ \text{Cluster covariance matrices:} \quad & \Sigma = (\Sigma_1, \ldots \Sigma_k) \end{aligned}$$



For now, **suppose all these parameters are known**.
We'll discuss how to **learn** or **estimate** them later.

Gaussian Mixture Model: Joint Distribution

- Factorize the joint distribution:

$$\begin{aligned} p(x,z) &= p(z)p(x \mid z) \\ &= \pi_z \mathcal{N}(x \mid \mu_z, \Sigma_z) \end{aligned}$$

  - π_z is probability of choosing cluster z.
  - $x \mid z$ has distribution $\mathcal{N}(\mu_z, \Sigma_z)$.
  - z corresponding to x is the true cluster assignment.

- Suppose we know the model parameters π_z, μ_z, Σ_z.

- Then we can easily compute the joint $p(x,z)$.

Latent Variable Model

- We observe x.
- In the intro problem we had labeled data. Here we don't observe z, the cluster assignment.
- Cluster assignment z is called a **hidden variable** or **latent variable**.

Definition

A **latent variable model** is a probability model for which certain variables are never observed.

e.g. The Gaussian mixture model is a latent variable model.

The GMM "Inference" Problem

- We observe x. We want to know z.
- The conditional distribution of the cluster z given x is

$$p(z \mid x) = p(x,z)/p(x)$$

- The conditional distribution is a **soft assignment** to clusters.
- A **hard assignment** is

$$z^* = \underset{z \in \{1,\ldots,k\}}{\arg\max}\; p(z \mid x).$$

- So if we have the model, clustering is trival.

Mixture Models

Gaussian Mixture Model: Marginal Distribution

- The **marginal distribution** for a single observation x is

$$
\begin{aligned}
p(x) &= \sum_{z=1}^{k} p(x,z) \\
&= \sum_{z=1}^{k} \pi_z \mathcal{N}\left(x \mid \mu_z, \Sigma_z\right)
\end{aligned}
$$

- Note that $p(x)$ is a convex combination of probability densities.
- This is a common form for a probability model...

Mixture Distributions (or Mixture Models)

Definition

A probability density $p(x)$ represents a **mixture distribution** or **mixture model**, if we can write it as a **convex combination** of probability densities. That is,

$$p(x) = \sum_{i=1}^{k} w_i p_i(x),$$

where $w_i \geqslant 0$, $\sum_{i=1}^{k} w_i = 1$, and each p_i is a probability density.

- In our Gaussian mixture model, x has a **mixture distribution**.
- More constructively, let S be a set of probability distributions:
  1. Choose a distribution randomly from S.
  2. Sample x from the chosen distribution.
- Then x has a mixture distribution.

Learning in Gaussian Mixture Models

The GMM "Learning" Problem

- Given data $x_1, \ldots, x_n$ drawn from a GMM,
- Estimate the parameters:

$$\begin{aligned}
\text{Cluster probabilities}: &\quad \pi = (\pi_1, \ldots, \pi_k) \\
\text{Cluster means}: &\quad \mu = (\mu_1, \ldots, \mu_k) \\
\text{Cluster covariance matrices:} &\quad \Sigma = (\Sigma_1, \ldots \Sigma_k)
\end{aligned}$$

- Once we have the parameters, we're done.
- Just do "inference" to get cluster assignments.

Estimating/Learning the Gaussian Mixture Model

- One approach to learning is **maximum likelihood**
  - find parameter values that give **observed data** the **highest likelihood**.
- The model likelihood for $\mathcal{D} = \{x_1, \ldots, x_n\}$ is

$$
\begin{aligned}
L(\pi, \mu, \Sigma) &= \prod_{i=1}^{n} p(x_i) \\
&= \prod_{i=1}^{n} \sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z).
\end{aligned}
$$

- As usual, we'll take our objective function to be the log of this:

$$
J(\pi, \mu, \Sigma) = \sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z) \right\}
$$

Properties of the GMM Log-Likelihood

- GMM log-likelihood:

$$J(\pi, \mu, \Sigma) \quad = \quad \sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}(x_i \mid \mu_z, \Sigma_z) \right\}$$

- Let's compare to the log-likelihood for a single Gaussian:

$$\begin{aligned} & \sum_{i=1}^{n} \log \mathcal{N}(x_i \mid \mu, \Sigma) \\ = \quad & -\frac{nd}{2} \log(2\pi) - \frac{n}{2} \log|\Sigma| - \frac{1}{2} \sum_{i=1}^{n} (x_i - \mu)' \Sigma^{-1} (x_i - \mu) \end{aligned}$$

- For a single Gaussian, the log cancels the exp in the Gaussian density.
  - $\implies$ Things simplify a lot.
- For the GMM, the sum inside the log prevents this cancellation.
  - $\implies$ Expression more complicated. No closed form expression for MLE.

Issues with MLE for GMM

Identifiability Issues for GMM

- Suppose we have found parameters

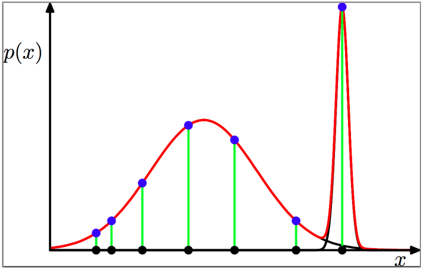
$$\begin{aligned} \text{Cluster probabilities}: \quad & \pi = (\pi_1, \ldots, \pi_k) \\ \text{Cluster means}: \quad & \mu = (\mu_1, \ldots, \mu_k) \\ \text{Cluster covariance matrices:} \quad & \Sigma = (\Sigma_1, \ldots \Sigma_k) \end{aligned}$$

  that are at a local minimum.

- What happens if we shuffle the clusters? e.g. Switch the labels for clusters 1 and 2.
- We'll get the same likelihood. How many such equivalent settings are there?
- Assuming all clusters are distinct, there are $k!$ equivalent solutions.
- Not a problem per se, but something to be aware of.

Singularities for GMM

- Consider the following GMM for 7 data points:



- Let σ^2 be the variance of the skinny component.
- What happens to the likelihood as $\sigma^2 \to 0$?
- In practice, we end up in local minima that do not have this problem.
  - Or keep restarting optimization until we do.
- Bayesian approach or regularization will also solve the problem.

From Bishop's *Pattern recognition and machine learning*, Figure 9.7.

Gradient Descent / SGD for GMM

- What about running gradient descent or SGD on

$$J(\pi, \mu, \Sigma) \quad = \quad -\sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \pi_z \mathcal{N}\left(x_i \mid \mu_z, \Sigma_z\right) \right\}?$$

- Can be done – but need to be clever about it.
- Each matrix $\Sigma_1, \ldots, \Sigma_k$ has to be positive semidefinite.
- How to maintain that constraint?
  - Rewrite $\Sigma_i = M_i M_i^T$, where M_i is an unconstrained matrix.
  - Then Σ_i is positive semidefinite.

The EM Algorithm for GMM

MLE for GMM

- From the intro questions, we know that we can solve the MLE problem if the cluster assignments z_i are known

$$\begin{aligned} n_z &= \sum_{i=1}^{n} \mathbf{1}(z_i = z) \\ \hat{\pi}(z) &= \frac{n_z}{n} \\ \hat{\mu}_z &= \frac{1}{n_z} \sum_{i:z_i=z} x_i \\ \hat{\Sigma}_z &= \frac{1}{n_z} \sum_{i:z_i=z} (x_i - \hat{\mu}_z)(x_i - \hat{\mu}_z)^T. \end{aligned}$$

- In the EM algorithm we will modify the equations to handle our evolving **soft assignments**, which we will call **responsibilities**.

Cluster Responsibilities: Some New Notation

- Denote the probability that observed value x_i comes from cluster j by

$$\gamma_i^j = \mathbb{P}\left(Z = j \mid X = x_i\right).$$

- The **responsibility** that cluster j takes for observation x_i.
- Computationally,

$$\begin{aligned}
\gamma_i^j &= \mathbb{P}\left(Z = j \mid X = x_i\right). \\
&= p\left(Z = j, X = x_i\right) / p(x) \\
&= \frac{\pi_j \mathcal{N}\left(x_i \mid \mu_j, \Sigma_j\right)}{\sum_{c=1}^{k} \pi_c \mathcal{N}\left(x_i \mid \mu_c, \Sigma_c\right)}
\end{aligned}$$

- The vector $\left(\gamma_i^1, \ldots, \gamma_i^k\right)$ is exactly the **soft assignment** for x_i.
- Let $n_c = \sum_{i=1}^{n} \gamma_i^c$ be the number of points "soft assigned" to cluster c.

EM Algorithm for GMM: Overview

- If we know π and μ_j, Σ_j for all j then we can easily find $\gamma_i^j = \mathbb{P}(Z = j \mid X = x_i)$.
- If we know the (soft) assignments, we can easily find estimates for π, μ_j, Σ_j for all j.
- Repeatedly alternate the previous 2 steps.

EM Algorithm for GMM: Overview

1. Initialize parameters μ, Σ, π.
2. "E step". Evaluate the responsibilities using current parameters:

$$\gamma_i^j = \frac{\pi_j \mathcal{N}(x_i \mid \mu_j, \Sigma_j)}{\sum_{c=1}^k \pi_c \mathcal{N}(x_i \mid \mu_c, \Sigma_c)}, \quad \text{for } i = 1, \dots, n \text{ and } j = 1, \dots, k.$$

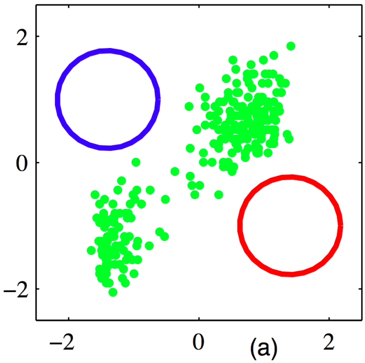
3. "M step". Re-estimate the parameters using responsibilities. [Compare with intro question.]

$$\begin{aligned} \mu_c^{\text{new}} &= \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c x_i \\ \Sigma_c^{\text{new}} &= \frac{1}{n_c} \sum_{i=1}^n \gamma_i^c (x_i - \mu_{\text{MLE}})(x_i - \mu_{\text{MLE}})^T \\ \pi_c^{\text{new}} &= \frac{n_c}{n}, \end{aligned}$$

4. Repeat from Step 2, until log-likelihood converges.

EM for GMM

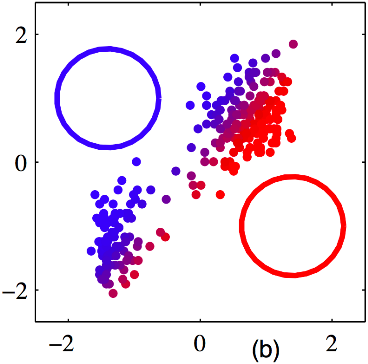
- Initialization



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

- First soft assignment:



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EM for GMM

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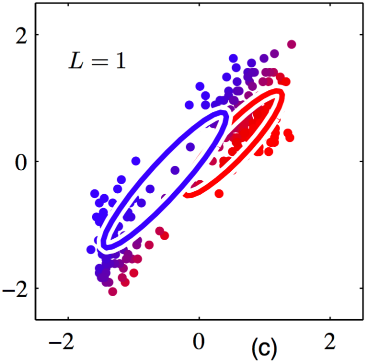
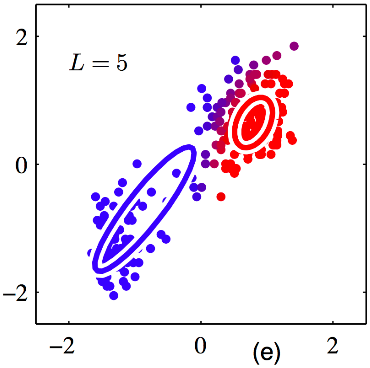


From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

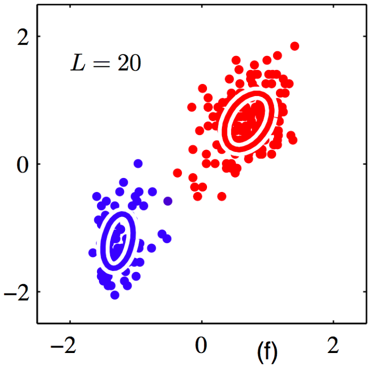
- After 5 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

EM for GMM

- After 20 rounds of EM:



From Bishop's *Pattern recognition and machine learning*, Figure 9.8.

Relation to K-Means

- EM for GMM seems a little like k-means.
- In fact, there is a precise correspondence.
- First, fix each cluster covariance matrix to be $\sigma^2 I$.
- As we take $\sigma^2 \to 0$, the update equations converge to doing k-means.
- If you do a quick experiment yourself, you'll find
  - Soft assignments converge to hard assignments.
  - Has to do with the tail behavior (exponential decay) of Gaussian.
- Can use k-means++ to initialize parameters of EM algorithm.