Gaussian Mixture Models (GMM)

ECE57000: Artificial Intelligence

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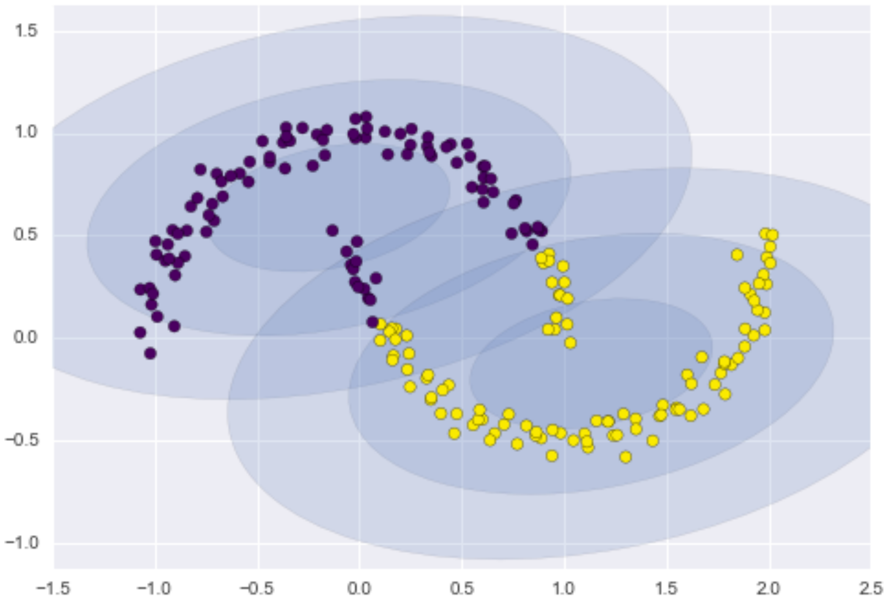
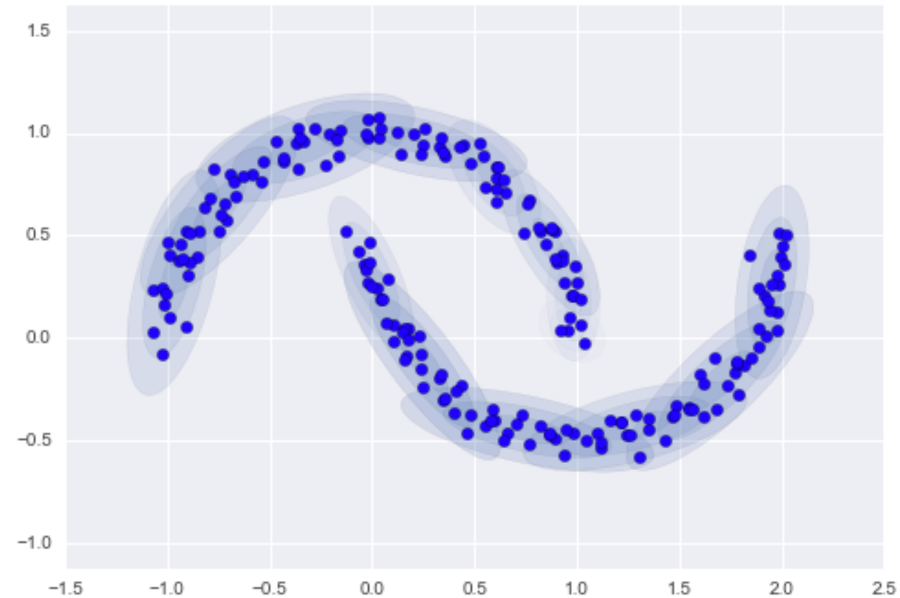
<u>Gaussian mixture models</u> (GMM) can be used for density estimation

1. General density estimation

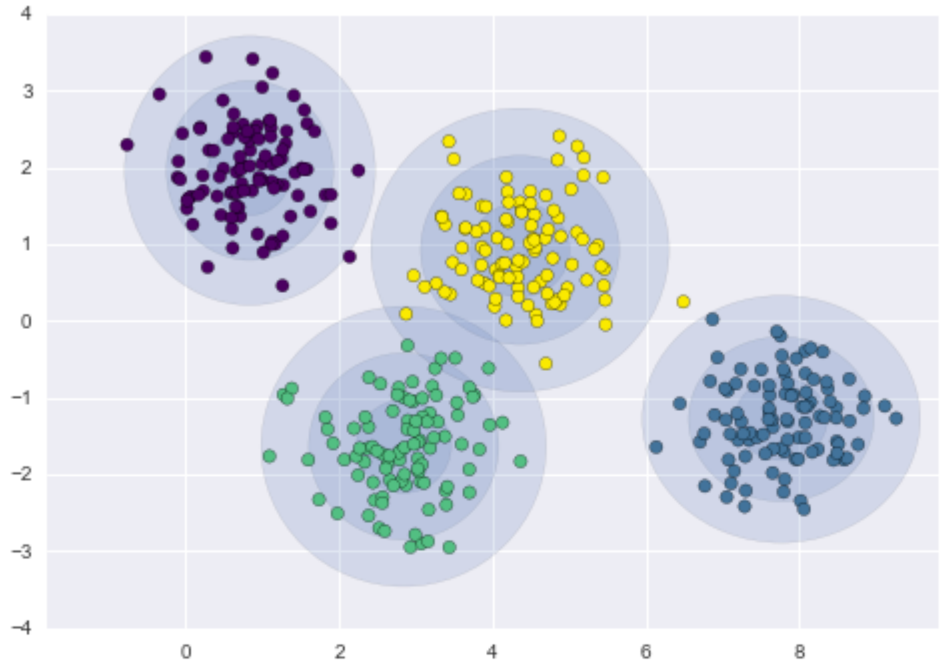




https://jakevdp.github.io/PythonDataScienceHandbook/05.12-gaussian-mixtures.html

Even if each component distribution is independent, the mixture may **not** be independent

- Each component distribution is spherical (i.e., independent)



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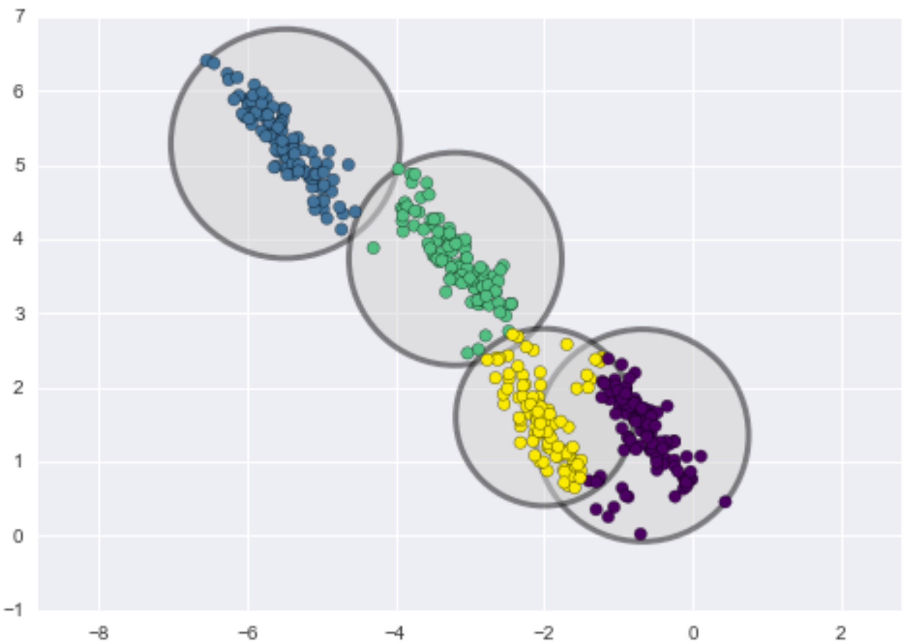
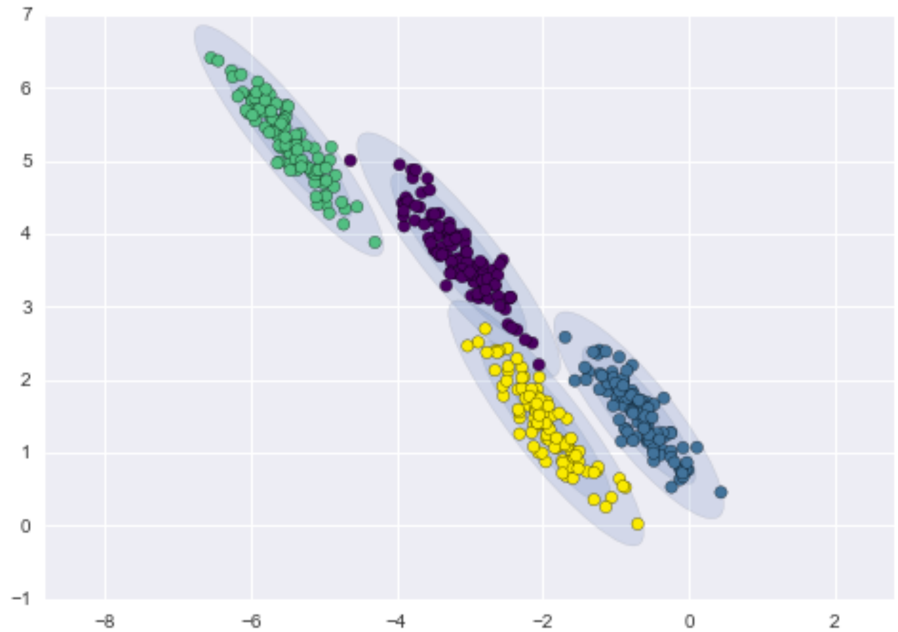
Gaussian mixture models (GMM) can be used for flexible clustering

2. Flexible clustering





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Mixture distributions are weighted averages of component distributions

- Mixture distribution
  - Component weights $0 \leq \pi_j, \leq 1 \text{ s.t. } \sum_{j=1}^{k} \pi_j = 1$
  - Component distributions $p_j(x)$
- Simple form of mixture

$$p_{\text{mixture}}(x) = \sum_{j=1}^{k} \pi_j p_j(x)$$

- Exercise: Check that p_{mixture} integrates to 1.

Mixture models can be viewed as <u>latent (or "hidden") variable models</u>

- Simple form of mixture

$$p_{\mathrm{mixture}}(x) = \sum_{j=1}^{k} \pi_j p_j(x)$$

- Let $z \in \{1, \dots, k\}$ be an *auxiliary* **<u>indicator variable</u>**

- Let $p(z = j) = \pi_j$, then the joint density model is:

$$p(x, z) = p(z)p(x|z)$$

- The distribution of x marginalizes over the latent variable z which is equivalent to the mixture above

$$p_{\mathrm{mixture}}(x) \equiv \sum_{z} p(x, z) = \sum_{z} p(z)p(x|z)$$

Gaussian mixture models (GMM) are one of the most common mixture distributions

- Form of Gaussian mixture model

$$p_{\mathrm{GMM}}(x) = \sum_{j=1}^{k} \pi_j p_{\mathcal{N}}(x; \mu_j, \Sigma_j) = \sum_{j=1}^{k} p(z = j) p_{\mathcal{N}}(x; z = j)$$

Machine Learning, Murphy, 2012.

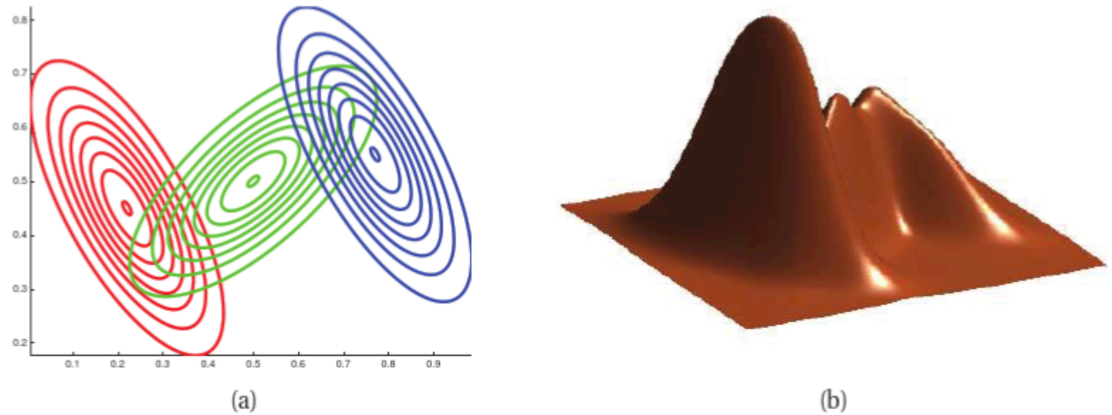


Figure 11.3 A mixture of 3 Gaussians in 2d. (a) We show the contours of constant probability for each component in the mixture. (b) A surface plot of the overall density. Based on Figure 2.23 of (Bishop 2006a). Figure generated by `mixGaussPlotDemo`.

MLE for mixtures is difficult
Reason 1: The algebraic form is more complex

- The mixture log likelihood cannot be simplified

$$\arg\max_{\pi,\mu_j,\Sigma_j} \log \prod_i p_{\text{GMM}}(x_i; \pi, \mu_1, \dots, \mu_k, \Sigma_1, \dots, \Sigma_k)$$

$$\sum_i \log p_{\text{GMM}}(x_i; \pi, \mu_1, \dots, \mu_k, \Sigma_1, \dots, \Sigma_k)$$

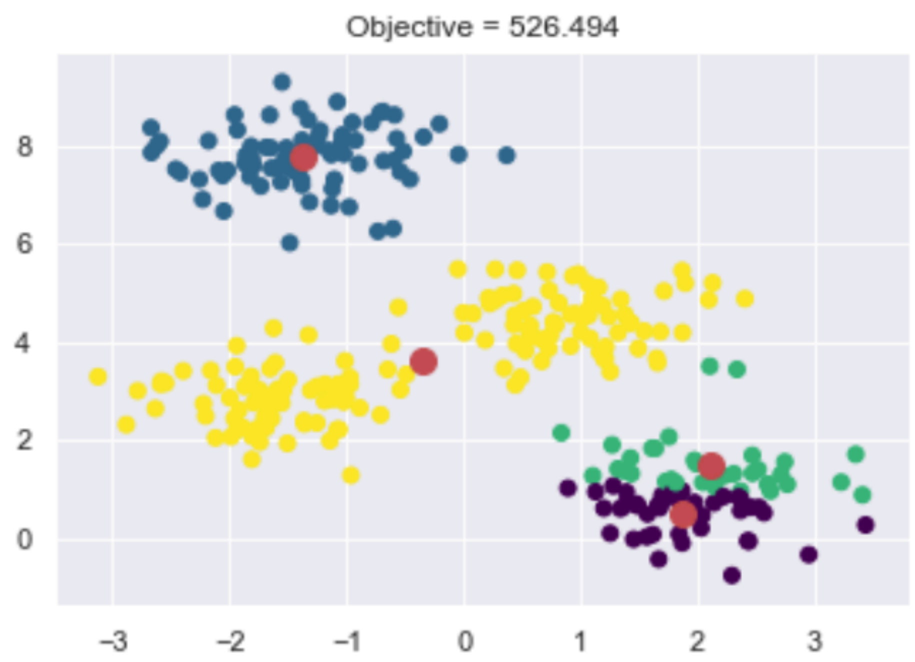
$$\sum_i \log \sum_{z_i} \pi_{z_i} p_{\mathcal{N}}\left(x_i \mid \mu_{z_i}, \Sigma_{z_i}\right)$$

$$\sum_i \log \sum_{z_i} p(z_i) p_{\mathcal{N}}(x_i | z_i)$$

- **Cannot exchange log and summation to cancel exp**

MLE for mixtures is difficult
Reason 2: Problem is non-convex
(and could have multiple local optima)

- The intuition is similar to the problem with k-means clustering



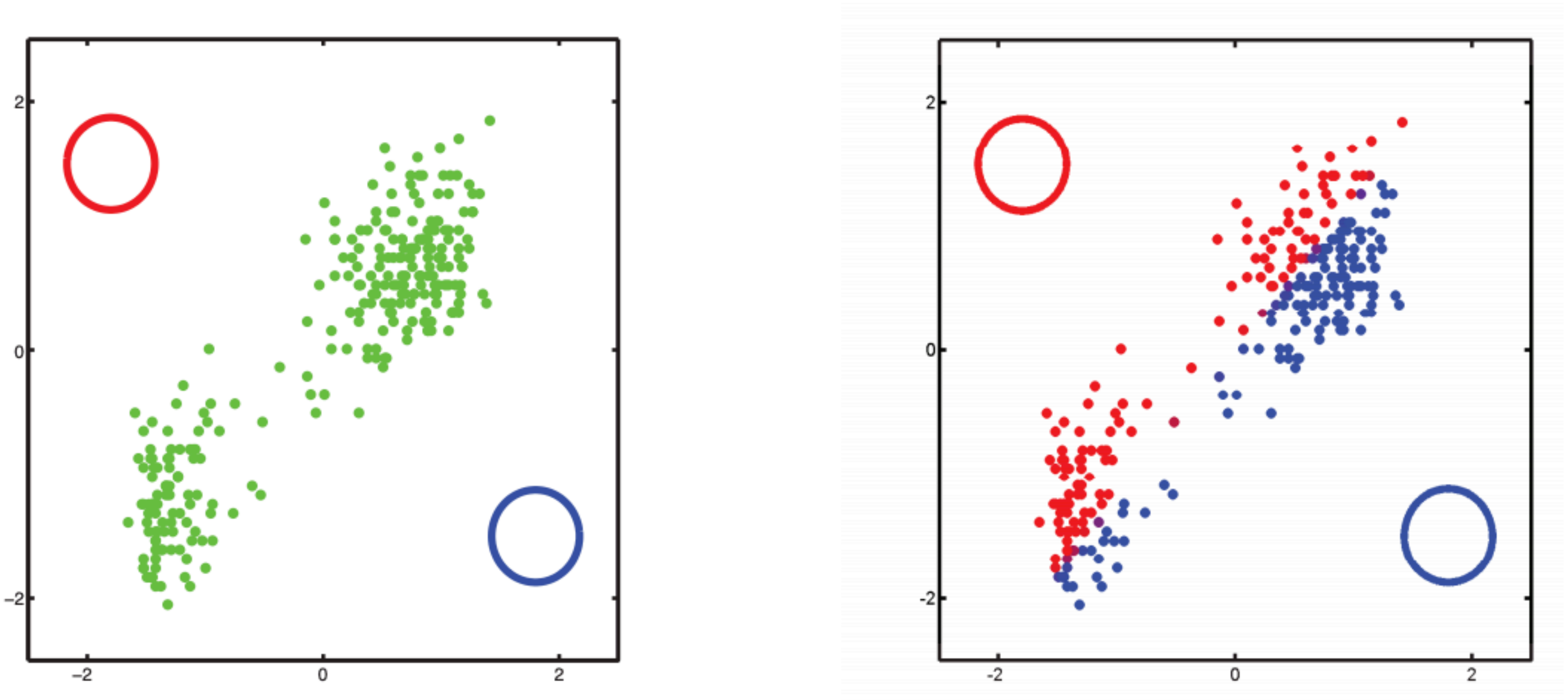
See [ML, Ch. 11, pp. 347-348] for more detailed analysis.

The Expectation-Maximization (EM) can estimate models and is a generalization of k-means

- The EM algorithm for GMM alternates between
  - Probabilistic/soft assignment of points
  - Estimation of Gaussian for each component

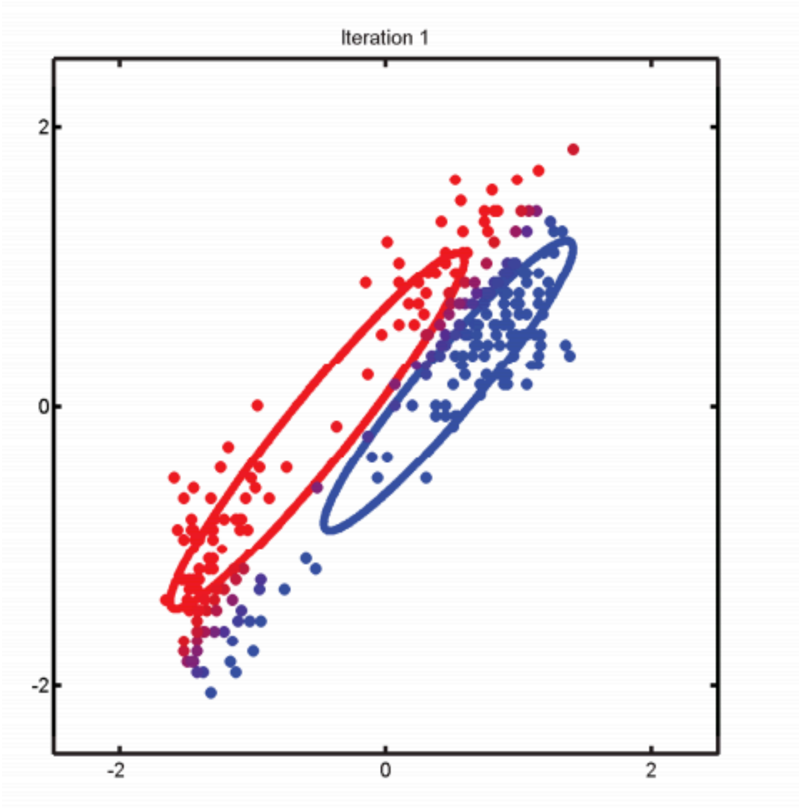
- Similar to k-means which alternates between
  - Hard assignment of points
  - Estimation of mean of points in each cluster

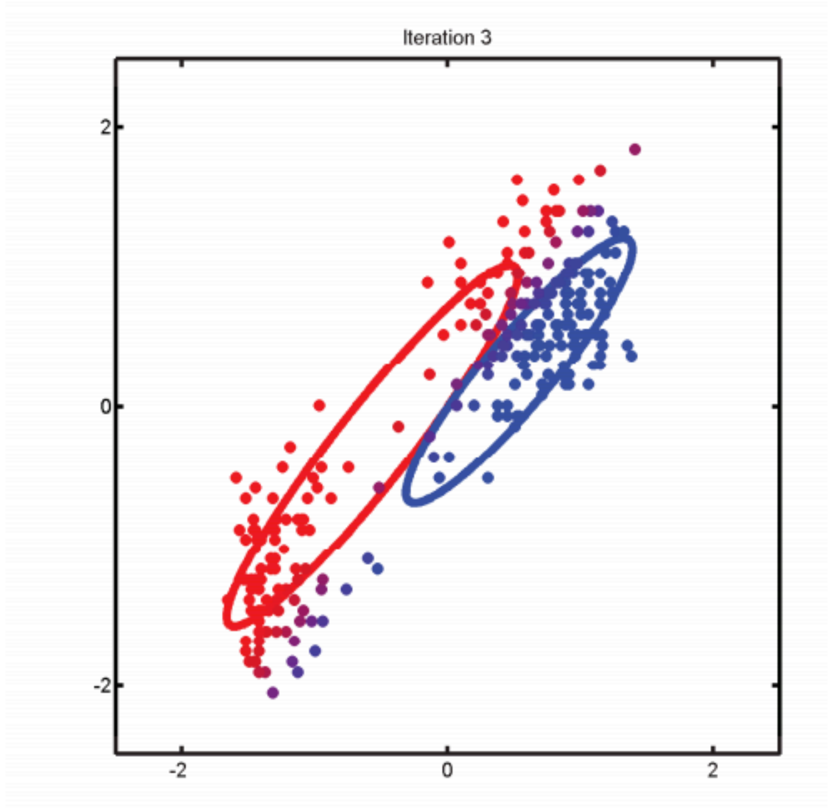
EM Algorithm: Initialization



Machine Learning: A probabilistic perspective, Murphy, 2012.

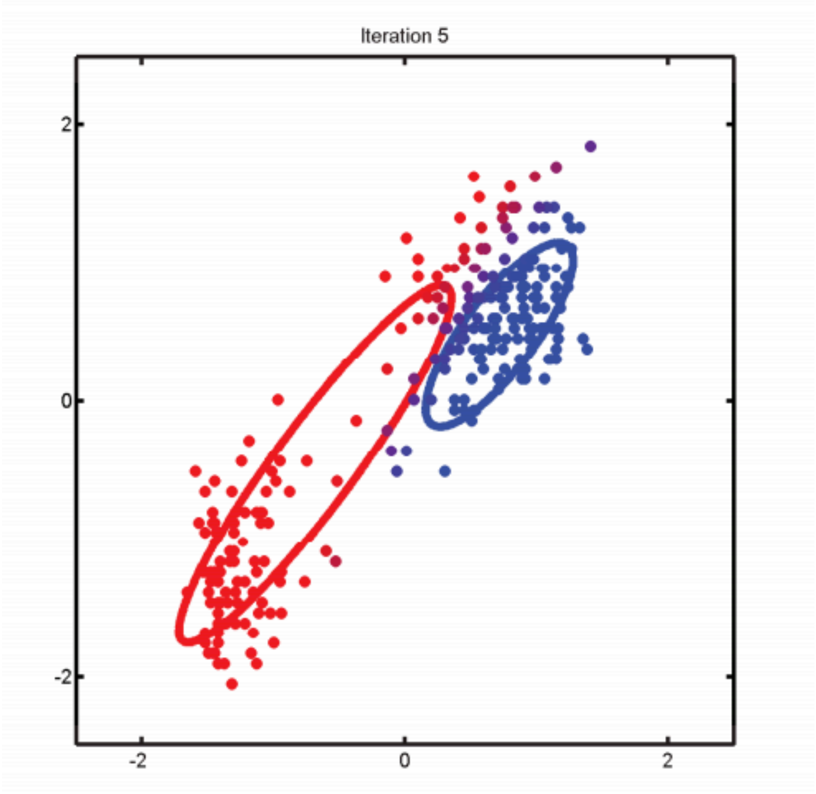
EM Algorithm: Iteration 1 and 3

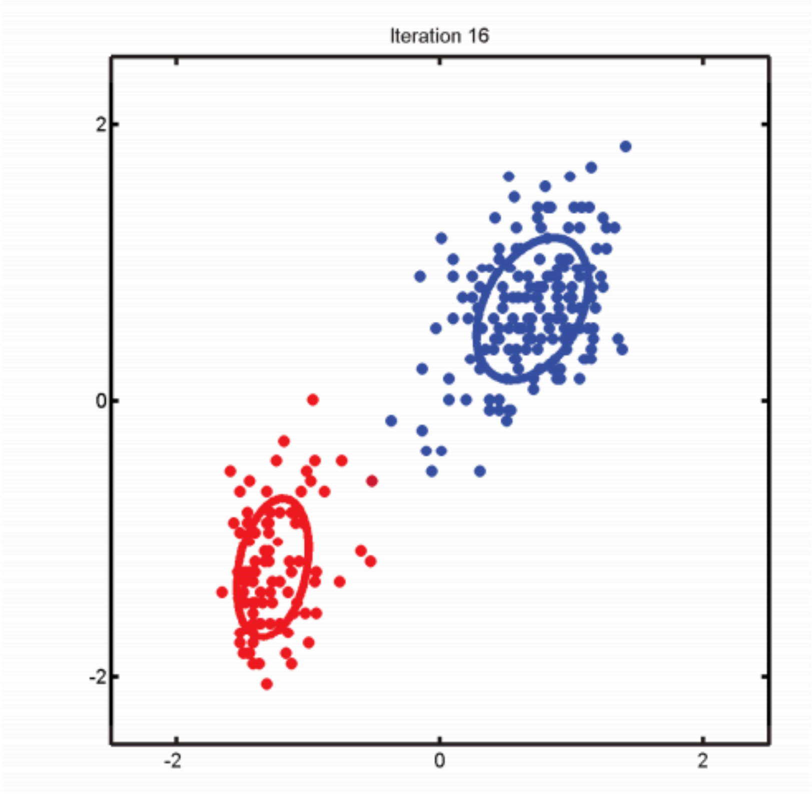




Machine Learning: A probabilistic perspective, Murphy, 2012.

EM Algorithm: Iteration 5 and 16





Machine Learning: A probabilistic perspective, Murphy, 2012.

EM algorithm for Gaussian mixture models Expectation step:

- Randomly initialize mixture components
- Expectation step (determine soft assignments)

$$r_{ij}^t = p(z_i = j | x_i, \theta^{t-1}) = \frac{p(z_i, x_i)}{p(x_i)} = \frac{p(z_i|\theta^{t-1})p(x_i|z_i, \theta^{t-1})}{\sum_{z_i} p(z_i|\theta^{t-1})p(x_i|z_i, \theta^{t-1})}$$

$$= \frac{\pi_j p_{\mathcal{N}}\left(x_i \middle| \mu_j^{t-1}, \Sigma_j^{t-1}\right)}{\sum_k \pi_k p_{\mathcal{N}}\left(x_i \middle| \mu_k^{t-1}, \Sigma_k^{t-1}\right)}$$

EM algorithm for Gaussian mixture models Maximization step

- Compute weighted mean and covariance using soft assignments from E step

$$\mu_j^t = \frac{\sum_i r_{ij}\, x_i}{\sum_i r_{ij}}$$

$$\Sigma_j^t = \frac{\sum_i r_{ij}\left(x_i - \mu_j^t\right)\left(x_i - \mu_j^t\right)^T}{\sum_i r_{ij}}$$

Observation: If z_i were **observed** (i.e., we knew the cluster labels), then optimizing the complete log likelihood is easy

- **Observed/marginal** log likelihood (if z_i is **unknown**)

$$\ell(\theta) = \sum_i \log \sum_{z_i} p(x_i, z_i; \theta)$$

- **Complete** log likelihood (if z_i is **known**)

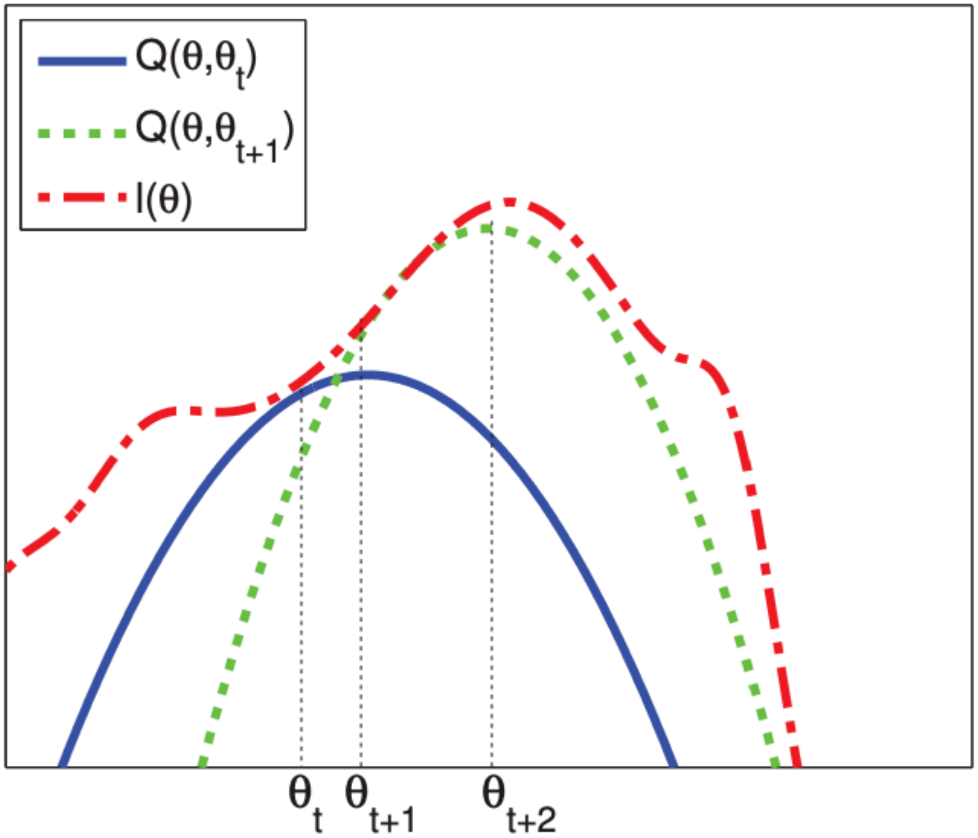
$$\ell_c(\theta) = \sum_i \log p(x_i, z_i; \theta) = \sum_i \log p(z_i) p_{\mathcal{N}}(x_i \mid z_i)$$

  - For GMMs, this is convex and easy to solve

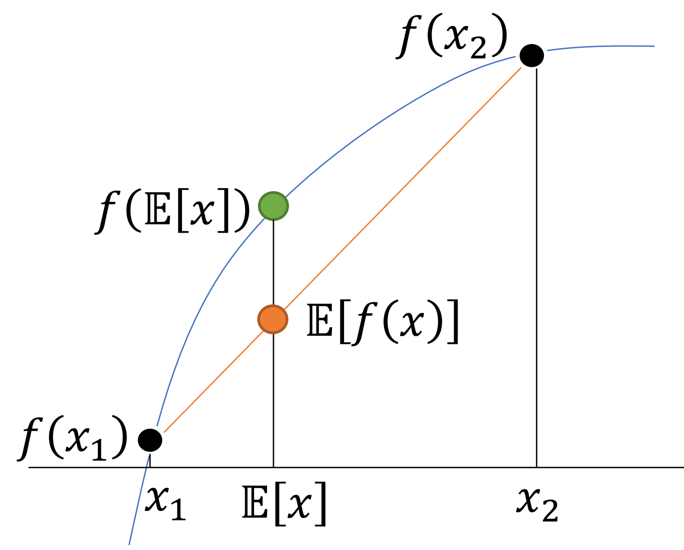
Derivation of EM iteration for GMM

- Complete log-likelihood
$$\ell_c(\theta) = \sum_i \log p(x_i, z_i|\theta)$$
- Expected complete log likelihood
$$Q(\theta; \theta^{t-1}) = Q_{\theta^{t-1}}(\theta) = \mathbb{E}_{\boldsymbol{z}_{\dots}|\boldsymbol{x}_{\dots}, \theta^{t-1}}[\ell_c(\theta)]$$
  - **NOTE:** Q is a function of θ **given** the previous parameter value θ^{t-1}
- Let's write the joint density of x and z as:
$$p(x_i, z_i|\theta) = \prod_j \left(\pi_j p\left(x_i|\theta_j\right)\right)^{I(z_i=j)}$$
  - $I(z_i = j)$ is an indicator function that is 1 if the inside expression is true or 0 otherwise
- See 11.22-11.26 pp. 351 of [ML] for derivation

EM algorithm is **guaranteed** to increase *observed* likelihood, i.e., $\prod_i p_{mixture}(x_i)$



Step 1: Use Jensen's inequality to get concave lower bound



- Jensen's inequality if f is *concave* (e.g., log)
$$f(\mathbb{E}[x]) \geq \mathbb{E}[f(x)]$$
- $\ell(\theta)$
- $= \sum_i \log \sum_{z_i} p(x_i, z_i; \theta)$
- $= \sum_i \log \sum_{z_i} q_i(z_i) \frac{p(x_i, z_i; \theta)}{q_i(z_i)}$
- $= \sum_i \log \mathbb{E}_{q_i} \left[\frac{p(x_i, z_i; \theta)}{q_i(z_i)} \right]$
- $\geq \sum_i \mathbb{E}_{q_i} \left[\log \frac{p(x_i, z_i; \theta)}{q_i(z_i)} \right]$
- $\equiv Q(\theta; q)$ for **any** distribution $q = (q_1, \cdots, q_n)$

Step 2: Choose **best** lower bound using the current parameters (for each point x_i)

- $L(\theta, q_i) = \sum_{z_i} q_i(z_i) \log \frac{p(x_i, z_i; \theta)}{q_i(z_i)}$
- $= \sum_{z_i} q_i(z_i) \log \frac{p(x_i\,;\theta) p(z_i\,|x_i\,;\theta)}{q_i(z_i)}$
- $= \sum_{z_i} q_i(z_i) \log \frac{p(z_i\,|x_i\,;\theta)}{q_i(z_i)} + \sum_{z_i} q_i(z_i) \log p(x_i\,;\;\theta)$
- $= \sum_{z_i} q_i(z_i) \log \frac{p(z_i\,|x_i\,;\theta)}{q_i(z_i)} + \log p(x_i\,;\;\theta)$
- $= -\sum_{z_i} q_i(z_i) \log \frac{q_i(z_i)}{p(z_i\,|x_i\,;\theta)} + \log p(x_i\,;\;\theta)$
- $= -KL(q_i(z_i), p(z_i|x_i\,;\theta)) + \log p(x_i\,;\;\theta)$
- Ideally, $q_i(z_i) = p(z_i|x_i, \theta\ )$ so KL is 0

Step 2: Lower bound is tight at current parameters θ^t if $q_i^t(z_i) = p(z_i|x_i, \theta^t)$

- The lower bound is **tight** with respect to the observed likelihood:
- $Q(\theta^t, \theta^t) = \sum_i L(\theta^t, q^t)$
- $= \sum_i -KL\left(q_i^t(z_i), p(z_i|x_i\,; \theta^t)\right) + \log p(x_i\,;\ \theta^t)$
- $= \sum_i -KL(p(z_i|x_i\,; \theta^t), p(z_i|x_i\,; \theta^t)) + \log p(x_i\,;\ \theta^t)$
- $= \sum_i \log p(x_i|\theta^t)$
- $= \ell(\theta^t)$
- Where last step is because KL is 0 if the same distribution
- In summary:

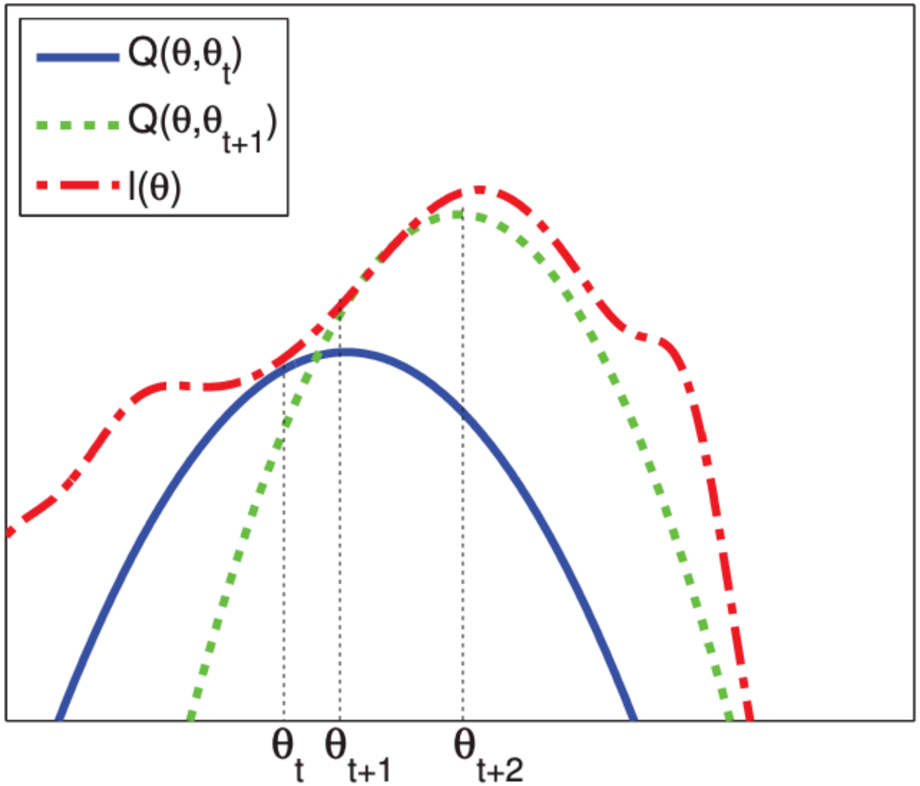
$$Q(\theta^t, \theta^t) = \ell(\theta^t)$$

Step 3: Maximize the lower bound

- We setup the optimization problem to update the parameter based on the lower bound
$$\theta^{t+1} = \arg\max_{\theta} Q(\theta, \theta^{t})$$
- By simple definition of maximization, we have:
$$Q(\theta^{t+1}, \theta^{t}) \geq Q(\theta^{t}, \theta^{t})$$

Putting all the steps together, we can prove monotonic increase of the EM algorithm

- **Lower bound, maximization, tightness**
  $$\ell(\theta^{t+1}) \geq Q(\theta^{t+1}, \theta^t) \geq Q(\theta^t, \theta^t) = \ell(\theta^t)$$



Proof that it monotonically increases likelihood

- See 11.4.7 in [ML] for full derivation of proof
- Show that $Q(\theta;\ q^t)$ is lower bound observed likelihood $\ell(\theta)$, i.e., $\ell(\theta) \geq Q(\theta; q^t), \forall\theta$
- Choose $q^t(z_i) = p(z_i|x_i, \theta^t)$, which corresponds to $Q(\theta; \theta^t)$
- Show that lower bound is tight at θ_t
- Combine three concepts
  1. Lower bound inequality
  2. Maximization inequality
  3. Tightness of lower bound