Gaussian Mixture Models

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Contents

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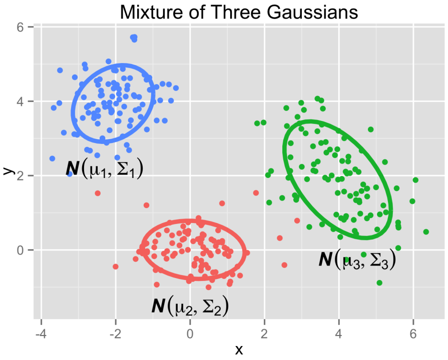
  1. Choose a random cluster $z \in \{1, 2, \ldots, k\}$.
  2. Choose a point from the distribution for cluster z.
- Data generated in this way is said to have a **mixture distribution.**

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)

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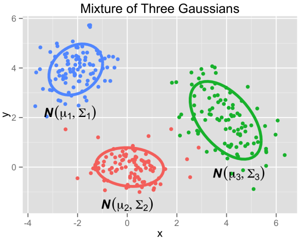

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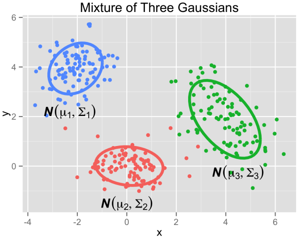

For now, **suppose all these parameters are known**.
We'll discuss how to **learn** or **estimate** them later.

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

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

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- So if we know the model parameters, clustering is trival.

Mixture Models

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- Note that p is a convex combination of the mixture component densities.
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- Conversely, if x has a density of this form, then x has a mixture distribution.

Gaussian Mixture Model (GMM): Marginal Distribution

For example:

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

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Learning in Gaussian Mixture Models

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- Estimate the parameters:

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- Just do "inference" to get cluster assignments.

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

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

Review: Estimating a Gaussian Distribution

- Recall that the density for $x \sim \mathcal{N}(\mu, \Sigma)$ is

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$$\sum_{i=1}^{n} \log p(x_i \mid \mu, \Sigma) = -\frac{n}{2}\log|2\pi\Sigma| - \frac{1}{2}\sum_{i=1}^{n}(x_i-\mu)^T \Sigma^{-1}(x_i-\mu)$$

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- We get a closed form solution:

$$\begin{aligned} \hat{\mu}_{\text{MLE}} &= \frac{1}{n} \sum_{i=1}^{n} x_i \\ \hat{\Sigma}_{\text{MLE}} &= \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mu}_{\text{MLE}})^T (x_i - \hat{\mu}_{\text{MLE}}) \end{aligned}$$

Properties of the GMM Log-Likelihood

- GMM log-likelihood:

$$J(\pi, \mu, \Sigma) = \sum_{i=1}^{n} \log \left\{ \sum_{z=1}^{k} \frac{\pi_z}{\sqrt{|2\pi\Sigma_z|}} \exp\left(-\frac{1}{2}(x-\mu_z)^T \Sigma_z^{-1}(x-\mu_z) \right) \right\}$$

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- 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

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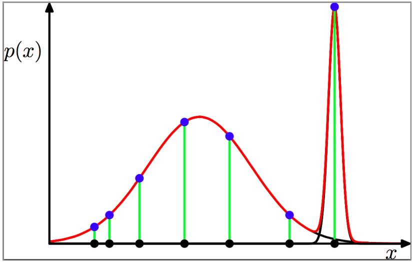
- We'll get the same likelihood. How many such equivalent settings are there?
- Assuming all clusters are distinct, there are $k!$ equivalent solutions.
- Not a problem *per se*, but something to be aware of.

Singularities for GMM

- Consider the following GMM for 7 data points:



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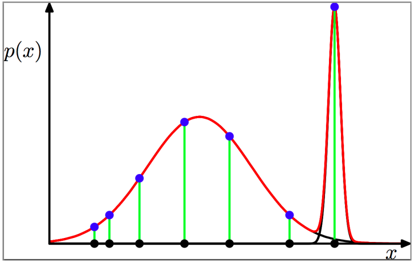

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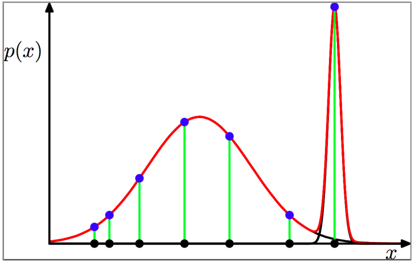

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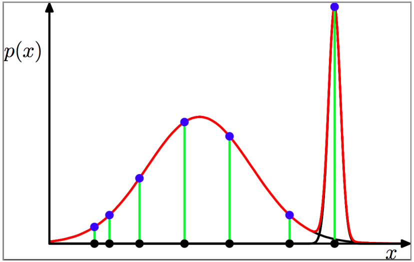
- What happens to the likelihood as $\sigma^2 \to 0$?
- In practice, we end up in local minima that do not have this problem.
  - Or keep restarting optimization until we do.

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

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

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

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- Even then, pure gradient-based methods have trouble.[1]

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The EM Algorithm for GMM

MLE for Gaussian Model

- Let's start by considering the MLE for the Gaussian model.
- For data $\mathcal{D} = \{x_1, \ldots, x_n\}$, the log likelihood is given by

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

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- For GMM, If we knew the cluster assignment z_i for each x_i,
  - we could compute the MLEs for each cluster.

Estimating a Fully-Observed GMM

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

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- The vector $\left(\gamma_i^1, \dots, \gamma_i^k\right)$ 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.

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- Repeatedly alternate these two steps.

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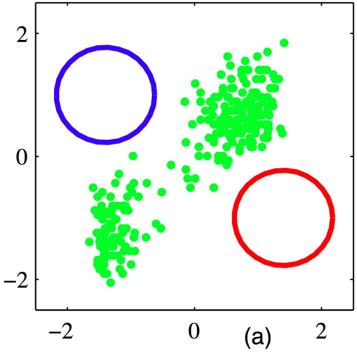
4. Repeat from Step 2, until log-likelihood converges.

EM for GMM

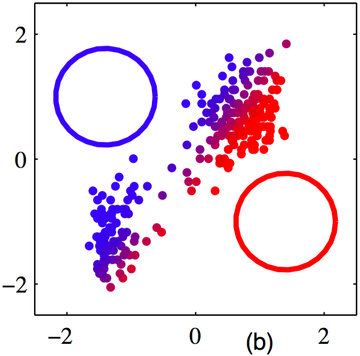
- Initialization



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

EM for GMM

- First soft assignment:



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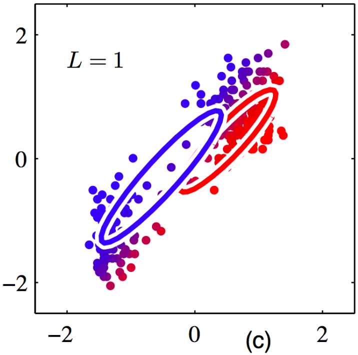

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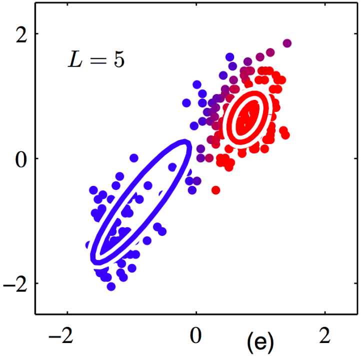
EM for GMM

- After 5 rounds of EM:



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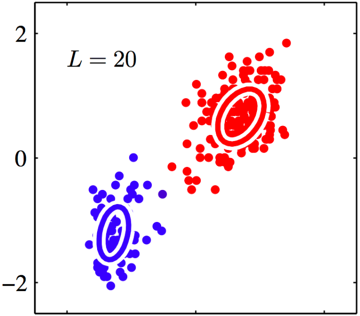
EM for GMM

- After 20 rounds of EM:



(f)

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- 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.