732A99/TDDE01 Machine Learning

Lecture 1b Block 2: Mixture Models

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Contents

Literature

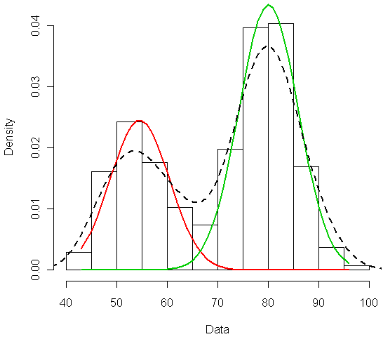
- Main source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Sections 2.3.9, 9.1-9.3.3 and 14.5.3.
- Additional source
  - Hastie, T., Tibshirani, R. and Friedman, J. *The Elements of Statistical Learning*. Springer, 2009. Section 8.5.

Mixture Models

- Sometimes the data do not follow any known probability distribution but a mixture of known distributions such as

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} p(k)p(\boldsymbol{x}|k)$$

where $p(\boldsymbol{x}|k)$ are called mixture components and $p(k)$ are called mixing coefficients, which are usually denoted by π_k and $0 \leq \pi_k \leq 1$ and $\sum_k \pi_k = 1$.



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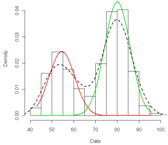

- We can also see a mixture model as an ensemble model of a population with subpopulations:
  1. Choose a subpopulation according to $Multinomial(k|\pi_1, \ldots, \pi_K)$.
  2. Sample an instance from the chosen subpopulation according to $p(\boldsymbol{x}|k)$.

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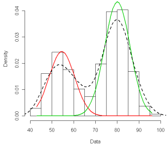

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- Mixture of multivariate Gaussian distributions:

$$p(\boldsymbol{x}) = \sum_k \pi_k \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \text{ and } \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \frac{1}{2\pi^{D/2}} \frac{1}{|\boldsymbol{\Sigma}_k|^{1/2}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1} (\boldsymbol{x}-\boldsymbol{\mu}_k)}$$

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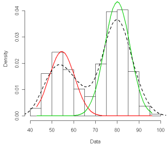

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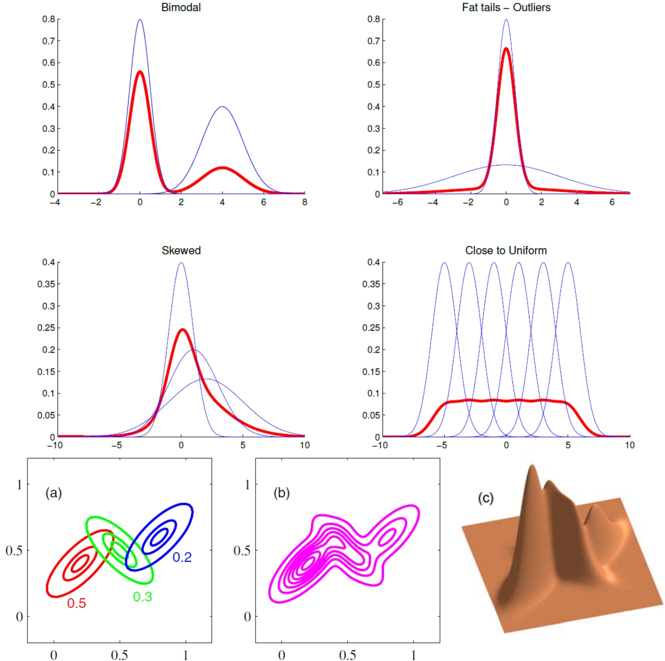
- Note that a mixture model defines a proper probability distribution:
$$0 \leq p(\boldsymbol{x}) \leq 1 \text{ and } \int p(\boldsymbol{x}) d\boldsymbol{x} = 1$$

Mixture Models



Mixture Models

- Mixture of multivariate Bernoulli distributions:

$$p(\boldsymbol{x}) = \sum_k \pi_k Bernoulli(\boldsymbol{x}|\boldsymbol{\mu}_k)$$

where we assume that

$$Bernoulli(\boldsymbol{x}|\boldsymbol{\mu}_k) = \prod_i Bernoulli(x_i|\mu_{ki}) = \prod_i \mu_{ki}^{x_i}(1-\mu_{ki})^{(1-x_i)}$$

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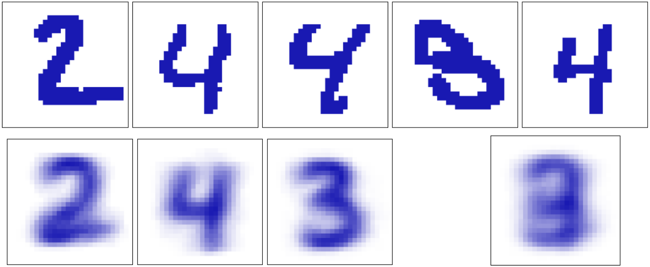

Figure 9.10 Illustration of the Bernoulli mixture model in which the top row shows examples from the digits data set after converting the pixel values from grey scale to binary using a threshold of 0.5. On the bottom row the first three images show the parameters μ_{ki} for each of the three components in the mixture model. As a comparison, we also fit the same data set using a single multivariate Bernoulli distribution, again using maximum likelihood. This amounts to simply averaging the counts in each pixel and is shown by the right-most image on the bottom row.

Maximum Likelihood

- Given a sample $\{\boldsymbol{x}_n, k_n\}$ of size N from a mixture of multivariate Bernoulli distributions, rewrite it as $\{\boldsymbol{x}_n, \boldsymbol{z}_n\}$ where $\boldsymbol{z}_n$ is a K-dimensional binary vector having only the k_n-th element equal to 1.

[1] Any stationary point of the Lagrangian function is a stationary point of the original function subject to the constraints. Unfortunately, the log likelihood function is typically not concave.

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- Let $x'_{ni} = 1 - x_{ni}$ and $\mu'_{ki} = 1 - \mu_{ki}$. To maximize the log likelihood function subject to the constraints $\sum_k \pi_k = 1$ and $\mu_{ki} + \mu'_{ki} = 1$, we maximize

$$\sum_n \sum_k z_{nk} [\log \pi_k + \sum_i [x_{ni} \log \mu_{ki} + x'_{ni} \log \mu'_{ki}]] + \lambda(\sum_k \pi_k - 1) + \sum_k \sum_i \lambda_{ki} (\mu_{ki} + \mu'_{ki} - 1)$$

where λ and λ_{ki} are called Lagrange multipliers.[1]

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- Setting to zero the derivatives with respect to π_k, μ_{ki} and μ'_{ki} gives

$$\pi_k = -\sum_n z_{nk}/\lambda \text{ and } \mu_{ki} = -\sum_n z_{nk} x_{ni}/\lambda_{ki} \text{ and } \mu'_{ki} = -\sum_n z_{nk} x'_{ni}/\lambda_{ki}$$

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- Replacing this into the constraint gives $\lambda = -N$ and $\lambda_{ki} = -\sum_n z_{nk}$ and, thus,

$$\pi_k^{ML} = \frac{\sum_n z_{nk}}{N} \text{ and } \mu_{ki}^{ML} = \frac{\sum_n z_{nk} x_{ni}}{\sum_n z_{nk}}$$

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- Given a sample $\{\boldsymbol{x}_n\}$ of size N from a mixture of multivariate Bernoulli distributions, the expected log likelihood function is

$$\mathbb{E}_{\boldsymbol{Z}}[\log p(\{\boldsymbol{x}_n, \boldsymbol{z}_n\}|\boldsymbol{\mu}, \boldsymbol{\pi})] = \sum_n \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi}) \log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\mu}, \boldsymbol{\pi})$$

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- Following a reasoning analogous to the complete-data case, we obtain that

$$\begin{aligned} \pi_k^{ML} &= \frac{\sum_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}{N} \\ \mu_{ki}^{ML} &= \frac{\sum_n x_{ni} p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}{\sum_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})} \end{aligned}$$

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- This is not a closed form solution because

$$p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi}) = \frac{p(z_{nk}, \boldsymbol{x}_n|\boldsymbol{\mu}, \boldsymbol{\pi})}{\sum_k p(z_{nk}, \boldsymbol{x}_n|\boldsymbol{\mu}, \boldsymbol{\pi})} = \frac{\pi_k p(\boldsymbol{x}_n|\boldsymbol{\mu}_k)}{\sum_k \pi_k p(\boldsymbol{x}_n|\boldsymbol{\mu}_k)}$$

but it suggests the following algorithm.

Expectation Maximization Algorithm

EM algorithm

Set $\boldsymbol{\pi}$ and $\boldsymbol{\mu}$ to some initial values
Repeat until $\boldsymbol{\pi}$ and $\boldsymbol{\mu}$ do not change
    Compute $p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})$ for all k and n /* E step */
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- The EM algorithm can also be obtained by maximizing $\log p(\{\boldsymbol{x}_n\}|\boldsymbol{\mu}, \boldsymbol{\pi})$.
- The EM algorithm is guaranteed to increase $\log p(\{\boldsymbol{x}_n\}|\boldsymbol{\mu}, \boldsymbol{\pi})$ in each iteration until a local maximum is reached. So, the algorithm aims for the ML estimates.

Expectation Maximization Algorithm

- We can derive the EM algorithm for mixtures of multivariate Gaussian distributions in much the same way. Simply,

$$
\begin{aligned}
\pi_k^{ML} &= \frac{\sum_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}{N} \\
\boldsymbol{\mu}_k^{ML} &= \frac{\sum_n \boldsymbol{x}_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}{\sum_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})} \\
\boldsymbol{\Sigma}_k^{ML} &= \frac{\sum_n (\boldsymbol{x}_n - \boldsymbol{\mu}_k^{ML})(\boldsymbol{x}_n - \boldsymbol{\mu}_k^{ML})^T p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}{\sum_n p(z_{nk}|\boldsymbol{x}_n, \boldsymbol{\mu}, \boldsymbol{\pi})}
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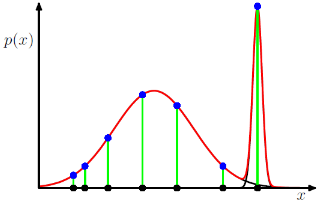
\end{aligned}$$

- Unlike in the case of mixture of multivariate Bernoulli distributions, there can be singularities, i.e. the log likelihood function goes to infinity when a component of the mixture collapses onto a single data point.

Figure 9.7 Illustration of how singularities in the likelihood function arise with mixtures of Gaussians. This should be compared with the case of a single Gaussian shown in Figure 1.14 for which no singularities arise.



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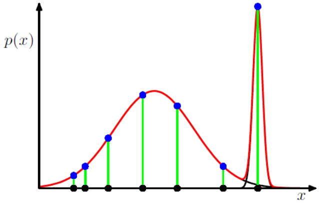
- Unlike in the case of mixture of multivariate Bernoulli distributions, there can be singularities, i.e. the log likelihood function goes to infinity when a component of the mixture collapses onto a single data point.

Figure 9.7 Illustration of how singularities in the likelihood function arise with mixtures of Gaussians. This should be compared with the case of a single Gaussian shown in Figure 1.14 for which no singularities arise.



- Solution: Reset the mean and covariance of the component to random and large values, respectively. Or adopt a Bayesian approach.

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- Nested cross-validations is also an option.

Model-Based Clustering

- A mixture model represents a mixture of subpopulations, a.k.a. clusters:
  1. Choose a subpopulation according to $\mathit{Multinomial}(k|\pi_1, \ldots, \pi_K)$.
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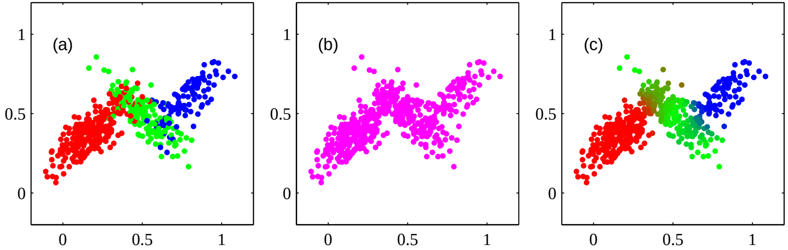
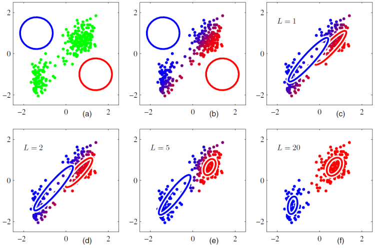


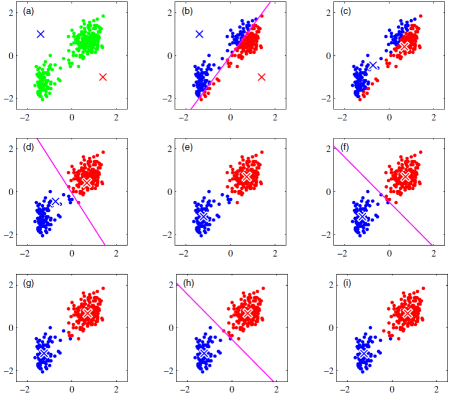
(a) Sample with cluster labels, (b) initial clustering, and (c) final clustering.

K-Means Algorithm

```
Assign each point to a cluster (a.k.a subpopulation) at random
Compute the cluster centroids as the averages of the points assigned to each cluster
Repeat until the centroids do not change
    Assign each point to the cluster with the closest centroid
    Update the cluster centroids as the averages of the points assigned to each cluster
```



EM algorithm



K-means algorithm

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- Recall that

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