Machine Learning

Lecture 20: Gaussian Mixture Models

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Context

1. Often times we need to analyse data for which we do not have their labels.
2. How can we find any structure in a collection of unlabelled data?
3. Clustering is an established category of methods for organising objects into groups whose members are similar in some way.

Context: K-means Solution

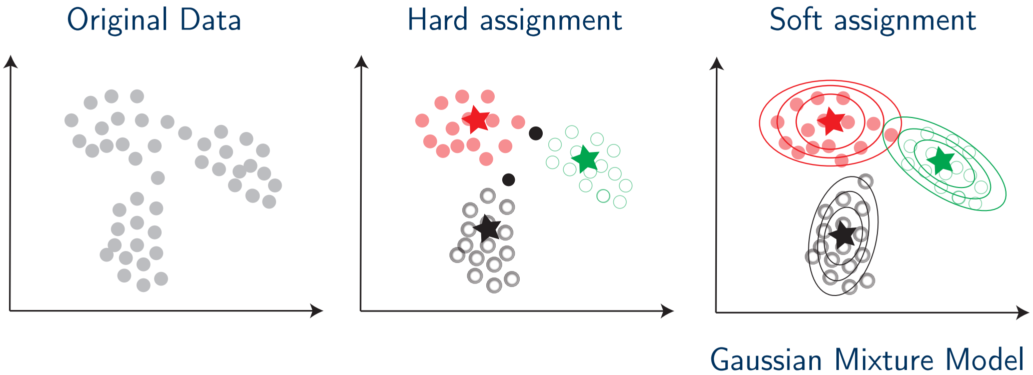
$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}$$

Context: K-means discussion

1. Too crude? Assumes that a cluster can be represented with a single point and a simple distance metric
2. A simple unsupervised method that enables clustering of data with no great computational complexity
3. Hard boundaries!
4. Q: How to generalise it to models that can cluster data of various types and shapes!

Context: Hard assignment vs. Soft assignment



Original Data

Hard assignment

Soft assignment

Gaussian Mixture Model

Learning Outcomes

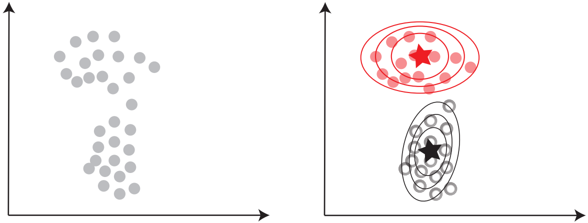
1. Understand the key motivations behind a Guassian Mixture Model (GMM).
2. Understand the formulation of a GMM and the need for the Expectation Maximisation (EM) solver.
3. Analyse the solution to a GMM.

References:

1. Bishop, *Pattern Recognition and Machine Learning*, Springer, 2008. (Section 9.1)
2. Rogers and Girolami, *A First Course in Machine Learning*, CRC Press, 2016. (Section 6.3)

Mixture Models

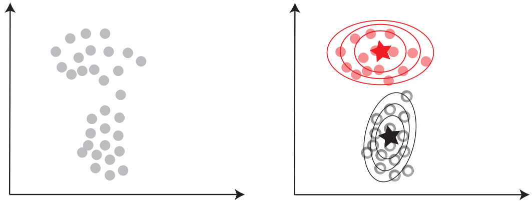
1. Models that can cluster data of various types and shapes!
2. Simple to compute
3. Clustering with statistical mixture models, similar to k-means, but offers richer representation of the data!



Mixture Models - A generative process

1. Let's assume we want to generate the below data with two Gaussians!
2. For data $\mathbf{x}_n$, Select one of the Gaussians (with probability π_k, assuming $\sum_k \pi_k = 1$). Set the parameter $z_{nk} = 1$
3. Sample data $\mathbf{x}_n$ from this Gaussian

$$p(\mathbf{x}_n | z_{nk} = 1, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



Mixture Models - A generative process

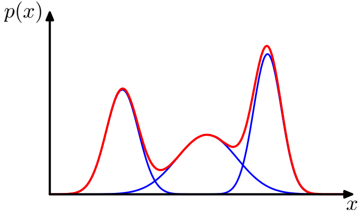
1. We described out data with a generative process
2. In a clustering context all data points with $z_{nk} = 1$ are in cluster k
3. But we need to learn/infer/calculate $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ from the observed data

BUT this is a circular argument

1. Trivial to calculate the component parameters $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
   if we knew the assignment rule $z_{nk} = 1$
2. Trivial to work out the assignment rule $z_{nk} = 1$
   if we knew the component parameters $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

Mixture of Gaussians

Complex probabilities can be approximated with a linear superposition of K Gaussian densities.

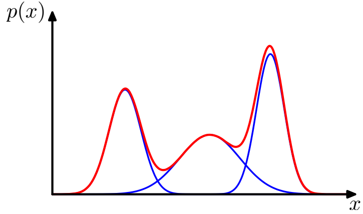


$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

We define $\mathbf{z} = \{z_1, z_2, \cdots, z_k\}$ where $z_k \in \{0, 1\}$ and $\sum_k z_k = 1$.

We know that $p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$ and $p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$.

Mixture of Gaussians



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- $p(z_k = 1) = \pi_k$: $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1$.
- $p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}$
- $p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$

Mixture of Gaussians

Another key quantity is $p(\mathbf{z}|\mathbf{x})$

$$\begin{aligned}\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) &= \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}\end{aligned}$$

$\gamma(z_k)$ is the *responsibility* that component k takes in explaining the observation $\mathbf{x}$.

A Maximum Likelihood solution to GMM? Not ideal!

Suppose we observe $\mathbf{X}_{N\times D} = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\}$. Assuming that the data points are drawn independently, the likelihood function of all N data points is

$$p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

and so the log-likelihood will be

$$L = \log p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

We can estimate $\pi_k, \boldsymbol{\mu}_k$, and $\boldsymbol{\Sigma}_k$ by differentiating L with respect to these variables and using gradient-based optimisation.

Expectation-Maximisation (EM) for GMMs

- The EM method can be used to overcome challenges of using Maximum Likelihood.
- EM derives a *lower bound* $\mathcal{B}$ on the likelihood L, that is $\mathcal{B} \leq L$.
- Instead of maximising L directly, EM maximises $\mathcal{B}$

- Question: How to determine $\mathcal{B}$? Using Jensen's inequality

$$\log \mathbf{E}_{p(z)}\{f(z)\} \geq \mathbf{E}_{p(z)}\{\log f(z)\}$$

- The logarithm of the expected value of $f(z)$ is always greater than or equal to the expected value of $\log f(z)$

EM - Derivation for GMMs

- Let's define γ_{nk} to be positive and satisfying $\sum_{k=1}^{K} \gamma_{nk} = 1$.
- γ_{nk} is some probability distribution over K components for the n-th data point.

$$\begin{aligned}
L &= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \\
&= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \frac{\gamma_{nk}}{\gamma_{nk}} \\
&= \sum_{n=1}^{N} \log \sum_{k=1}^{K} \gamma_{nk} \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \\
&= \sum_{n=1}^{N} \log \mathbf{E}_{\gamma_{nk}} \left\{ \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \right\}
\end{aligned}$$

Apply Jensen's inequality

$$\log \mathbf{E}_{p(z)}\{f(z)\} \geq \mathbf{E}_{p(z)}\{\log f(z)\}$$

$$\begin{aligned} L &= \sum_{n=1}^{N} \log \mathbf{E}_{\gamma_{nk}} \left\{ \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \right\} \\ &\geq \sum_{n=1}^{N} \mathbf{E}_{\gamma_{nk}} \left\{ \log \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \right\} = \mathcal{B} \end{aligned}$$

Apply Jensen's inequality

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$$\begin{aligned} L &= \sum_{n=1}^{N} \log \mathbf{E}_{\gamma_{nk}} \left\{ \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \right\} \\ &\geq \sum_{n=1}^{N} \mathbf{E}_{\gamma_{nk}} \left\{ \log \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\gamma_{nk}} \right\} = \mathcal{B} \end{aligned}$$

$$\mathcal{B} = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \log \pi_k + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \log \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) - \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \log \gamma_{nk}.$$

EM - Derivation for GMMs

$$\mathcal{B} = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma_{nk}\log\pi_k + \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma_{nk}\log\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) - \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma_{nk}\log\gamma_{nk}.$$

- EM is an iterative process, maximising the bound $\mathcal{B}$, until convergence.
- For each update, we take the partial derivative of the bound $\mathcal{B}$ wrt parameters, set it to zero and solve.
- See Rogers and Girolami (2016) [pp.218-222] for full derivations

EM Solution for GMMs

E-step

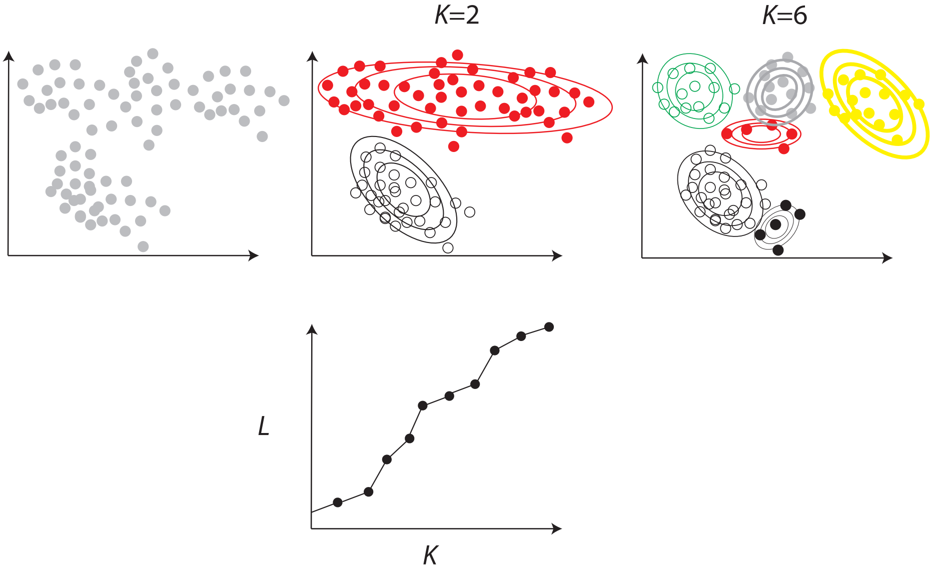
$$\gamma_{nk} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

M-step

$$\begin{aligned} \pi_k &= \frac{1}{N} \sum_{n=1}^{N} \gamma_{nk} \\ \boldsymbol{\mu}_k &= \frac{\sum_{n=1}^{N} \gamma_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} \gamma_{nk}} \\ \boldsymbol{\Sigma}_k &= \frac{\sum_{n=1}^{N} \gamma_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T}{\sum_{n=1}^{N} \gamma_{nk}} \end{aligned}$$

Some intution ...

Choosing the Number of components K for GMMs



GMM: Summary

- Hard boundaries are exchanged for flexible and probabilistic soft boundaries
- Immense flexibility: $p(\mathbf{x}_n|\cdots)$ can take the form of any probability density including Bernoulli distribution (binary data)
- The choice of K remains ad-hoc

Next lecture:

- Delving [a bit] deeper into the EM method