Mixture of Gaussians Clustering

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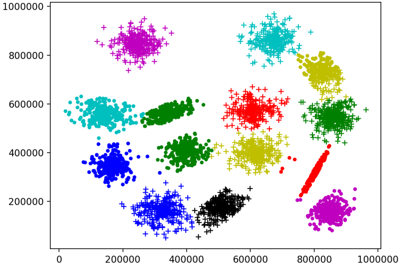
Unsupervised Learning



- Data is unlabeled (no “ground truth”).
- Problems: clustering, density estimation, and pattern detection.

Clustering

- Most common unsupervised problem is clustering.
- Can we separate the data into different clusters, each with a given (but not necessarily the same class) distribution?
- We can then analyze the underlying properties of each cluster.

Hard vs. Soft Clustering

- Hard clustering: assign each point to a cluster.
- Soft clustering: assign a probability γ_{ik} that each point x_i belongs to the k^{th} cluster.

Density Estimation

- Can we determine the underlying probability distribution(s) on unlabeled data?

Example

- Crime is happening on the streets of Gotham City!
- There are $n = 2$ criminals: Bane and the Joker. Suppose every night, one of the two decides to commit a series of crimes.
- Bane succeeds 50% of the time, and the Joker 70% (the Joker is more skilled). That is, $P(success) = 0.5$ for Bane and $P(success) = 0.7$ for the Joker on each attempt.
- Neither criminal is identified nor caught during each attempt.
- Over a series of $m = 100$ nights, $j = 10$ crimes are attempted by one of the two criminals.

Example

- Suppose we know there are $n = 2$ criminals, and the number of crimes (from $j = 10$ attempts) succeeded during each of $m = 100$ nights.
- However, we don't know which criminal committed the series of crimes each night, and $P(success)$ for each criminal.
- Can we recover a probability that a night's crimes were committed by a given criminal, and $P(success)$ for each criminal?
- Yes! Utilize the expectation-maximization (EM) algorithm.

EM Algorithm

- Powerful algorithm to estimate maximum likelihood for various model parameters, even with several missing data or unobserved latent variables.
- In our example, cluster assignments are the unobserved latent variables: on a given night, which criminal committed the series of crimes?
- Mixture of Gaussians clustering (GMM) is a soft clustering and density estimation algorithm that allows us to maximize likelihood (of the parameters of the cluster distributions) even with these latent variables.

EM Algorithm

- Randomly initialize the parameters θ of the n distributions (clusters).
- E-step: compute the probabilities γ_{ik} that each point x_i belongs to the k^{th} cluster:

$$\gamma_{ik} = P(z_i = k | x_i, \theta^{(t)}).$$

- M-step: maximize a lower bound on the likelihood of an estimate of the new parameters $\theta^{(t+1)}$.
- Repeat until convergence.

Mixture of Gaussians

- Specific case of EM-algorithm: assumes each cluster is normally distributed with mean μ and variance Σ.
- E-step: compute $\gamma_{ik}^{(t+1)} = \frac{P(X_i=x_i|z_i=k,\theta^{(t)})P(z_i=k|\theta^{(t)})}{P(X_i=x_i|\theta^{(t)})}$.
- M-step: update w_k, μ_k, and Σ_k:

$$w_k^{(t+1)} = \frac{\sum_i \gamma_{ik}^{(t+1)}}{n}, \mu_k^{(t+1)} = \frac{\sum_i x_i \gamma_{ik}^{(t+1)}}{\sum_i \gamma_{ik}^{(t+1)}}, \text{ and}$$

$$\Sigma_k^{(t+1)} = \frac{\sum_i \gamma_{ik}^{(t+1)}(x_i - \mu_k^{(t+1)})(x_i - \mu_k^{(t+1)})^T}{\sum_i \gamma_{ik}^{(t+1)}}.$$

Mixture of Gaussians

- Understanding the derivations of the formulas is beyond the scope of this class.
- Instead, understand the interpretation of the EM algorithm, with GMM as a specific case, and when it can be utilized.
- We can also apply it to our example.

Example

- Let's return to our example: $n = 2$ criminals, and $j = 10$ attempted crimes from $m = 100$ nights.
- We don't know which criminal committed the series of crimes each night, and $P(success)$ for each criminal.
- Today's notebook contains a snippet of code to generate this data. Let's assume it is normally distributed.

Example

- We can implement a mixture of Gaussians model. Let's do that using the notebook.
- Observe γ_{ik}, w_k, μ_k over the k criminals. What is the interpretation of each of these values?

Interpretation

- γ_{ik}: probability criminal k committed a crime on night i.
- w_k: proportion of nights criminal k commits a crime.
- μ_k: average number of successful crimes per night for criminal k.

Applications

- But we still don't have labels on the clusters! We don't know whether it was Bane or the Joker who is criminal k.
- In general, this is a problem for unlabeled data. What (or who) do the clusters represent?
- We can correlate the parameters of each cluster (distribution). Say the data also included the locations (in coordinates) where the crime was committed, and the hour at which it was committed.
- Questions we can ask: at what hour does criminal k commit a crime, and where?

Applications

- Say over a few of the j nights, a witness comes out to identify the criminal who performed the crime on that night.
- We can then assign a probability that Bane and the Joker are criminal k, and probabilities that they committed crimes over each of the j nights.
- Predictions of assigning Bane or the Joker to criminal k get stronger the more identifications (labels) we have. But the more labeled data we have, the less the need for the EM algorithm.

Limitations

- Assumes clusters arise from the same distribution (in the mixture of Gaussians case, from the normal distribution).
- Can be extremely slow: works well for low-dimensional data.