Machine Learning

4771

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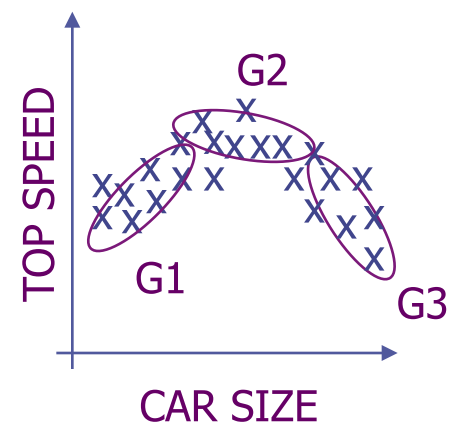
Topic 12

- Mixture Models and Hidden Variables
- Clustering
- K-Means
- Expectation Maximization

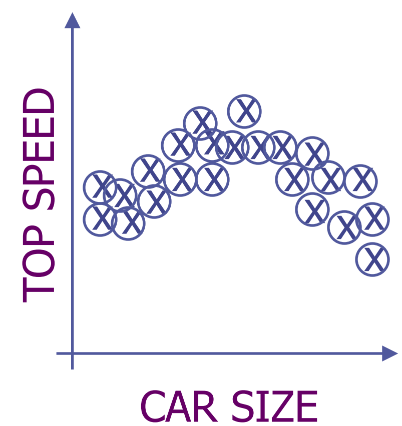
Mixtures for More Flexibility

- With mixtures (e.g. mixtures of Gaussians) we can handle more complicated (e.g. multi-bump, nonlinear) distributions.



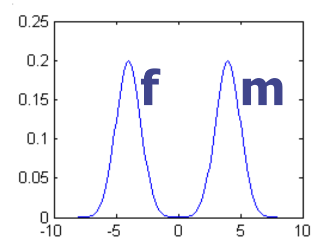
subpopulations: G1=compact car
G2=mid-size car
G3=cadillac

- In fact, if we have enough Gaussians (maybe infinite) we can approximate any distribution...

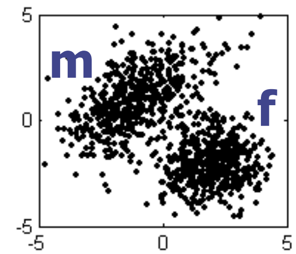


Mixtures as Hidden Variables

- Consider a dataset with K subpopulations but don't know which subpopulation each point belongs to



I.e. looking at height of adult people, we see K=2 subpopulations: males & females



I.e. looking at weight and height of people we see K=2 subpopulations: males & females

- Because of the 'hidden' variable (y can be 1 or 2), these distributions are not Gaussians but Mixture of Gaussians

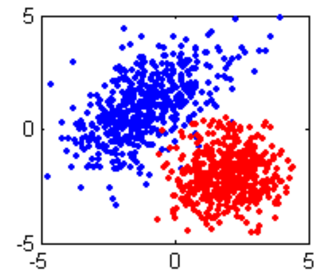
$$p\left(\vec{x}\right) = \sum_y p(\vec{x}, y) = \sum_y p\left(y\right) p\left(\vec{x} \mid y\right) = \sum_y \pi_y N\left(\vec{x} \mid \vec{\mu}_y, \Sigma_y\right)$$

$$= \sum_{y=1}^{K} \pi_y \frac{1}{\left(2\pi\right)^{D/2} \sqrt{\left|\Sigma_y\right|}} \exp\left(-\frac{1}{2}\left(\vec{x} - \vec{\mu}_y\right)^T \Sigma_y^{-1} \left(\vec{x} - \vec{\mu}_y\right)\right)$$

Hidden / Unlabeled = Clustering

- Recall classification problem:

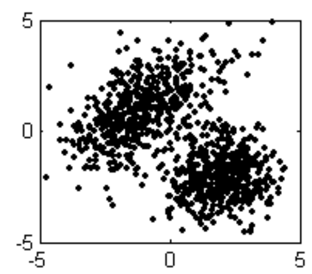
  maximize the log-likelihood of data given models:



$$l = \sum_{n=1}^{N} \log p\left(\vec{x}_n, y_n \mid \pi, \mu, \Sigma\right)$$
$$= \sum_{n=1}^{N} \log \pi_{y_n} N\left(\vec{x}_n \mid \vec{\mu}_{y_n}, \Sigma_{y_n}\right)$$

- If we don't know the class treat it as a hidden variable

  maximize the log-likelihood with unlabeled data:

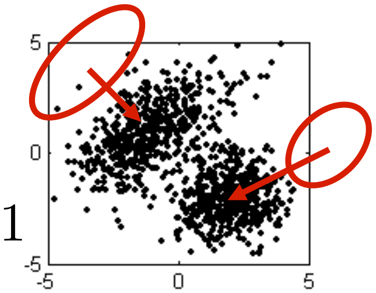


$$l = \sum_{n=1}^{N} \log p\left(\vec{x}_n \mid \pi, \mu, \Sigma\right) = \sum_{n=1}^{N} \log \sum_{y=1}^{K} p\left(\vec{x}_n, y \mid \pi, \mu, \Sigma\right)$$
$$= \sum_{n=1}^{N} \log\left(\pi_1 N\left(\vec{x}_n \mid \vec{\mu}_1, \Sigma_1\right) + \ldots + \pi_K N\left(\vec{x}_n \mid \vec{\mu}_K, \Sigma_K\right)\right)$$

- Instead of classification, we now have a clustering problem

Hidden / Unlabeled = Clustering

- Represent each hidden y integer (1 to K) with a hidden binary indicator vector z



$$\vec{z} \in \mathbb{B}^K, \sum_{i=1}^K \vec{z}(i) = 1 \quad or \ \vec{z} \in \left\{\vec{\delta}_1, \ldots, \vec{\delta}_K\right\} \ where \ \vec{\delta}_i(i) = 1$$

- Each likelihood requires summing over the possible z

$$p(\vec{x} \mid \theta) = \sum_z p(\vec{z} \mid \theta) p(\vec{x} \mid \vec{z}, \theta) = \sum_{i=1}^K p(\vec{z} = \vec{\delta}_i \mid \pi) p(\vec{x} \mid \vec{z} = \vec{\delta}_i, \theta)$$

mixing proportions (prior) = $\pi_i = p(\vec{z} = \vec{\delta}_i \mid \theta)$

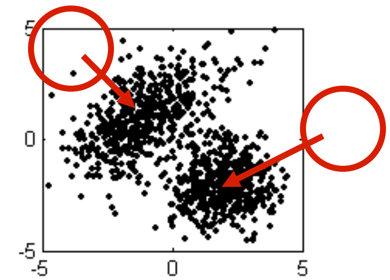
mixture components = $p(\vec{x} \mid \vec{z} = \vec{\delta}_i, \theta)$

posteriors (responsibilities) = $\tau_{n,i} = p(\vec{z} = \vec{\delta}_i \mid \vec{x}_n, \theta) = \frac{p(\vec{x}_n \mid \vec{z} = \vec{\delta}_i, \theta) p(\vec{z} = \vec{\delta}_i \mid \theta)}{p(\vec{x}_n \mid \theta)}$

log likelihood = $\sum_{n=1}^N \log p(\vec{x}_n \mid \alpha, \mu, \Sigma) = \sum_{n=1}^N \log \sum_{i=1}^K \pi_i N(\vec{x}_n \mid \vec{\mu}_i, \Sigma_i)$

- Can't easily take derivatives of log-likelihood and set to 0.
- Not nice, seems to need gradient ascent…
- Or, can we break up mixture into smaller Gaussian steps?

K-Means Clustering



- An old "heuristic" clustering algorithm
- Gobble up data with a divide & conquer scheme
- Assume each point x has an discrete multinomial vector z
- Chicken and Egg problem:

  If know classes, we can get model (max likelihood!)

  If know the model, we can predict the classes (classifier!)

- K-means Algorithm:

0) Input dataset $\left\{\vec{x}_1,\ldots,\vec{x}_N\right\}$

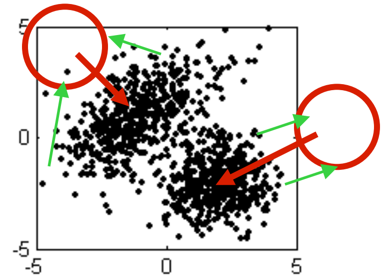
1) Randomly initialize means $\vec{\mu}_1,\ldots,\vec{\mu}_K$

2) Find closest mean for each point $\vec{z}_n(i) = \begin{cases} 1 & \textit{if } i = \arg\min_j \left\|\vec{x}_n - \vec{\mu}_j\right\|^2 \\ 0 & \textit{otherwise} \end{cases}$

3) Update means $\vec{\mu}_i = \sum_{n=1}^N \vec{x}_n \vec{z}_n(i) \Big/ \sum_{n=1}^N \vec{z}_n(i)$

4) If any z has changed go to 2

K-Means Clustering

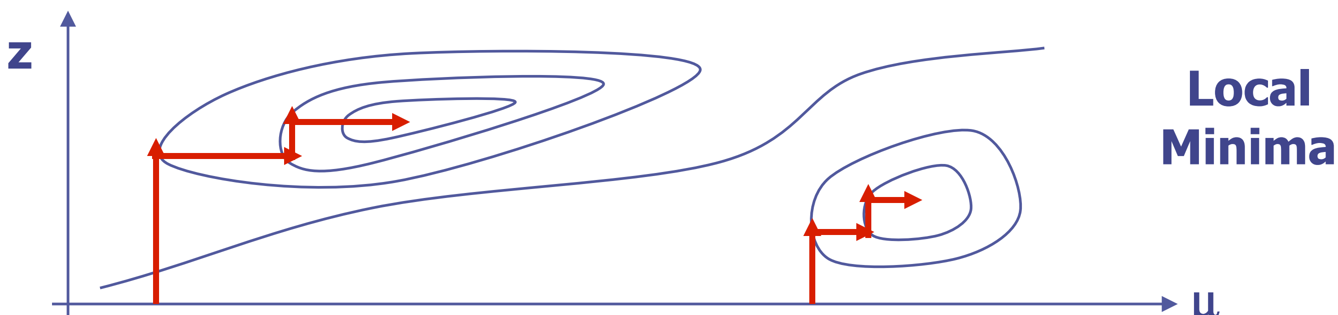


- Geometric, each point goes to closest Gaussian
- Recompute the means by their assigned points
- Essentially minimizing the following cost function:

$$\min_{\mu} \min_{z} J\left(\vec{\mu}_1,\ldots,\vec{\mu}_K,\vec{z}_1,\ldots,\vec{z}_N\right) = \sum_{n=1}^{N}\sum_{i=1}^{K} \vec{z}_n\left(i\right)\left\|\vec{x}_n - \vec{\mu}_i\right\|^2$$

$$\vec{z}_n\left(i\right) = \begin{cases} 1 & if\ i = \arg\min_j \left\|\vec{x}_n - \vec{\mu}_j\right\|^2 \\ 0 & otherwise \end{cases} \qquad \vec{\mu}_i = \frac{\sum_{n=1}^{N} \vec{x}_n \vec{z}_n\left(i\right)}{\sum_{n=1}^{N} \vec{z}_n\left(i\right)}$$

- Guaranteed to improve per iteration and converge
- Like Coordinate Descent (lock one var, maximize the other)
- A.k.a. Axis-Parallel Optimization or Alternating Minimization



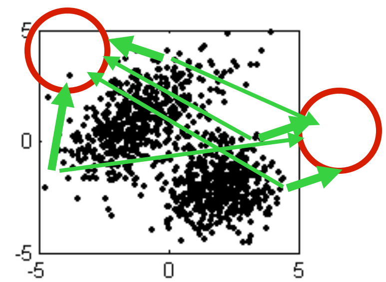
Expectation-Maximization (EM)

- EM is a soft/fuzzy version of K-Means (which does winner-takes-all, closest Gaussian Mean completely wins datapoint)

$$\vec{z}_n(i) = \begin{cases} 1 & if\ i = \arg\min_j \left\| \vec{x}_n - \vec{\mu}_j \right\|^2 = \arg\max_j N\left(\vec{x}_n \mid \vec{\mu}_j, I\right) = \arg\max_j p\left(\vec{x}_n \mid \vec{\mu}_j\right) \\ 0 & otherwise \end{cases}$$

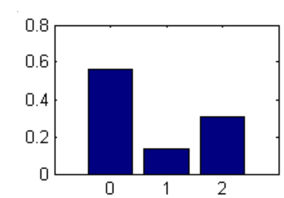
- Instead, consider soft percentage assignment of datapoint

$$assign \propto \pi_j \frac{1}{(2\pi)^{D/2}} \exp\left(-\frac{1}{2}\left\| \vec{x}_n - \vec{\mu}_j \right\|^2\right)$$



- EM is 'less greedy' than K-Means uses $\tau_{n,i} = p\left(\vec{z} = \vec{\delta}_i \mid \vec{x}_n, \theta\right)$ as shared responsibility for $\vec{x}_n$

$$\tau_{n,1}, \ldots, \tau_{n,K} =$$



- Update for the means are then 'weighted' by responsibilities:

$$\mu_i = \frac{\sum_{n=1}^{N} \tau_{n,i} \vec{x}_n}{\sum_{n=1}^{N} \tau_{n,i}}$$

Expectation-Maximization

- EM uses expected value of $\vec{z}_n(i)$ rather than max

$$\tau_{n,i} = E\left\{\vec{z}_n(i) \mid \vec{x}_n\right\} = p\left(\vec{z}_n = \vec{\delta}_i \mid \vec{x}_n, \theta\right)$$

- EM updates covariances, mixing proportions AND means…
- The algorithm for Gaussian mixtures:

EXPECTATION:

$$\tau_{n,i}^{(t)} = \frac{\pi_i N\left(\vec{x}_n \mid \vec{\mu}_i^{(t)}, \Sigma_i^{(t)}\right)}{\sum_j \pi_j N\left(\vec{x}_n \mid \vec{\mu}_j^{(t)}, \Sigma_j^{(t)}\right)}$$

MAXIMIZATION:

$$\vec{\mu}_i^{(t+1)} = \frac{\sum_n \tau_{n,i}^{(t)} \vec{x}_n}{\sum_n \tau_{n,i}^{(t)}} \qquad \pi_i^{(t+1)} = \frac{\sum_n \tau_{n,i}^{(t)}}{N}$$

$$\Sigma_i^{(t+1)} = \frac{\sum_n \tau_{n,i}^{(t)} \left(\vec{x}_n - \vec{\mu}_i^{(t+1)}\right)\left(\vec{x}_n - \vec{\mu}_i^{(t+1)}\right)^T}{\sum_n \tau_{n,i}^{(t)}}$$

- DEMO… like an iterative divide-and-conquer algorithm
- But, divide&conquer is not a guarantee. Can we prove EM?