Lecture 22. Gaussian Mixture Models.

COMP90051 Statistical Machine Learning

Semester 1, 2021
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This lecture

- Unsupervised learning
  - Diversity of problems
  - *k*-means refresher
- Gaussian mixture model (GMM)
  - A probabilistic approach to clustering
  - The GMM model
  - GMM clustering as an optimisation problem
- Starting Expectation-Maximisation (EM) algorithm

Unsupervised Learning

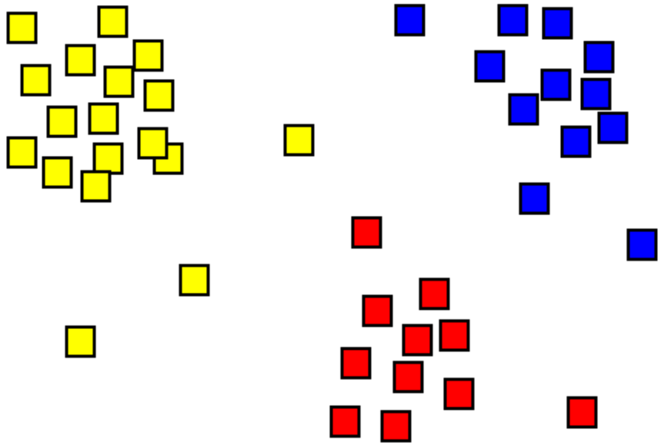
A large branch of ML that concerns with learning the structure of the data in the absence of labels

Main learning paradigms so far

- Supervised learning: Overarching aim is making predictions from data
- We studied methods in the context of this aim: e.g. linear/logistic regression, DNN, SVM
- We had instances $\boldsymbol{x}_i \in \boldsymbol{R}^m, i = 1, \dots, n$ and corresponding labels y_i for model fitting, aiming to predict labels for new instances
- Can be viewed as a function approximation problem, but with a big caveat: ability to generalise is critical
- Bandits: a setting of partial supervision where subroutine in contextual bandits requires supervised learning

Now: Unsupervised learning

- In unsupervised learning, there is no dedicated variable called a "label"
- Instead, we just have a set of points $\boldsymbol{x}_i \in \boldsymbol{R}^m, i = 1, \dots, n$
- Aim of unsupervised learning is to explore the structure (patterns, regularities) of data



public domain

- The aim of "exploring the structure" is vague

Unsupervised learning tasks

- Diversity of tasks fall into unsupervised learning category
  * Clustering (now)
  * Dimensionality reduction (autoencoders)
  * Learning parameters of probabilistic models (before/now)
- Applications and related tasks are numerous :
  * Market basket analysis. E.g., use supermarket transaction logs to find items that are frequently purchased together
  * Outlier detection. E.g., find potentially fraudulent credit card transactions
  * Often unsupervised tasks in (supervised) ML pipelines

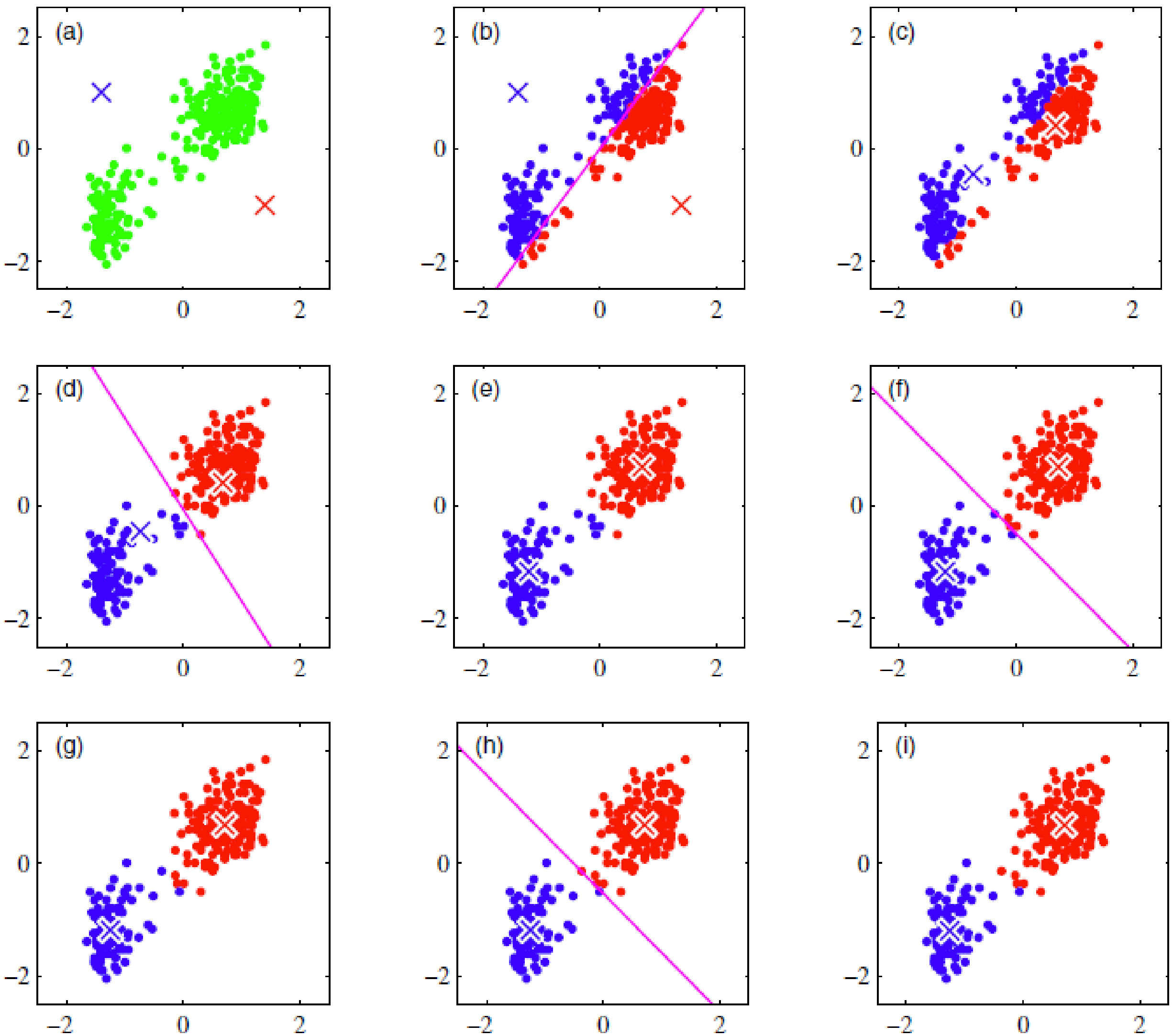
Refresher: *k*-means clustering

1. Initialisation: choose k cluster centroids randomly
2. Update:
   a) Assign points to the nearest* centroid
   b) Compute centroids under the current assignment
3. Termination: if no change then stop
4. Go to Step 2

*Distance represented by choice of metric typically L_2

Still one of the most popular data mining algorithms.

Refresher: *k*-means clustering



Requires specifying the number of clusters in advance

Measures "dissimilarity" using Euclidean distance

Finds "spherical" clusters

An iterative optimization procedure

Data: Old Faithful Geyser Data: waiting time between eruptions and the duration of eruptions

Figure: Bishop, Section 9.1

Mini Summary

- Unsupervised learning
  - Face value: drop labels from training. That’s it
  - Actually: catch-all for many many ML tasks, even as steps in supervised learning pipelines
- Refresher: *k*-means
  - Import next as we introduce GMMs

Next time: The Gaussian mixture model

Gaussian Mixture Model

A probabilistic view of clustering.
Simple example of a latent variable model.

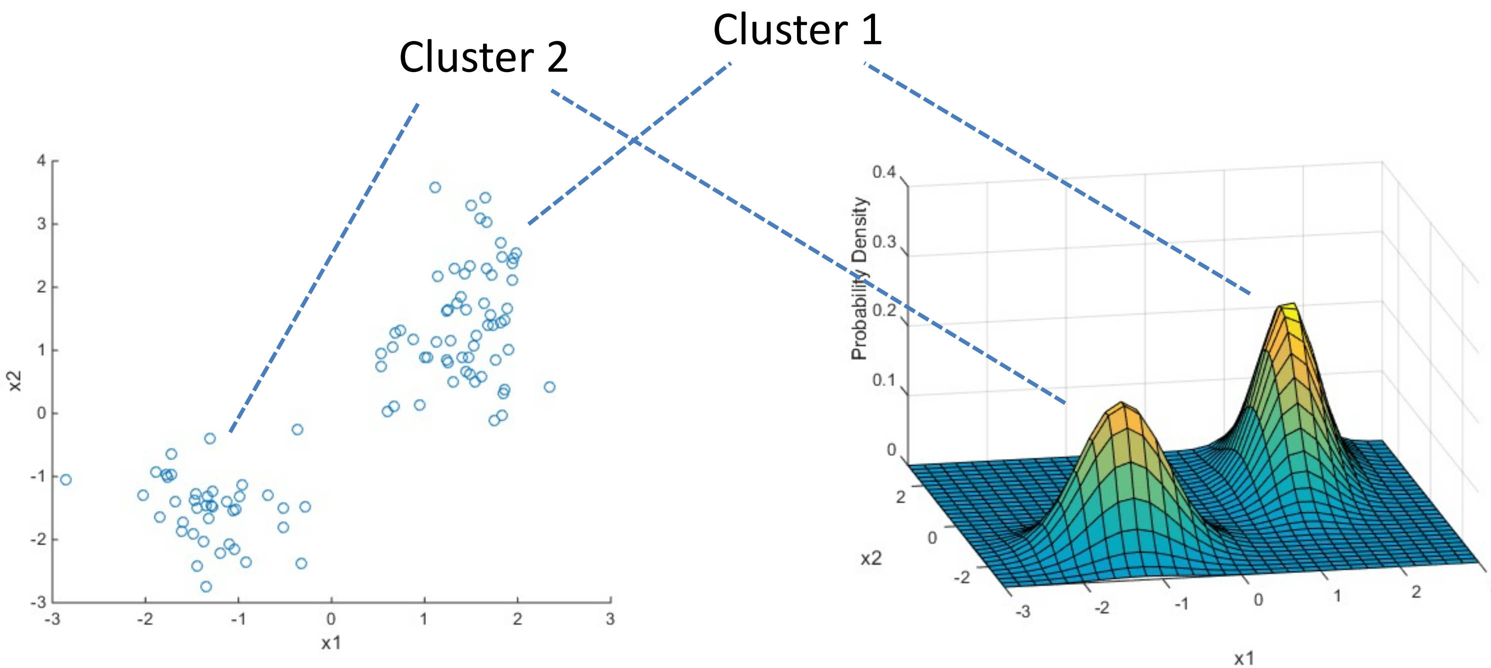
Modelling uncertainty in data clustering

- *k*-means clustering assigns each point to exactly one cluster
  - Does this make sense for points that are between two clusters?
  - Clustering is often not well defined to begin with!
- Like *k*-means, a probabilistic mixture model requires the user to choose the number of clusters in advance
- Unlike *k*-means, the probabilistic model gives us a power to express uncertainly about the origin of each point
  - Each point originates from cluster c with probability w_c, $c = 1, \ldots, k$
- That is, each point still originates from one particular cluster (aka component), but we are not sure from which one
- Next
  - Clustering becomes model fitting in probabilistic sense. Philosophically satisfying.
  - Individual components modelled as Gaussians
  - Fitting illustrates general Expectation Maximization (EM) algorithm

Clustering: probabilistic model

Data points $\boldsymbol{x}_i$ are independent and identically distributed (i.i.d.) samples from a mixture of K distributions (components)

Each component in the mixture is what we call a cluster



In principle, we can adopt any probability distribution for the components, however, the normal distribution is a common modelling choice → Gaussian Mixture Model

Normal (aka Gaussian) distribution

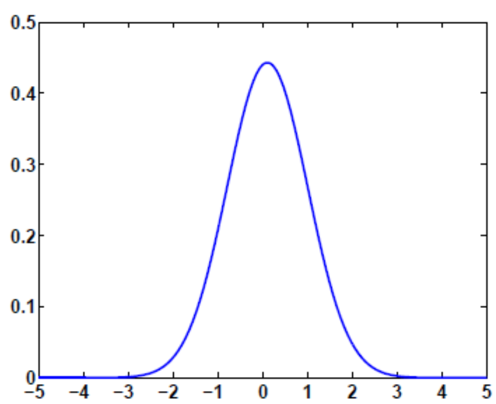
- Recall that a 1D Gaussian is

$$\mathcal{N}(x|\mu,\sigma) \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

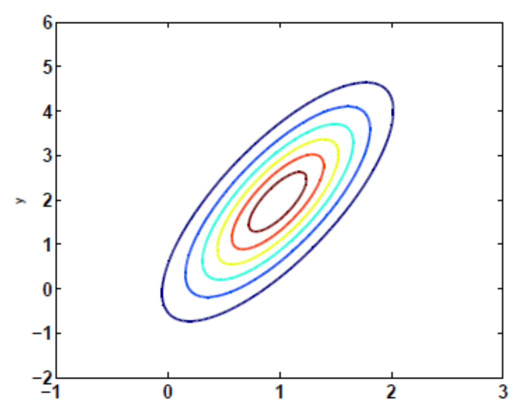
- And a d-dimensional Gaussian is

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) \equiv (2\pi)^{-\frac{d}{2}}|\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$

  - $\boldsymbol{\Sigma}$ is a PSD symmetric $d \times d$ matrix, the covariance matrix
  - $|\boldsymbol{\Sigma}|$ denotes determinant
  - No need to memorize the full formula.



(a) 1-Dim

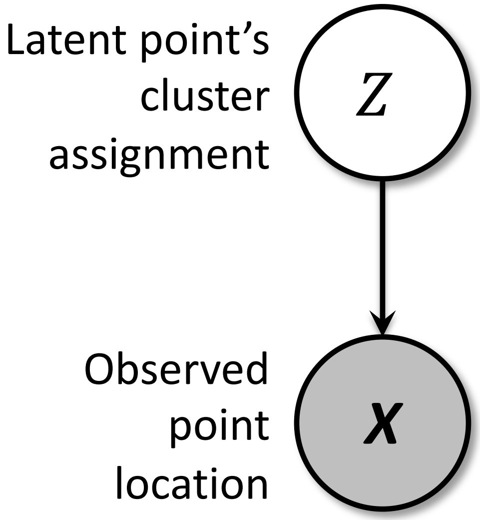


(b) 2-Dim

Figure: Bishop

Gaussian mixture model (GMM): One point

- Cluster assignment of point
  - Categorical distribution on *k* outcomes
  - $P(Z = j)$ described by $\mathrm{P}(C_j) = w_j \geq 0$ with $\sum_{j=1}^{k} w_j = 1$
- Location of point
  - Each cluster has its own Gaussian distribution
  - Location of point governed by its cluster assignment
  - $P(\boldsymbol{X}|Z = j) = \mathcal{N}\left(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)$ class conditional density
- Model's parameters: $w_j, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j, j = 1, \dots, k$



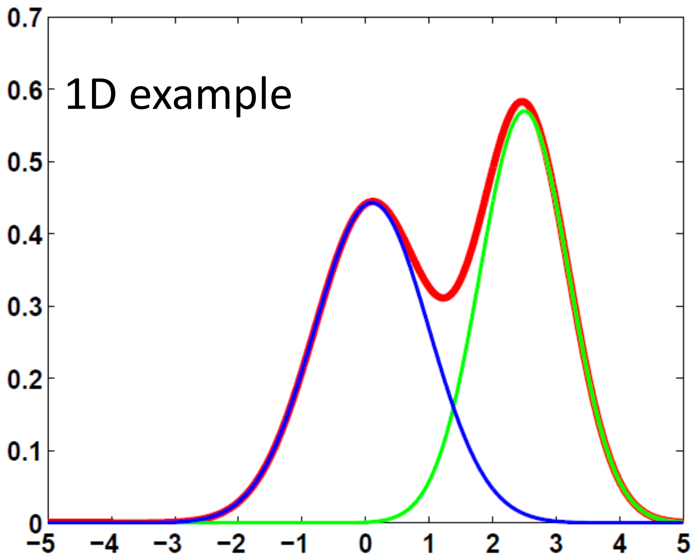
From marginalisation to mixture distribution

- When fitting the model to observations, we'll be maximising likelihood of observed portions of the data (the **X**'s) not the latent parts (the *Z*'s)
- Marginalising out the *Z*'s derives the "familiar" mixture distribution
- Gaussian mixture distribution:

$$P(\boldsymbol{x}) \equiv \sum_{j=1}^{k} w_j \mathcal{N}\left(\boldsymbol{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)$$

$$\equiv \sum_{j=1}^{k} \mathrm{P}(C_j)\, P\,(\boldsymbol{x}|\boldsymbol{C}_j)$$

- A convex combination of Gaussians
- Simply marginalization at work

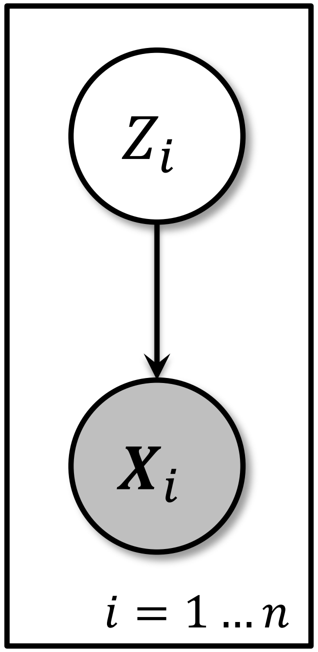


Mixture and individual component densities are re-scaled for visualisation purposes

Figure: Bishop

Clustering as model estimation

- Given a set of data points, we assume that data points are generated by a GMM
  - Each point in our dataset originates from our mixture distribution
  - Shared parameters between points: *w00t* independence assumption
- Clustering now amounts to finding parameters of the GMM that "best explains" observed data
- Call upon old friend MLE principle to find parameter values that maximise $p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n)$



Mini Summary

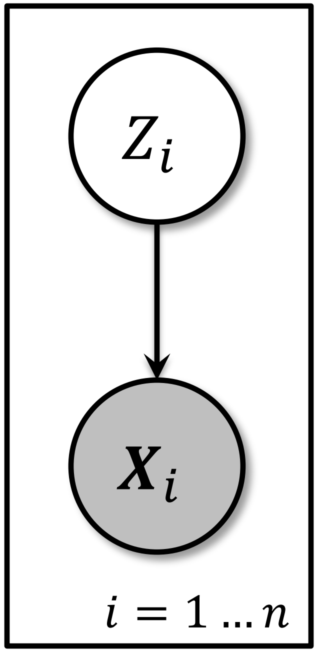
- GMM is just another D-PGM
- Some variables are observed some latent
- Convenient to model location as generated by cluster assignment
- Shared clusters arise from independence b/w points
- Mixture distribution arises algebraically from marginalisation

Next: MLE to fit the model, again motivating EM algorithm

Motivating (again) Expectation-Maximisation Algorithm

We want to implement MLE but we have unobserved r.v.'s that prevent clean decomposition as happens in fully observed settings

Fitting the GMM



- Modelling the data points as independent, aim is to find $\boldsymbol{P(C_j)}, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j, j = 1, \dots, k$ that maximise

  $P(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n) = \prod_{i=1}^{n} \sum_{j=1}^{k} \mathrm{P}(C_j)\, P(\boldsymbol{x}_i | C_j)$

  where $P(\boldsymbol{x}|\boldsymbol{C}_j) \equiv \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$

  Can be solved analytically?

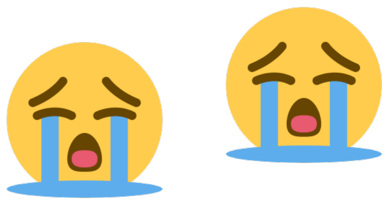
- Taking the derivative of this expression is pretty awkward, try the usual log trick

$$\log P(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n) = \sum_{i=1}^{n} \log \left(\sum_{j=1}^{k} \mathrm{P}(C_j)\, P\big(\boldsymbol{x}_i | \mathbf{C}_j\big) \right)$$

→ Expectation-Maximisation (EM)

Motivation of EM

- Consider a parametric probabilistic model $p(\boldsymbol{X}|\boldsymbol{\theta})$, where $\boldsymbol{X}$ denotes data and $\boldsymbol{\theta}$ denotes a vector of parameters
- According to MLE, we need to maximise $p(\boldsymbol{X}|\boldsymbol{\theta})$ as a function of $\boldsymbol{\theta}$
  * equivalently maximise $\log p(\boldsymbol{X}|\boldsymbol{\theta})$
- There can be a couple of issues with this task



1. Sometimes we don't observe some of the variables needed to compute the log likelihood
   * Example: GMM cluster membership Z is not known in advance
2. Sometimes the form of the log likelihood is inconvenient to work with
   * Example: taking a derivative of GMM log likelihood results in a cumbersome equation

art: Ebrahim at Wikimedia Commons (CC4)

Expectation-Maximisation (EM) Algorithm

- <u>Initialisation Step</u>:
  - Initialize K clusters: $C_1, \ldots, C_K$

    (μ_j, Σ_j) and $P(C_j)$ for each cluster j.

- <u>Iteration Step</u>:
  - Estimate the cluster of each datum → Expectation

    $$p(C_j \mid x_i)$$

  - Re-estimate the cluster parameters → Maximisation

    $(\mu_j, \Sigma_j), p(C_j)$ for each cluster j

Summary

- Unsupervised learning
  - Diversity of problems
- Gaussian mixture model (GMM)
  - A probabilistic approach to clustering
  - The GMM model
  - GMM clustering as an optimisation problem
- MLE: Motivating Expectation Maximization (EM)

Next lecture: Getting to the bottom of EM