Lecture 13. Clustering. Gaussian Mixture Model

COMP90051 Statistical Machine Learning

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This lecture

- Unsupervised learning
  - Diversity of problems
  - Pipelines
- Clustering
  - Problem formulation
  - Algorithms
  - Choosing the number of clusters
- Gaussian mixture model (GMM)
  - A probabilistic approach to clustering
  - GMM clustering as an optimisation problem

Unsupervised Learning

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

Previously: Supervised learning

- Supervised learning: Overarching aim is making predictions from data
- We studied methods such as random forest, ANN and SVM in the context of this aim
- We had instances $\boldsymbol{x}_i \in \boldsymbol{R}^m$, $i = 1, \ldots, n$ and corresponding labels y_i as inputs, and the aim was to predict labels for new instances
- Can be viewed as a function approximation problem, but with a big caveat
- The ability to generalise is critical

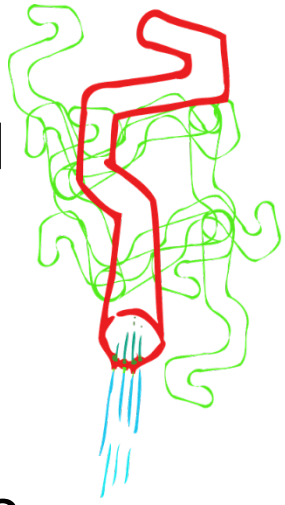
Now: Unsupervised learning

- Next few lectures: unsupervised learning methods
- In unsupervised learning, there is no dedicated variable called a "label"
- Instead, we just have a set of points $\boldsymbol{x}_i \in \boldsymbol{R}^m$, $i = 1, \ldots, n$
  - And often data cannot be reduced to points in $\boldsymbol{R}^m$ (e.g., data is a set of variable length sequences)
- The aim of unsupervised learning is to explore the structure (patterns, regularities) of the data
- The aim of "exploring the structure" is vague

Applications of unsupervised learning

- Diversity of tasks fall into unsupervised learning category
- This subject covers some common applications of unsupervised learning:
  - Clustering (this week)
  - Dimensionality reduction (next week)
  - Learning parameters of probabilistic models (after break)
- A few other applications not covered in this course:
  - Marked 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

Data analysis pipelines



- Clustering and dimensionality reduction are listed as separate problems
- In many cases, these can be viewed as distinct unsupervised learning tasks
- However, different methods can be combined into powerful data analysis *pipelines*
- E.g., we will use these pipelines for data points where patterns are obscure, or for datasets that are not points in $\boldsymbol{R}^m$
- Before getting to this stage, we first consider a classical clustering problem

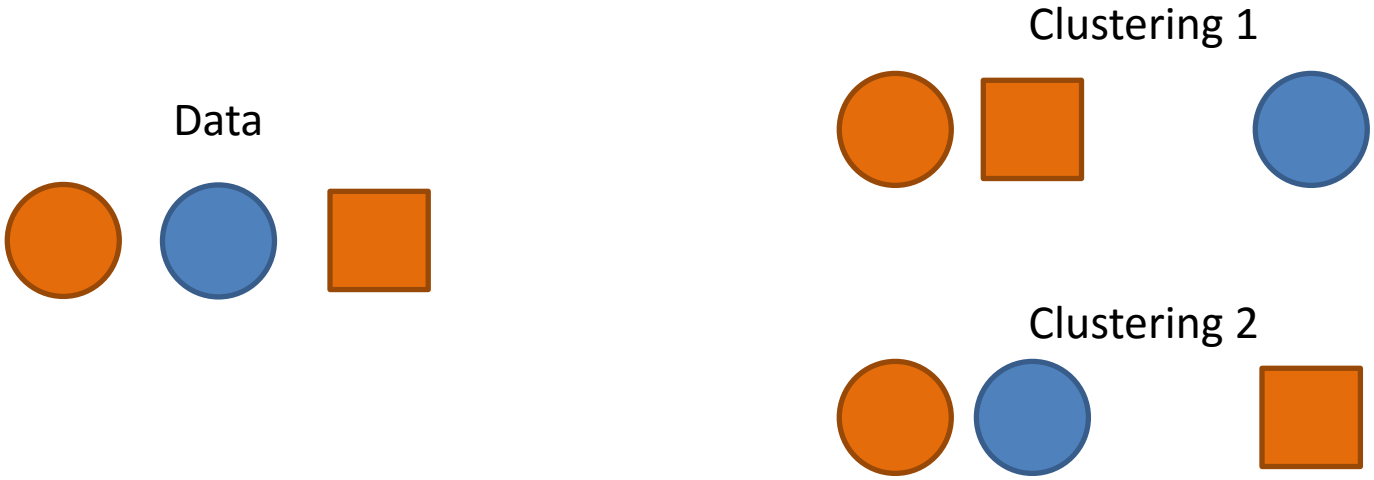
art: adapted from Clker-Free-Vector-Images at pixabay.com (CC0)

Clustering

A fundamental task in Machine Learning. Thousands of algorithms, yet no definitive universal solution

Introduction to clustering

- *Clustering* is automatic grouping of objects such that the objects within each group (cluster) are more similar to each other than objects from different groups
  - An extremely vague definition that reflects the variety of real-world problems that require clustering
- The key to this definition is defining what "*similar*" means



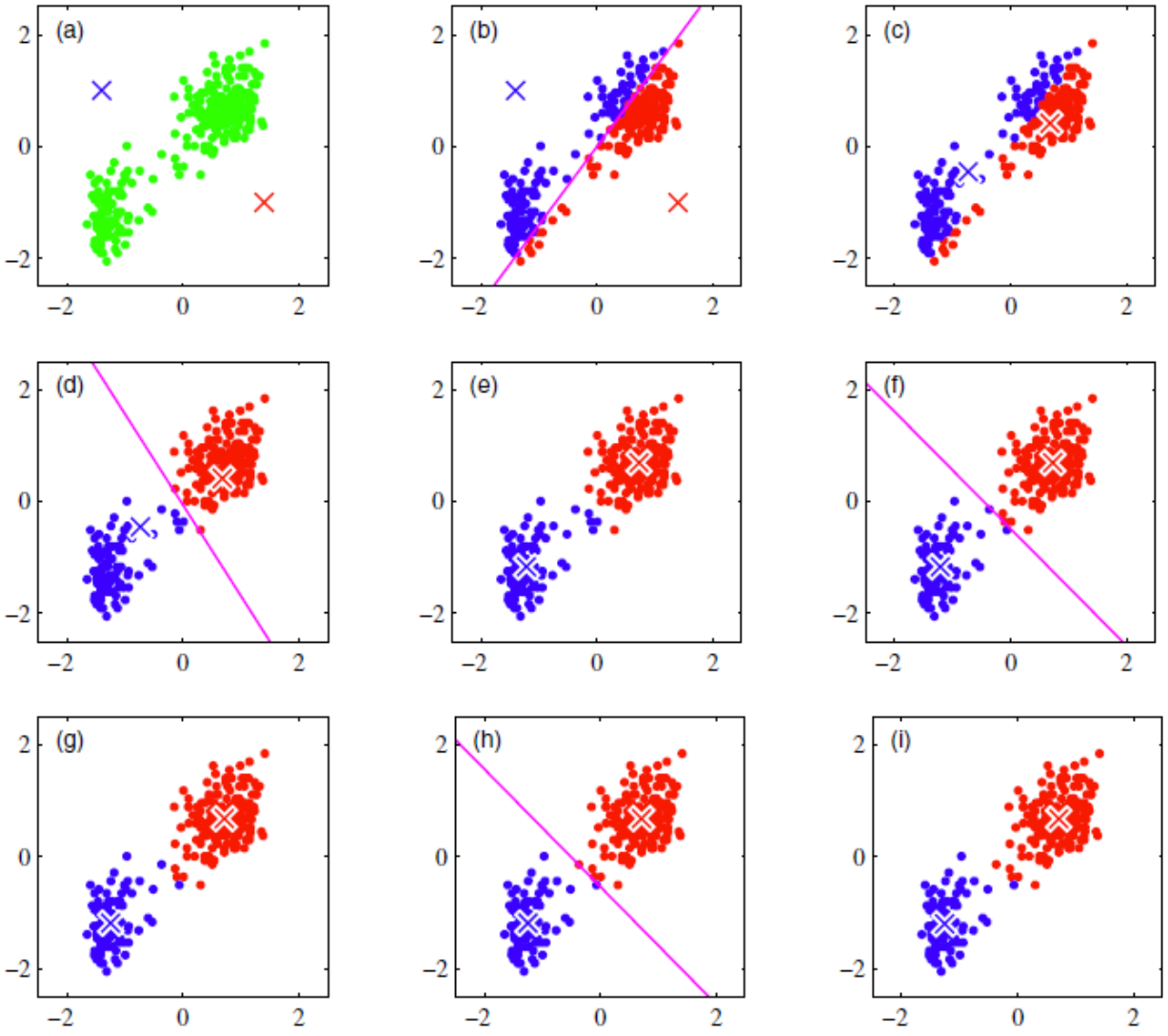
Measuring (dis)similarity

- Consider a "classical" setting where the data is a set of points $\boldsymbol{x}_i \in \boldsymbol{R}^m$, $i = 1, \ldots, n$
- Instead of "similarity", it is sometimes more convenient to use an opposite concept of "dissimilarity" or "difference"
- A natural choice for formalising the "difference" between a pair of points is Euclidean distance

$$d_{ij} \equiv \|\boldsymbol{x}_i - \boldsymbol{x}_j\| = \sqrt{\sum_{l=1}^{m} \left((\boldsymbol{x}_i)_l - (\boldsymbol{x}_j)_l \right)^2}$$

- Here $\boldsymbol{x}_i$ is a vector and $(\boldsymbol{x}_i)_l$ denotes the l-th element of that vector

Refresher on 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

K-means as iterative optimisation

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

Clustering algorithms

- There are thousands (!) of clustering algorithms
  - *Jain A.K. et al., Data clustering: 50 years beyond K-means, 2010, Pattern recognition letters*
- K-means is still one of the most popular algorithms (perhaps the most popular)
  - *Wu X. et al., Top 10 algorithms in data mining, 2008, Knowledge and information systems*
- Many popular algorithms do not require specifying k
  - Hierarchical clustering (*e.g., see Hastie at al., The elements of statistical learning*)
  - DBSCAN (*Ester M. et al., A density-based algorithm for discovering clusters in large spatial databases with noise, 1996, KDD conference*)
  - Affinity propagation (*Brendan J.F. and Dueck D., Clustering by passing messages between data points, 2007, Science*)

Consensus clustering (1/3)

- Unsupervised learning counterpart of bagging
  - *Monti S. et al., Consensus clustering: a resampling-based method for class discovery and visualization of gene expression microarray data, 2003, Machine Learning*
- Consider a dataset $D = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}$, and some pre-defined number of iterations T
- The algorithm creates sampled versions $D_1, \dots, D_T$ of the original data
  - In principle, one can use bootstrapping (sampling with replacement), resulting in $|D_t| = n$
  - For consensus clustering authors consider subsampling (without replacement), resulting in $|D_t| < n$

Consensus clustering (2/3)

- $D_1, \ldots, D_T$ are sampled versions of original data
- Define an $n \times n$ indicator matrix $\boldsymbol{I}_t$, such that $\boldsymbol{I}_t(i,j) = 1$ if $\boldsymbol{x}_i, \boldsymbol{x}_j \in D_t$ and $\boldsymbol{I}_t(i,j) = 0$ otherwise
- Apply clustering independently on each D_t
- Define an $n \times n$ association matrix $\boldsymbol{M}_t$, such that $\boldsymbol{M}_t(i,j) = 1$ if $\boldsymbol{x}_i, \boldsymbol{x}_j$ are in the same cluster, and $\boldsymbol{M}_t(i,j) = 0$ otherwise
  - If $\boldsymbol{x}_i \notin D_t$ or $\boldsymbol{x}_j \notin D_t$ then $\boldsymbol{M}_t(i,j) = 0$
- The consensus matrix $\boldsymbol{\mathcal{M}}$ is defined as $\boldsymbol{\mathcal{M}}(i,j) \equiv \frac{\sum_{t=1}^{T} \boldsymbol{M}_t(i,j)}{\sum_{t=1}^{T} \boldsymbol{I}_t(i,j)}$
  - Proportion of clustering runs in which two items cluster together

Consensus clustering (3/3)

- Algorithm
  1. Choose a clustering algorithm
  2. For $t = 1 \ldots T$
     a) Sample D_t from D (this can also be done by sampling features rather than data points)
     b) Apply clustering on D_t
     c) Save connectivity matrix $\boldsymbol{M}_t$ and indicator matrix $\boldsymbol{I}_t$
  3. Construct consensus matrix $\mathcal{M}$
  4. Cluster D using $\mathcal{M}$ as a similarity matrix (e.g., apply hierarchical clustering)

Compare with random forest generation

Choosing the number of clusters

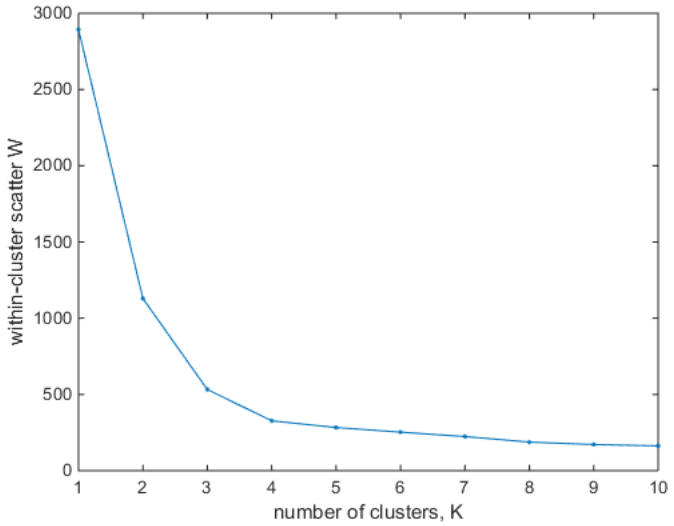
- Many clustering algorithms do not require k, but require specifying some other parameters that influence resulting number of clusters
- Suppose that we are using the algorithm that does require k
- The number of clusters can be known from context
  - E.g., clustering genetic profiles from a group of cells that is known to contain a certain number of cell types
- Visualising the data (e.g., using multidimensional reduction, next week) can help to estimate the number of clusters
- Another strategy is to try a few plausible values and see whether it makes difference to the analysis

Number of clusters and overfitting

- In the context of k-means it might be appealing to treat k as an parameter to be optimised
- This does not work because larger k results in a more flexible model that will always fit the data better
  - This is analogous to overfitting in supervised learning
- Instead, approaches that can work are:
  - Cross-validation-like strategies for determining k
  - Try several possible k and look at the trend
  - Information-theoretic results
- Example of the second approach is shown in the next slide
- Examples of the third approach are given in green slides after that

Kink method and gap statistics

- Manual inspection of minimised within cluster variation as a function of k
- The real number of clusters is indicated by the kink in this curve
- The gap statistics (*Hastie et al. book*) developed for k-means clustering is an automated version of the kink method
- This method measures the gaps between each k and analyses their distribution



Akaike information criterion

- This and next methods are only applicable for parametric probabilistic models $p(\boldsymbol{X}|\boldsymbol{\theta})$. Let $\widehat{\boldsymbol{\theta}}$ be MLE for this model, and let $L^* \equiv p\left(\boldsymbol{X}|\widehat{\boldsymbol{\theta}}\right)$
- Akaike information criterion (AIC) is defined as

$$AIC = 2N_{par} - 2\ln L^*$$

- Here N_{par} is the number of free parameters
- The equation is simple, but the derivation is very complicated. AIC is one of fundamental results in statistic
- AIC estimates divergence between the true unknown model (e.g., GMM with true number of clusters), and the current model

Akaike information criterion

- Method: consider several different k, and their corresponding GMM. Find MLE parameters for each model
- Compute AIC for each model and choose k that resulted in the smallest AIC
- The smallest AIC is preferable because AIC is an estimator of divergence between the true and current models
- AIC estimator was shown to be biased for finite sample sizes, thus a correction has been proposed which should be used in practice instead AIC (n is the number of data points)

$$AICc = 2N_{par} + \ln L^* + \frac{2N_{par}\left(N_{par}+1\right)}{n - N_{par} - 1}$$

Bayesian information criterion

- AIC was derived from a frequentist standpoint. Bayesian information criterion (BIC) represents the Bayesian approach to model selection
- Bayesian model selection is based on marginal likelihood $p(data|model)$
- BIC is an approximate computation of the marginal likelihood
- BIC is defined as

$$BIC = N_{par} \ln n - 2 \ln L^*$$

- One should choose a model with the smallest BIC

Gaussian Mixture Model

A probabilistic view of clustering

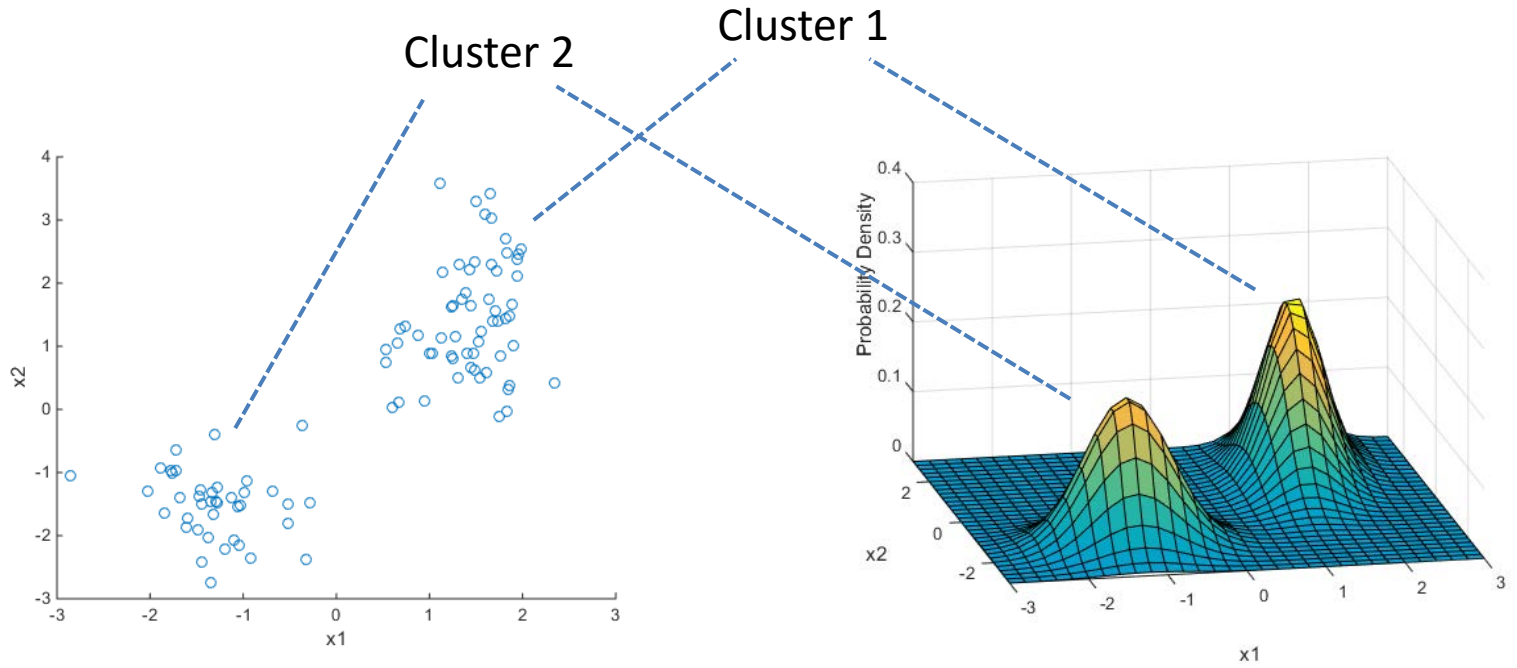
Why GMM clustering

- K-means algorithm is one of the most popular algorithms, GMM clustering is a generalisation of k-means
- Empirically, works well in many cases
  - Moreover, it can be used in a manifold learning pipeline (coming soon)
- Reasonably simple and mathematically tractable
- Example of a probabilistic approach
- Example application of Expectation Maximisation (EM) algorithm
  - EM algorithm is a generic technique, not only for GMM clustering

Clustering: Probabilistic interpretation

Clustering can be viewed as identification of components of a probability density function that generated the data

Identifying cluster centroids can be viewed as finding modes of distributions



Modelling uncertainty in data clustering

- K-means clustering assigns each point to exactly one cluster
  - In other words, the result of such a clustering is partitioning into k subsets
- Similar to 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, $c = 1, \dots, k$
- That is, each point still originates from one particular cluster (aka component), but we are not sure from which one
- Next, for each individual component, the normal distribution is a common modelling choice

Normal (aka Gaussian) distribution

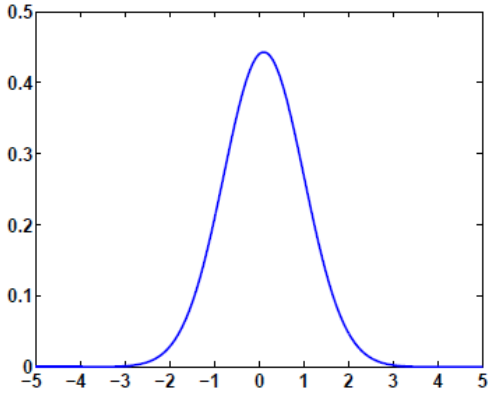
- Recall that a 1D Gaussian is

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

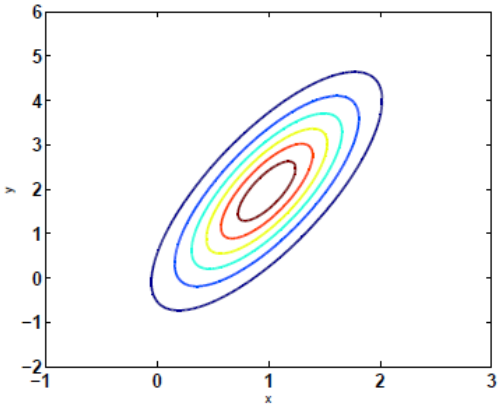
- And a m-dimensional Gaussian is

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

  - $\boldsymbol{\Sigma}$ is a symmetric $m \times m$ matrix that is assumed to be positive definite
  - $\det \boldsymbol{\Sigma}$ denotes matrix determinant



(a) 1-Dim



(b) 2-Dim

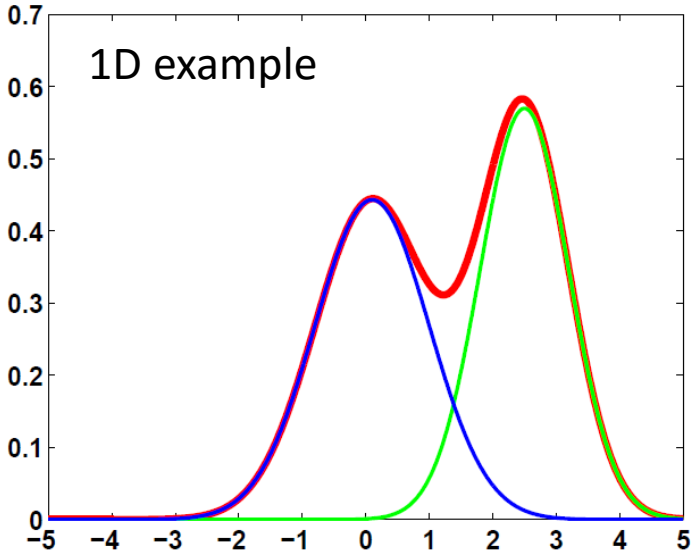
Figure: Bishop

Gaussian mixture model (GMM)

- Gaussian mixture distribution (for one data point):

$$p(\boldsymbol{x}) \equiv \sum_{c=1}^{k} w_c \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

- Here $w_c \geq 0$ and $\sum_{c=1}^{k} w_c = 1$
- That is, $w_1, \ldots, w_k$ is a probability distribution over components
- Parameters of the model are $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \ldots, k$



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

Figure: Bishop

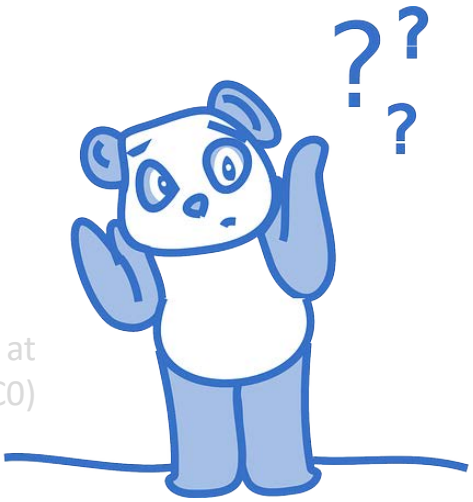
Checkpoint

- Consider a GMM with five components for 3D data. How many independent parameters does this model have?

$6 \times 5 + 3 \times 5 + 4$

$6 \times 5 + 3 \times 5 + 5$

$9 \times 5 + 3 \times 5 + 5$



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Clustering as an optimisation problem

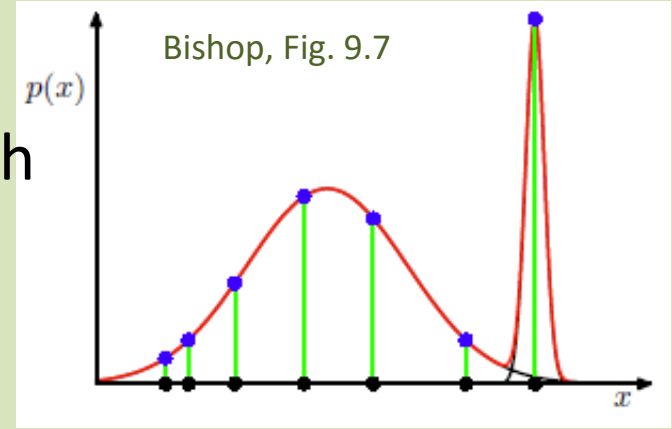
- Given a set of data points, we assume that data points are generated by a GMM
  - Each point in our dataset originates from the c-th normal distribution component with probability w_c
- Clustering now amounts to finding parameters of the GMM that "best explain" the observed data
- But what does "best explain" mean?
- We are going to call upon another old friend: MLE principle tells us to use parameter values that maximise $p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)$

Fitting a GMM model to data

- Assuming that data points are independent, our aim is to find $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \ldots, k$ that maximise

$$p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \prod_{i=1}^{n} \sum_{c=1}^{k} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

- This is actually an ill-posed problem
  - Singularities (points at which the likelihood is not defined)
  - Non-uniqueness
- Theoretical cure – Bayesian approach
- Practical cure – heuristically avoid singularities



Fitting a GMM model to data

- Yet again, we are facing an optimisation problem
- Assuming that data points are independent, our aim is to find $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \ldots, k$ that maximise

$$p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \prod_{i=1}^{n} \sum_{c=1}^{k} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

- Let's see if this can be solved analytically
- Taking the derivative of this expression is pretty awkward, try the usual log trick

Attempting the log trick for GMM

- Our aim is to find $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \ldots, k$ that maximise

$$\log p(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \sum_{i=1}^{n} \log \left(\sum_{c=1}^{k} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) \right)$$

- The log cannot be pushed inside the sum. The derivative of the log likelihood still going to have a cumbersome form
- We should use an iterative procedure

Fitting a GMM using iterative optimisation

- So there's little prospect in analytical solution
- At this point, we could use the gradient descent algorithm
- But it still requires taking partial derivatives
- Another problem of using the gradient descent are complicated constraints on parameters
- We aim to find w_c, $\boldsymbol{\mu}_c$, $\boldsymbol{\Sigma}_c$, $c = 1, \ldots, k$, where $\boldsymbol{\Sigma}_c$ are symmetric and positive definite for each c, and where w_c add up to one

Introduction to Expectation Maximisation

- Expectation Maximisation (EM) algorithm is a common way to find parameters of a GMM
- EM is a generic algorithm for finding MLE of parameters of a probabilistic model
- Broadly speaking, as "input" EM requires
  - A probabilistic model that is can be specified by a fixed number of parameters
  - Data ☺
- EM is widely used outside clustering and GMMs (another application of EM coming soon)

MLE vs EM

- MLE is a frequentist *principle* that suggests that given a dataset, the "best" parameters to use are the ones that maximise the probability of the data
  - MLE is a way *to formally pose* the problem
- EM is an *algorithm*
  - EM is a way *to solve* the problem posed by MLE
- MLE can be found by other methods such as gradient descent (but gradient descent is not always the most convenient method)

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  - GMM clustering as an optimisation problem