Lecture 14.
Gaussian Mixture Model.
Expectation Maximization.

COMP90051 Statistical Machine Learning

Semester 2, 2018
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THE UNIVERSITY OF MELBOURNE

This lecture

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

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: ability to generalise is critical
- Bandits: a setting of partial supervision

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 $\boldsymbol{x}_i \in \boldsymbol{R}^m, i = 1, \dots, n$
- The aim of unsupervised learning is to explore the structure (patterns, regularities) of the data
- The aim of "exploring the structure" is vague

Unsupervised learning tasks

- Diversity of tasks fall into unsupervised learning category
  - Clustering (now)
  - Dimensionality reduction (soon)
  - Learning parameters of probabilistic models (later)
- Applications and related tasks are numerous :
  - 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
  - Often unsupervised tasks in (supervised) ML pipelines

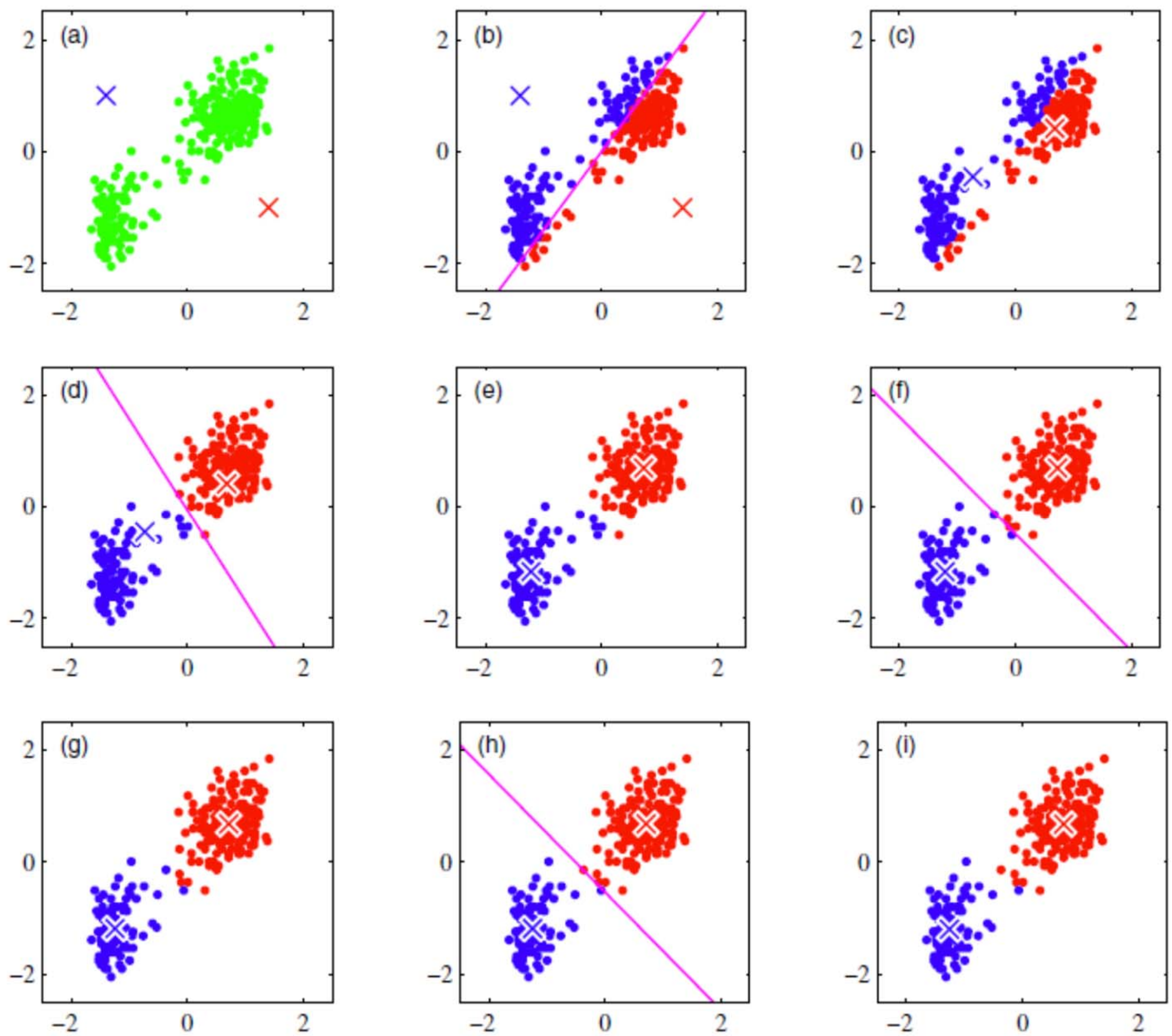
Refresher: K-means clustering

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

Gaussian Mixture Model

A probabilistic view of clustering

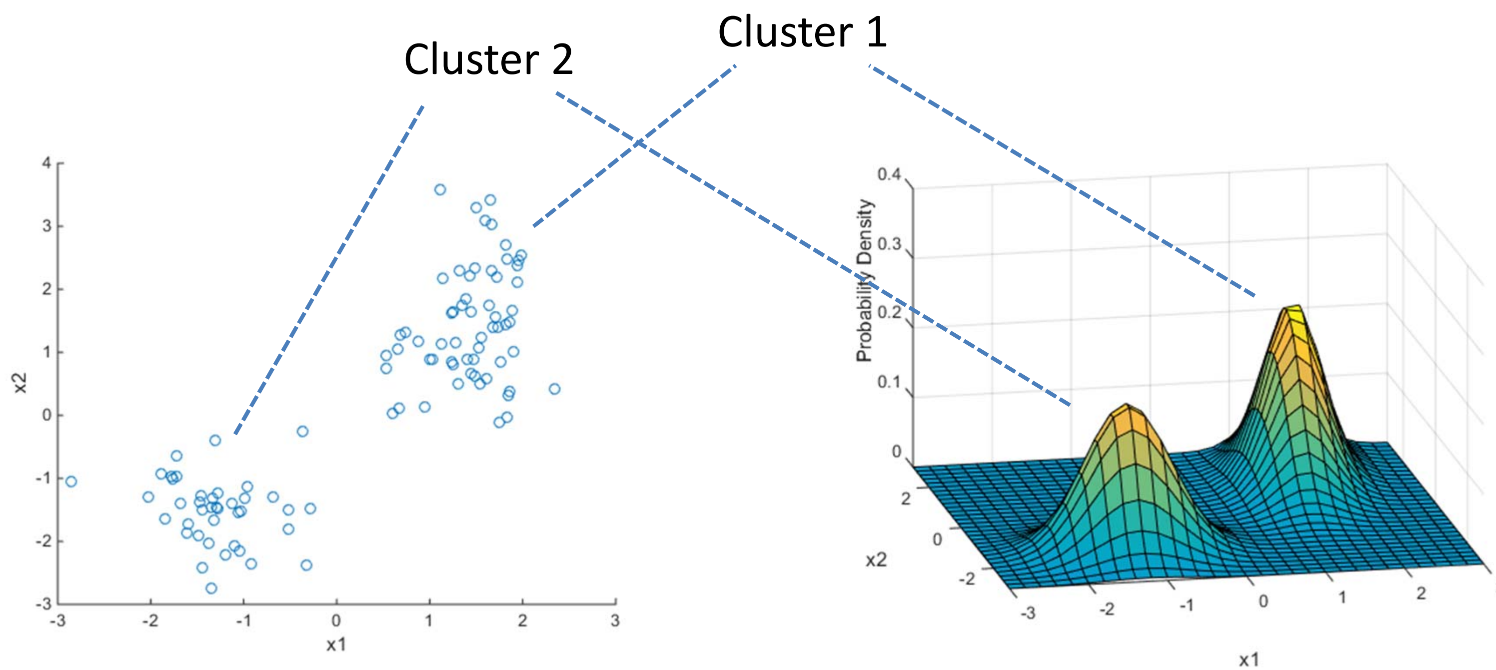
Modelling uncertainty in data clustering

- K-means clustering assigns each point to exactly one cluster
- 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
  * Individual components modelled as Gaussians
  * Fitting illustrates general Expectation Maximization (EM) algorithm

Clustering: Probabilistic interpretation

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

Identifying cluster centroids can be viewed as finding modes/components of distributions



Normal (aka Gaussian) distribution

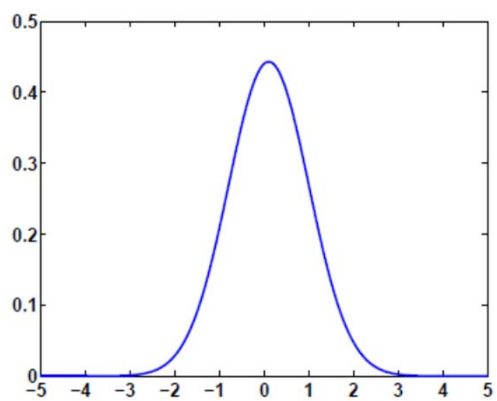
- Recall that a 1D Gaussian is

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

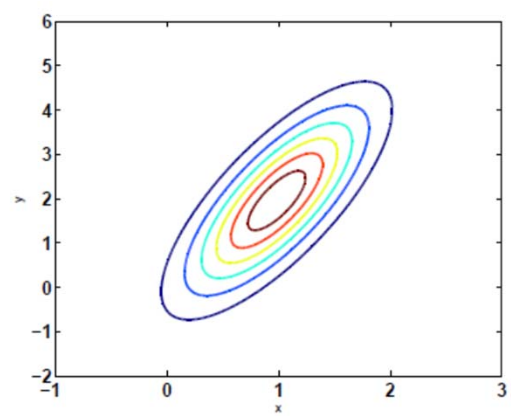
- And a m-dimensional Gaussian is

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

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



(a) 1-Dim



(b) 2-Dim

Figure: Bishop

Gaussian mixture model (GMM)

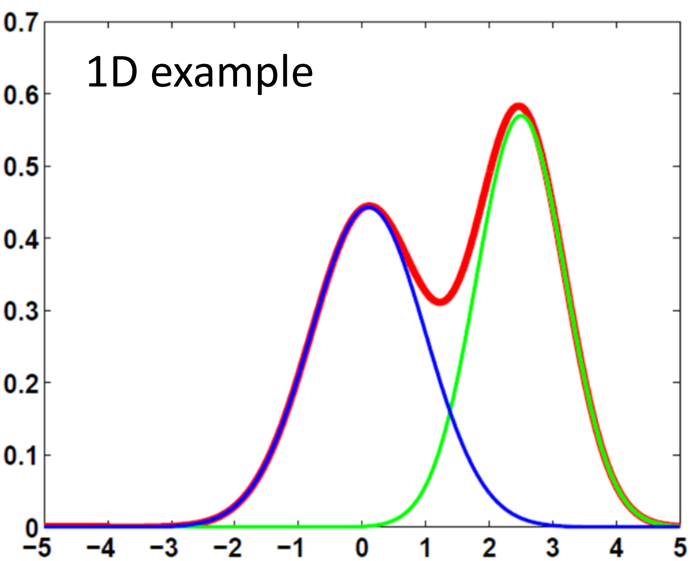
Gaussian mixture density (at one data point):

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

The w_c are component probabilities

- $w_c \geq 0$ and $\sum_{c=1}^{k} w_c = 1$
- Components can be rare (small prob.) or common (high prob.)

Parameters of the model are w_c, $\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \dots, k$



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

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

$$49 = 6 \times 5 + 3 \times 5 + 4$$

$$50 = 6 \times 5 + 3 \times 5 + 5$$

$$65 = 9 \times 5 + 3 \times 5 + 5$$

Clustering as model estimation

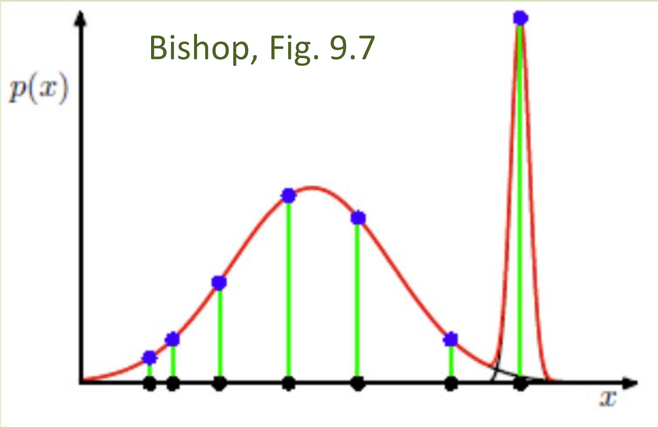
- Given a set of data points, we assume that data points are generated by a GMM
  - Each point in our dataset originates from the c-th normal distribution component with probability w_c
- Clustering now amounts to finding parameters of the GMM that “best explain” the observed data
- But what does “best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

Fitting a GMM model to data

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

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

- 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

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

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

- Can 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

- Find $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \dots, k$ that maximise

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

- The log cannot be pushed inside the sum. The derivative of log likelihood has unworkable form

- Should use an iterative procedure
  * We could use the gradient descent algorithm
  * But it still requires taking partial derivatives
  * Another problem of using gradient descent are complicated constraints on parameters
  * I.e. We aim to find $w_c, \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c, c = 1, \dots, k$, where $\boldsymbol{\Sigma}_c$ are symmetric and positive definite for each c, and where w_c add up to one

Look 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 can be specified by a fixed number of parameters
  - Data ☺
- EM is widely used outside clustering and GMMs

Expectation Maximisation Algorithm

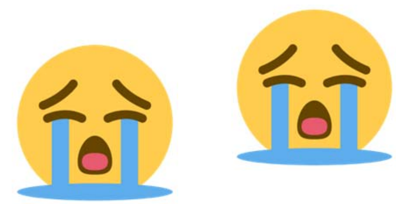
For a moment, let’s put GMM problem aside – to come back to later.

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)

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 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

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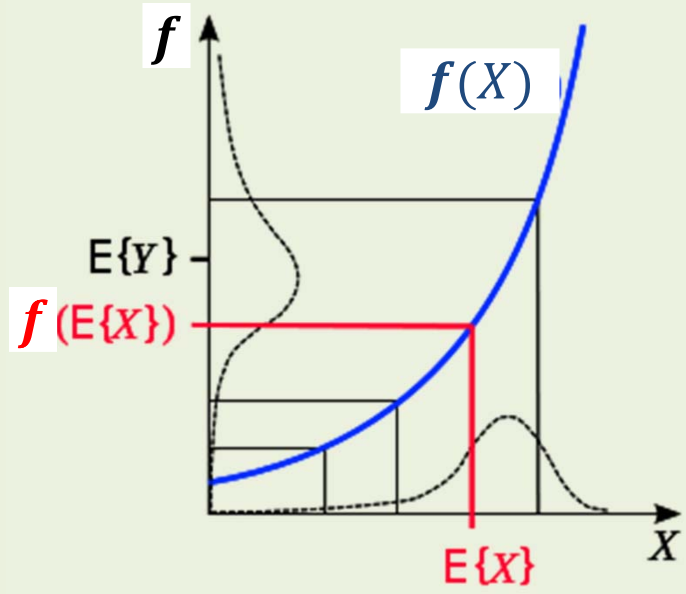
Key idea: Introduce latent variables

- Assume that the data consists of observed variables $\boldsymbol{X}$ and unobserved (aka *latent*) variables collectively denoted as $\boldsymbol{Z}$
- Such an approach directly models the situation where some variables are indeed unobserved
- Introducing additional variables might seem redundant
- However, a smart choice of latent variables can make calculations easier
  - Example: in GMM, if we let z_i denote true cluster membership for each point $\boldsymbol{x}_i$, computing the likelihood with known values $\boldsymbol{z}$ is simplified (see next section)

Needed tool: Jensen's inequality

- Compares effect of averaging before and after applying a convex function: $f\left(Average(\boldsymbol{x})\right) \leq Average\left(f(\boldsymbol{x})\right)$
- Example:
  * Let f be some convex function, such as $f(x) = x^2$
  * Consider $\boldsymbol{x} = [1,2,3,4,5]'$, then $f(\boldsymbol{x}) = [1,4,9,16,25]'$
  * Average of input $Average(\boldsymbol{x}) = 3$
  * $f\left(Average(\boldsymbol{x})\right) = 9$
  * Average of output $Average\left(f(\boldsymbol{x})\right) = 12.4$
- Proof follows from the definition of convexity
  * Proof by induction
- General statement:
  * If $\boldsymbol{X}$ random variable, f is a convex function
  * $f(\mathbb{E}[\boldsymbol{X}]) \leq \mathbb{E}[f(\boldsymbol{X})]$



plot: MHz'as at Wikimedia Commons (public domain)

Putting the latent variables in use

- We want to maximise $\log p(\boldsymbol{X}|\boldsymbol{\theta})$. We don't observe $\boldsymbol{Z}$ (here discrete), but can introduce it nonetheless.
- $\boxed{\log p(\boldsymbol{X}|\boldsymbol{\theta})} = \log \sum_{\boldsymbol{Z}} p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})$ ← Marginalisation (here $\sum_{\boldsymbol{Z}}$ … iterates over all possible values of $\boldsymbol{Z}$)
- $= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta}) \frac{p(\boldsymbol{Z})}{p(\boldsymbol{Z})} \right)$ ← Need $\boldsymbol{Z}$ to have non-zero marginal
- $= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{Z}) \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right)$
- $= \log \mathbb{E}_{\boldsymbol{Z}} \left[\frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$
- $\geq \mathbb{E}_{\boldsymbol{Z}} \left[\log \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$ ← Jensen's inequality holds since $\log(\ldots)$ is a concave function
- $= \boxed{\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]}$

Maximising the lower bound (1/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- The right hand side (RHS) is a lower bound on the original log likelihood
  - This holds for any $\boldsymbol{\theta}$ and any non zero $p(\boldsymbol{Z})$
- Intuitively, we want to push the lower bound up
- This lower bound is a function of two "variables" $\boldsymbol{\theta}$ and $p(\boldsymbol{Z})$. We want to maximise the RHS as a function of these two "variables"
- It is hard to optimise with respect to both at the same time, so EM resorts to an iterative procedure

Maximising the lower bound (2/2)

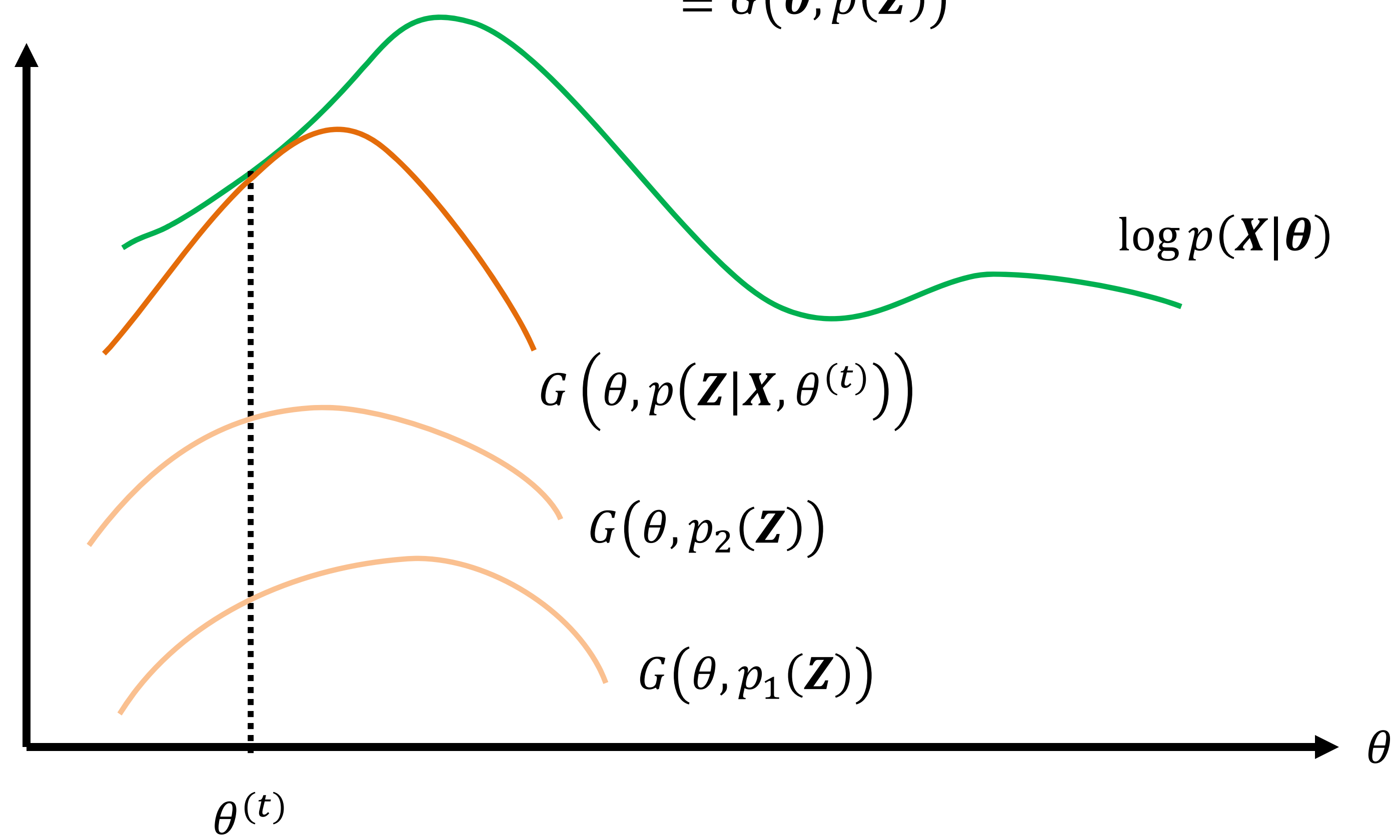
- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- EM is essentially coordinate ascent:
  * Fix $\boldsymbol{\theta}$ and optimise the lower bound for $p(\boldsymbol{Z})$
  * Fix $p(\boldsymbol{Z})$ and optimise for $\boldsymbol{\theta}$
- The convenience of EM comes from the following

we will prove this shortly

- For any point $\boldsymbol{\theta}^*$, it can be shown that setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$ makes the lower bound tight
- For any $p(\boldsymbol{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$, the first term can usually be maximised as a function of $\boldsymbol{\theta}$ in a closed-form
  * If not, then probably don't use EM

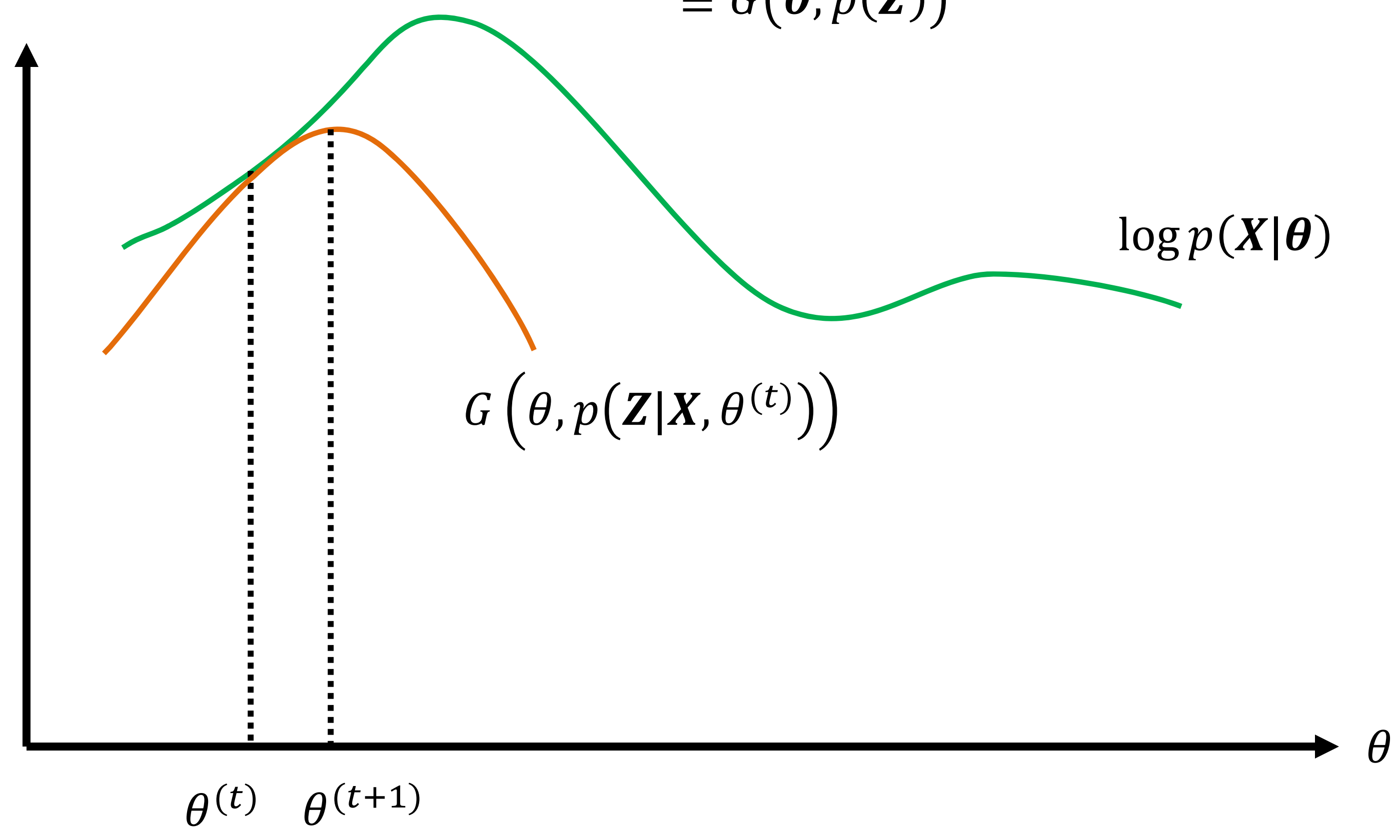
Example (1/3)

$$\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \underbrace{\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]}_{\equiv G(\boldsymbol{\theta}, p(\boldsymbol{Z}))}$$



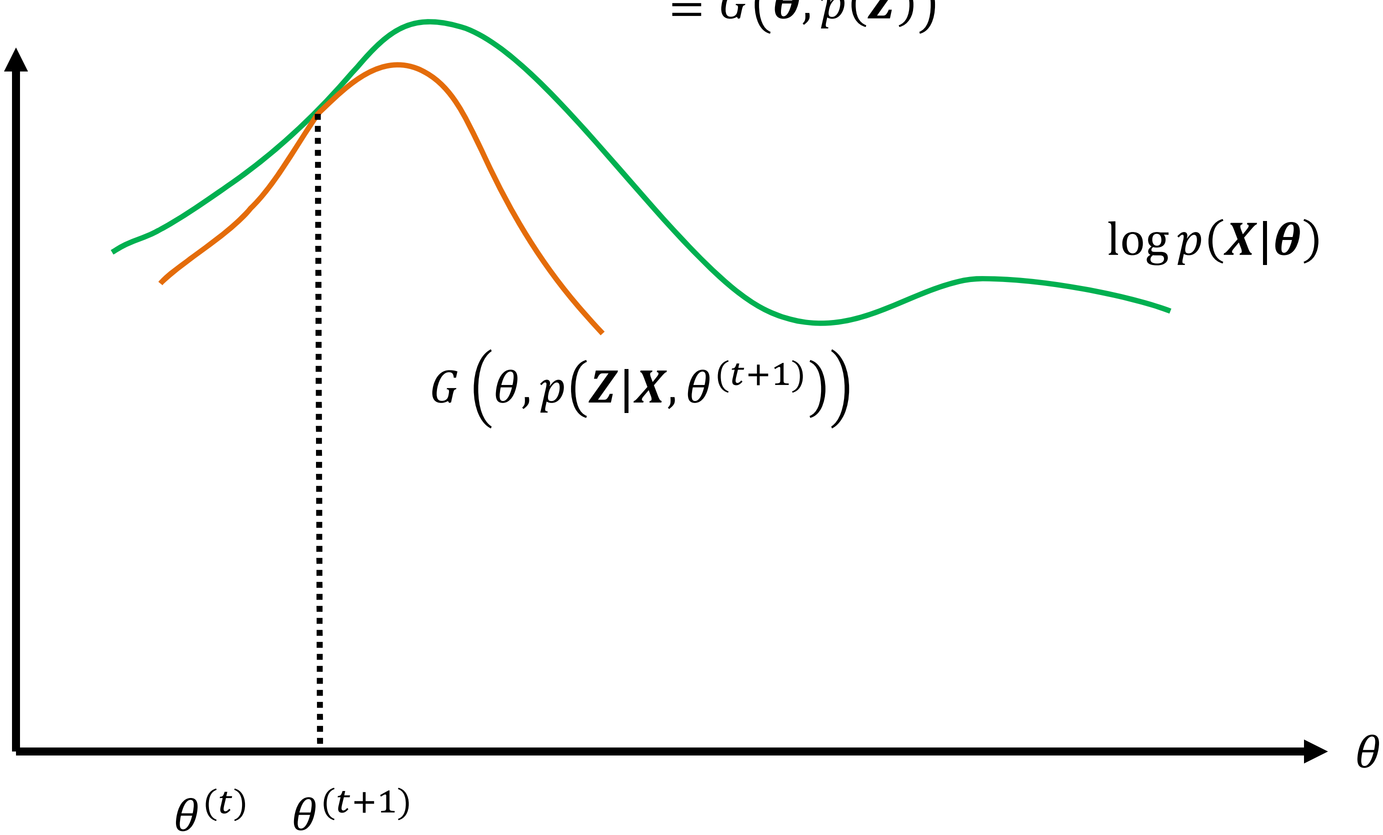
Example (2/3)

$$\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \underbrace{\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]}_{\equiv G(\boldsymbol{\theta}, p(\boldsymbol{Z}))}$$



Example (3/3)

$$\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \underbrace{\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]}_{\equiv G(\boldsymbol{\theta},p(\boldsymbol{Z}))}$$



EM as iterative optimisation

1. Initialisation: choose (random) initial values of $\boldsymbol{\theta}^{(1)}$
2. Update:
   * E-step: compute $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right) \equiv \mathbb{E}_{\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})]$
   * M-step: $\boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$
3. Termination: if no change then stop
4. Go to Step 2

This algorithm will eventually stop (converge), but the resulting estimate can be only a local maximum

Maximising the lower bound (2/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- EM is essentially coordinate descent:
  * Fix $\boldsymbol{\theta}$ and optimise the lower bound for $p(\boldsymbol{Z})$
  * Fix $p(\boldsymbol{Z})$ and optimise for $\boldsymbol{\theta}$

we will prove this now

- The convenience of EM follows from the following
- For any point $\boldsymbol{\theta}^*$, it can be shown that setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$ makes the lower bound tight
- For any $p(\boldsymbol{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$, the first term can usually be maximised as a function of $\boldsymbol{\theta}$ in a closed-form
  * If not, then probably don't use EM

Putting the latent variables in use

We want to maximise $\log p(\boldsymbol{X}|\boldsymbol{\theta})$. We don't know $\boldsymbol{Z}$, but consider an arbitrary non-zero distribution $p(\boldsymbol{Z})$

$$\boxed{\log p(\boldsymbol{X}|\boldsymbol{\theta})} = \log \sum_{\boldsymbol{Z}} p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})$$

← Rule of marginal distribution (here $\sum_{\boldsymbol{Z}}$ … iterates over all possible values of $\boldsymbol{Z}$)

$$= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta}) \frac{p(\boldsymbol{Z})}{p(\boldsymbol{Z})} \right)$$

$$= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{Z}) \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right)$$

$$= \log \mathbb{E}_{\boldsymbol{Z}} \left[\frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$$

← Jensen's inequality holds since $\log(\dots)$ is a concave function

$$\boxed{\geq \mathbb{E}_{\boldsymbol{Z}} \left[\log \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]}$$

$$= \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$$

Setting a tight lower bound (1/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]$
  - $= \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})p(\boldsymbol{X}|\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]$ ← Chain rule of probability
  - $= \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})} + \log p(\boldsymbol{X}|\boldsymbol{\theta})\right]$
  - $= \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}|\boldsymbol{\theta})]$ ← Linearity of $\mathbb{E}[.]$
  - $= \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \log p(\boldsymbol{X}|\boldsymbol{\theta})$ ← $\mathbb{E}[.]$ of a constant
- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \log p(\boldsymbol{X}|\boldsymbol{\theta})$

Setting a tight lower bound (2/2)

$$\underbrace{\log p(\boldsymbol{X}|\boldsymbol{\theta})}^{\text{Ultimate aim: maximise this}} \geq \overbrace{\underbrace{\mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]}_{\text{First, note that this term* } \leq 0} + \log p(\boldsymbol{X}|\boldsymbol{\theta})}^{\text{Lower bound of what we want to maximise}}$$

Second, note that if $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})$, then

$$\mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}\right] = \mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}[\log 1] = 0$$

For any $\boldsymbol{\theta}^*$, setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^*)$ maximises the lower bound on $\log p(\boldsymbol{X}|\boldsymbol{\theta}^*)$ and makes it tight

*Negative Kullback-Leibler divergence between $p(\boldsymbol{Z})$ and $p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})$

Estimating Parameters of Gaussian Mixture Model

A classical application of the
Expectation Maximisation algorithm

Latent variables of GMM

- Let $z_1, \dots, z_n$ denote true origins of the corresponding points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$. Each z_i is a discrete variable that takes values in $1, \dots, k$, where k is a number of clusters

- Now compare the original log likelihood

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

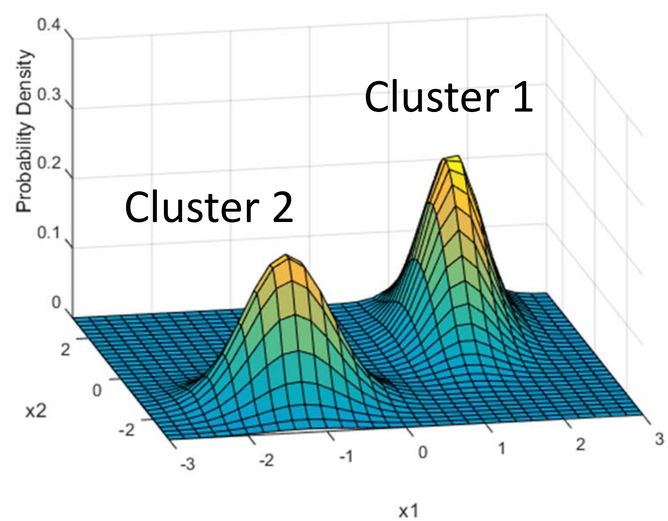
- With *complete log likelihood* (if we knew $\boldsymbol{z}$)

$$\log p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n, \boldsymbol{z}) = \sum_{i=1}^{n} \log\left(w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i | \boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)\right)$$

- Recall that taking a log of a normal density function results in a tractable expression

Handling uncertainty about $\boldsymbol{z}$

- We cannot compute complete log likelihood because we don't know $\boldsymbol{z}$
- EM algorithm handles this uncertainty replacing $\log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})$ with expectation $\mathbb{E}_{\boldsymbol{z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})]$
- This in turn requires the distribution of $p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right)$ given current parameter estimates
- Assuming that z_i are pairwise independent, we need $P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right)$
- E.g., suppose $\boldsymbol{x}_i = (-2, -2)$. What is the probability that this point originated from Cluster 1



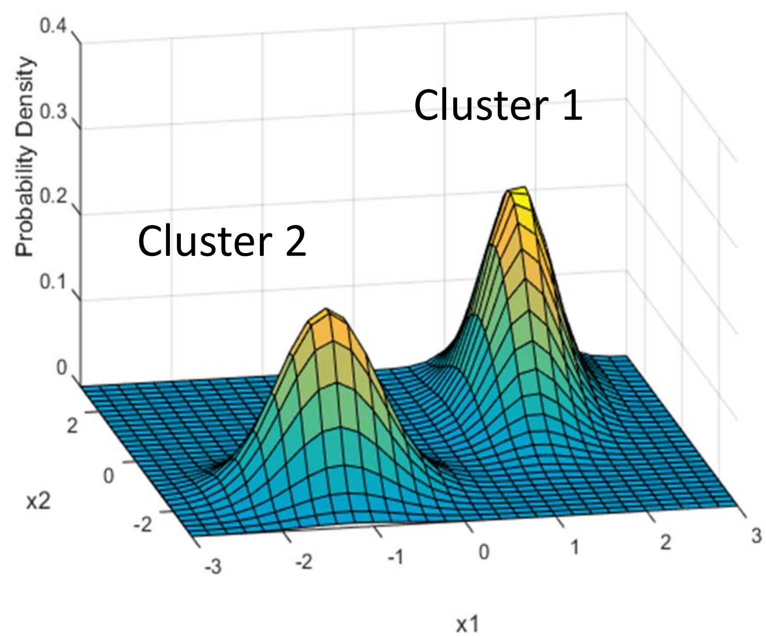
Defining cluster responsibilities

- Setting latent Z as originating cluster, yields (via Bayes rule)

$$P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right) = \frac{w_c \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)}{\sum_{l=1}^{k} w_l \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)}$$

- This probability is called *responsibility* that cluster c takes for data point i

$$r_{ic} \equiv P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right)$$



Expectation step for GMM

To simplify notation, we denote $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$ as $\boldsymbol{X}$

$$Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right) \equiv \mathbb{E}_{\boldsymbol{z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})]$$

$$= \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})$$

$$= \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \sum_{i=1}^{n} \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

$$= \sum_{i=1}^{n} \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

$$= \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

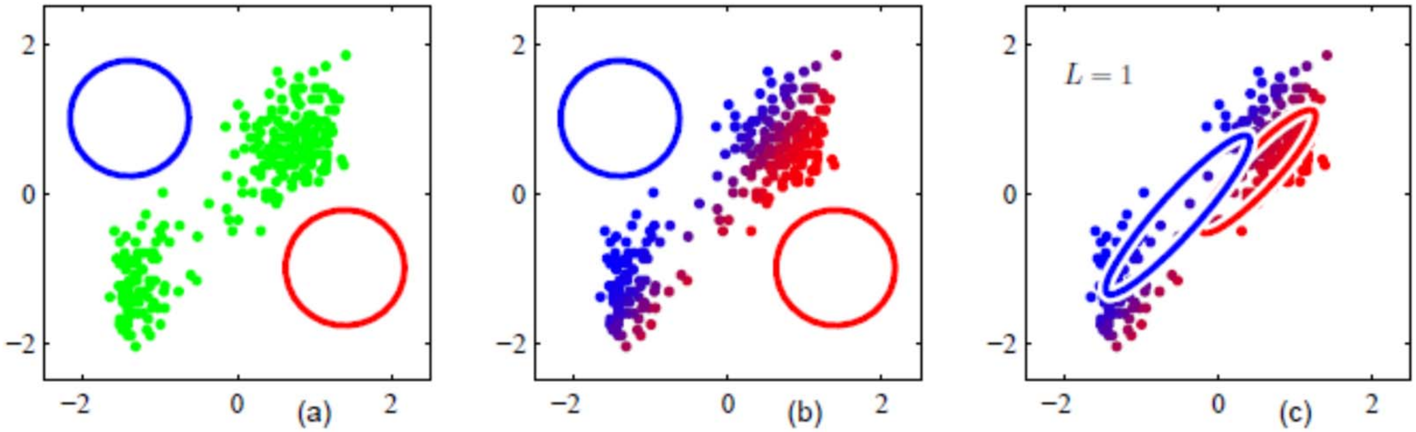
$$= \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log w_{z_i}$$

$$+ \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

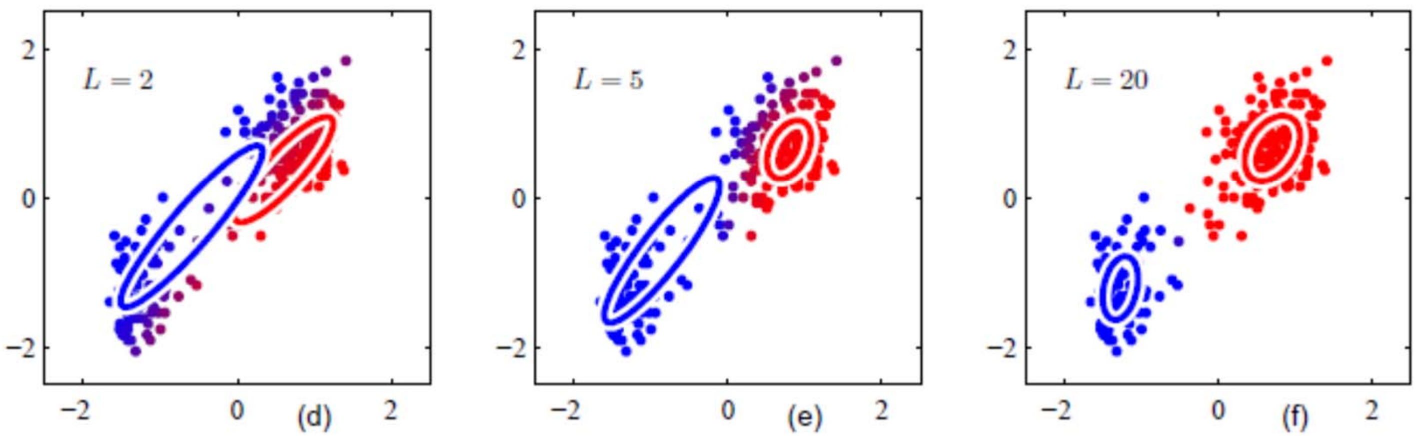
Maximisation step for GMM

- In the maximisation step, take partial derivatives of $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$ with respect to each of the parameters and set the derivatives to zero to obtain new parameter estimates
- $w_c^{(t+1)} = \frac{1}{n}\sum_{i=1}^{n} r_{ic}$
- $\boldsymbol{\mu}_c^{(t+1)} = \frac{\sum_{i=1}^{n} r_{ic}\boldsymbol{x}_i}{r_c}$
  - Here $r_c \equiv \sum_{i=1}^{n} r_{ic}$
- $\boldsymbol{\Sigma}_c^{(t+1)} = \frac{\sum_{i=1}^{n} r_{ik}\boldsymbol{x}_i\boldsymbol{x}_i'}{r_k} - \boldsymbol{\mu}_c^{(t)}\left(\boldsymbol{\mu}_c^{(t)}\right)'$
- Note that these are the estimates for step $(t+1)$

Example of fitting Gaussian Mixture model



(a) Initial (b) E-step (c) M-step



(d) 2 cycles (e) 5-cyclces (f) 20-cycles

K-means as a EM for a restricted GMM

- Consider a GMM model in which all components have the same fixed probability $w_c = 1/k$, and each Gaussian has the same fixed covariance matrix $\boldsymbol{\Sigma}_c = \sigma^2 \boldsymbol{I}$, where $\boldsymbol{I}$ is the identity matrix
- In such a model, only component centroids $\boldsymbol{\mu}_c$ need to be estimated
- Next approximate a probabilistic cluster responsibility $r_{ic} = P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\mu}_c^{(t)}\right)$ with a deterministic assignment $r_{ic} = 1$ if centroid $\boldsymbol{\mu}_c^{(t)}$ is closest to point $\boldsymbol{x}_i$, and $r_{ic} = 0$ otherwise
- Such a formulation results in a E-step where $\boldsymbol{\mu}_c$ should be set as a centroid of points assigned to cluster c
- In other words, k-means algorithm is a EM algorithm for the restricted GMM model described above*!!!*

This lecture

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

- Next lecture: More unsupervised with dim reduction