Introduction to

Machine Learning and Data Mining

(Học máy và Khai phá dữ liệu)

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Content

- Introduction to Machine Learning & Data Mining
- Unsupervised learning
- Supervised learning
- **Probabilistic modeling**
  - **Expectation maximization**
- Practical advice

Difficult situations

- No closed-form solution for the learning/inference problem? (không tìm được ngay công thức nghiệm)
  - The examples before are easy cases, as we can find solutions in a closed form by using gradient.
  - Many models (e.g., GMM) do not admit a closed-form solution
- No explicit expression of the density/mass function? (không có công thức tường minh để tính toán)
- Intractable inference (bài toán không khả thi)
  - Inference in many probabilistic models is NP-hard [Sontag & Roy, 2011; Tosh & Dasgupta, 2019]

Expectation maximization

The EM algorithm

GMM revisit

- Consider learning GMM, with K Gaussian distributions, from the training data $\mathbf{D} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M\}$.
- The density function is $p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
  - $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_K)$ represents the weights of the Gaussians, $P(z = k| \boldsymbol{\phi}) = \phi_k$.
  - Each multivariate Gaussian has density $\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma}_k)}} \exp\left[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x} - \boldsymbol{\mu}_k)\right]$
- MLE tries to maximize the following log-likelihood function

$$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = \sum_{i=1}^{M} \log \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- We cannot find a closed-form solution!
- **Naïve gradient decent:** repeat until convergence
  - Optimize $L(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$ w.r.t $\boldsymbol{\phi}$, when fixing $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.
  - Optimize $L(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$ w.r.t $(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, when fixing $\boldsymbol{\phi}$.

Still hard

GMM revisit: K-means

- **GMM:** we need to know
  - Among K gaussian components, which generates an instance $\boldsymbol{x}$?
    the index z of the gaussian component
  - The parameters of individual gaussian components: $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \phi_k)$

- **K-means:**
  - Among K clusters, to which an instance $\boldsymbol{x}$ belongs?
    the cluster index z
  - The parameters of individual clusters: the mean

- Idea for GMM?
  - $P(z|\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$?
    (note $\sum_{k=1}^{K} P(z = k|\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = 1$)

    (soft assignment)
  - Update the parameters of individual gaussians: $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \phi_k)$

- **K-means training:**
  - Step 1: assign each instance $\boldsymbol{x}$ to the nearest cluster
    (the cluster index z for each $\boldsymbol{x}$)
    (hard assignment)
  - Step 2: recompute the means of the clusters

GMM: lower bound

- Idea for GMM?
  - Step 1: compute $P(z|\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$? (note $\sum_{k=1}^{K} P(z = k|\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = 1$)
  - Step 2: Update the parameters of the gaussian components: $\boldsymbol{\theta} = (\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$

- Consider the log-likelihood function

$$L(\boldsymbol{\theta}) = \log P(\boldsymbol{D}|\boldsymbol{\theta}) = \sum_{i=1}^{M} \log \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x}_i |\, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

  - Too complex if directly using gradient
  - Note that $\log P(\boldsymbol{x}|\boldsymbol{\theta}) = \log P(\boldsymbol{x}, z|\boldsymbol{\theta}) - \log P(z|\boldsymbol{x}, \boldsymbol{\theta})$. Therefore

$$\log P(\boldsymbol{x}|\boldsymbol{\theta}) = \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(\boldsymbol{x}, z|\boldsymbol{\theta}) - \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(z|\boldsymbol{x}, \boldsymbol{\theta}) \geq \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(\boldsymbol{x}, z|\boldsymbol{\theta})$$

- Maximizing $L(\boldsymbol{\theta})$ can be done by *maximizing the lower bound*

$$LB(\boldsymbol{\theta}) = \sum_{\boldsymbol{x} \in \boldsymbol{D}} \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(\boldsymbol{x}, z|\boldsymbol{\theta}) = \sum_{\boldsymbol{x} \in \boldsymbol{D}} \sum_{z} P(z|\boldsymbol{x}, \boldsymbol{\theta}) \log P(\boldsymbol{x}, z|\boldsymbol{\theta})$$

GMM: maximize the lower bound

- Step 1: compute $P(z|\boldsymbol{x},\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\phi})$? (note $\sum_{k=1}^{K} P(z=k|\boldsymbol{x},\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\phi})=1$)
- Step 2: Update the parameters of the gaussian components: $\boldsymbol{\theta}=(\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\phi})$

- Bayes' rule: $P(z|\boldsymbol{x},\boldsymbol{\theta}) = P(\boldsymbol{x}|z,\boldsymbol{\theta})P(z|\boldsymbol{\phi})/P(\boldsymbol{x}) = \phi_z \mathcal{N}(\boldsymbol{x}|\,\boldsymbol{\mu}_z,\boldsymbol{\Sigma}_z)/C$, where $C=\sum_k \phi_k \mathcal{N}(\boldsymbol{x}|\,\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)$ is the normalizing constant.
  - Meaning that one can compute $P(z|\boldsymbol{x},\boldsymbol{\theta})$ if $\boldsymbol{\theta}$ is known
  - Denoting $T_{ki}=P(z=k|\boldsymbol{x}_i,\boldsymbol{\theta})$ for any index $k=\overline{1,K}, i=\overline{1,M}$
- How about $\boldsymbol{\phi}$?
  - $\phi_z = P(z|\boldsymbol{\phi}) = P(z|\boldsymbol{\theta}) = \int P(z,\boldsymbol{x}|\boldsymbol{\theta})d\boldsymbol{x} = \int P(z|\boldsymbol{x},\boldsymbol{\theta})P(\boldsymbol{x}|\boldsymbol{\theta})d\boldsymbol{x} = \mathbb{E}_{\boldsymbol{x}}\big(P(z|\boldsymbol{x},\boldsymbol{\theta})\big) \approx \frac{1}{M}\sum_{\boldsymbol{x}\in D} P(z|\boldsymbol{x},\boldsymbol{\theta}) = \frac{1}{M}\sum_{i=1}^{M} T_{zi}$
- Then the lower bound can be maximized w.r.t individual $(\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)$:

$$LB(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}\in \boldsymbol{D}} \sum_{z} P(z|\boldsymbol{x},\boldsymbol{\theta}) \log[P(\boldsymbol{x}|z,\boldsymbol{\theta})P(z|\boldsymbol{\theta})]$$

$$= \sum_{i=1}^{M}\sum_{k=1}^{K} T_{ki}\left[-\frac{1}{2}(\boldsymbol{x}_i-\boldsymbol{\mu}_k)^T\boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_i-\boldsymbol{\mu}_k) - \log\sqrt{\det(2\pi\boldsymbol{\Sigma}_k)}\right] + constant$$

GMM: EM algorithm

- **Input:** training data $\boldsymbol{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_M\}, \quad K > 0$
- **Output:** model parameter $(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi})$
- Initialize $\left(\boldsymbol{\mu}^{(0)}, \boldsymbol{\Sigma}^{(0)}, \boldsymbol{\phi}^{(0)}\right)$ randomly
  - $\boldsymbol{\phi}^{(0)}$ must be non-negative and sum to 1.
- At iteration t:
  - **E step:** compute $T_{ki} = P\left(z = k \middle| \boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right) = \phi_k^{(t)} \mathcal{N}(\boldsymbol{x} | \, \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})/C$ for any index $k = \overline{1, K}, i = \overline{1, M}$
  - **M step:** update for any *k*,

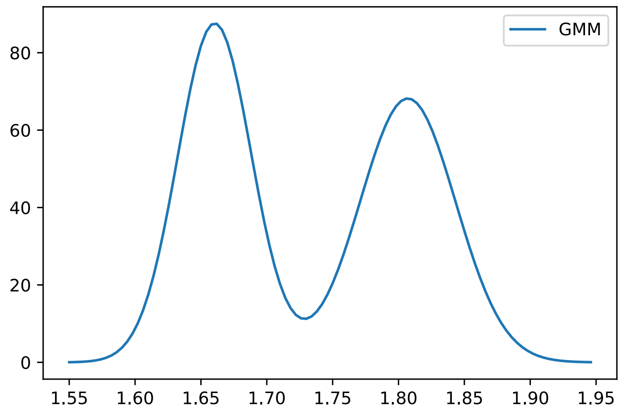
$$\phi_k^{(t+1)} = \frac{a_k}{M}, \qquad \text{where } a_k = \sum_{i=1}^{M} T_{ki} \, ;$$

$$\boldsymbol{\mu}_k^{(t+1)} = \frac{1}{a_k} \sum_{i=1}^{M} T_{ki} \boldsymbol{x}_i \, ; \quad \boldsymbol{\Sigma}_k^{(t+1)} = \frac{1}{a_k} \sum_{i=1}^{M} T_{ki} \left(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)}\right) \left(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)}\right)^T$$

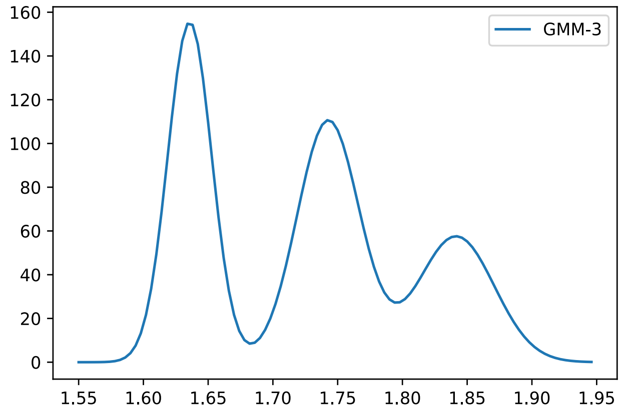
- If not convergence, go to iteration $t + 1$.

GMM: example 1

- We wish to model the height of a person
  - We had collected a dataset from 10 people in Hanoi + 10 people in Sydney
    D={1.6, 1.7, 1.65, 1.63, 1.75, 1.71, 1.68, 1.72, 1.77, 1.62, 1.75, 1.80, 1.85, 1.65, 1.91, 1.78, 1.88, 1.79, 1.82, 1.81}



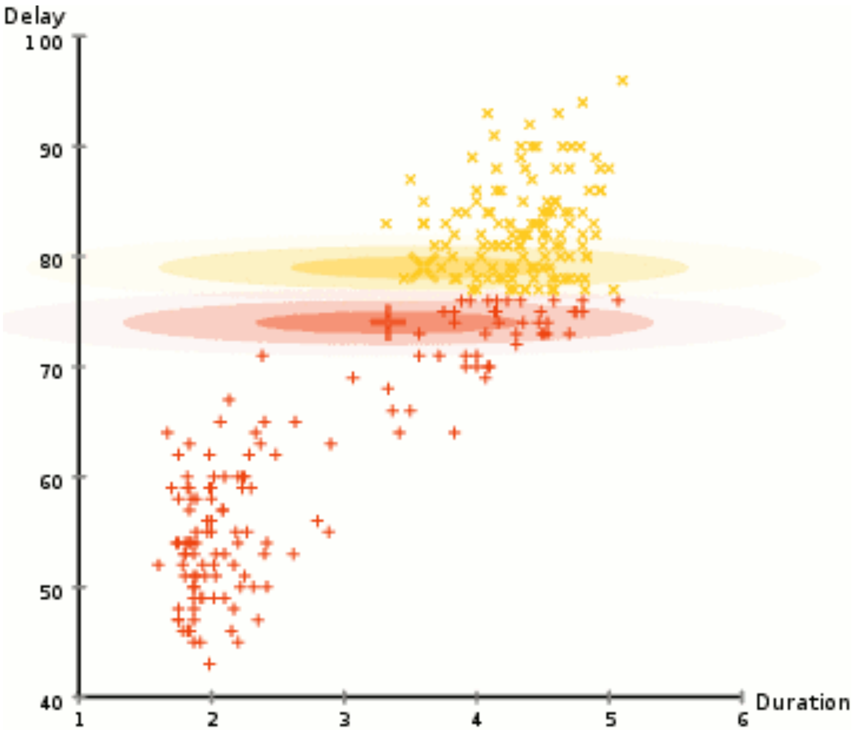
GMM with
2 components



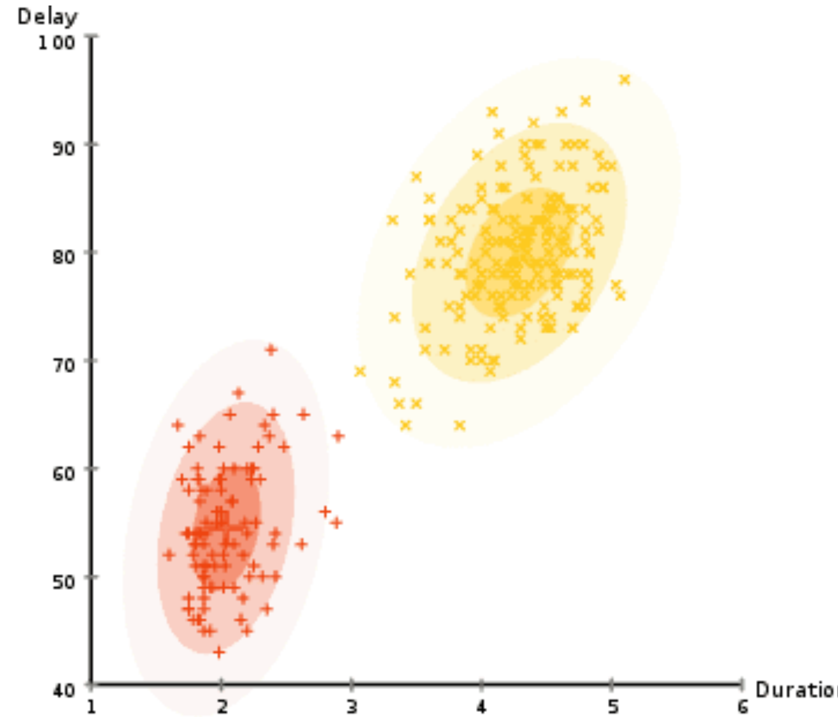
GMM with
3 components

GMM: example 2

- A GMM is fitted in a 2-dimensional dataset to do clustering.



From initialization



To convergence

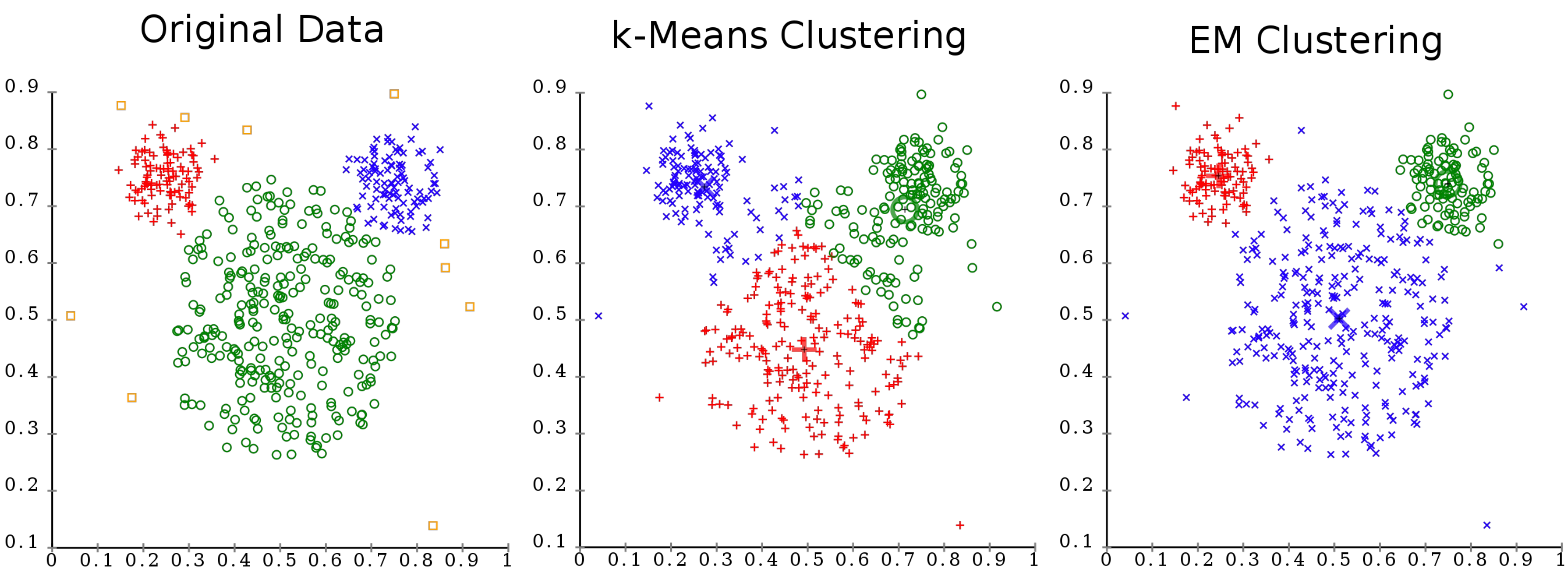
https://en.wikipedia.org/wiki/Expectation-maximization_algorithm

GMM: comparison with K-means

- **K-means:**
  - Step 1: hard assignment
  - Step 2: the means
    → similar shape for the clusters?

- GMM clustering
  - Soft assignment of data to the clusters
  - Parameters $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \phi_k)$
    →different shapes for the clusters

Different cluster analysis results on "mouse" data set:



https://en.wikipedia.org/wiki/Expectation-maximization_algorithm

General models

- We can make the EM algorithm in more general cases.
- Consider a model $B(\boldsymbol{x}, \boldsymbol{z};\ \boldsymbol{\theta})$ with observed variable **x**, hidden variable **z**, and parameterized by $\boldsymbol{\theta}$
  (mô hình có một biến **x** quan sát được, biến ẩn **z**, và tham số $\boldsymbol{\theta}$)
  - **x** depends on **z** and $\boldsymbol{\theta}$, while **z** may depend on $\boldsymbol{\theta}$
  - Mixture models: each observed data point has a corresponding latent variable, specifying the mixture component which generated the data point
- The learning task is to find a specific model, from the model family parameterized by $\boldsymbol{\theta}$, that maximizes the log-likelihood of training data **D**:
$$\boldsymbol{\theta}^* = \mathrm{argmax}_{\boldsymbol{\theta}} \log P(\boldsymbol{D}|\boldsymbol{\theta})$$
- We assume **D** consists of i.i.d samples of **x**, the the log-likelihood function can be expressed analytically, $LB(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}\in\boldsymbol{D}} \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(\boldsymbol{x}, z|\boldsymbol{\theta})$ can be computed easily (hàm log-likelihood có thể viết một cách tường minh)
  - Since there is a latent variable, MLE may not have a close form solution

The Expectation Maximization algorithm

- The Expectation maximization (EM) algorithm was introduced in 1977 by Arthur Dempster, Nan Laird, and Donald Rubin.
- The EM algorithm maximizes the lower bound of the log-likelihood

$$\mathrm{L}(\boldsymbol{\theta}; \boldsymbol{D}) = \log P(\boldsymbol{D}|\boldsymbol{\theta}) \geq LB(\boldsymbol{\theta}) = \sum_{\boldsymbol{x} \in \boldsymbol{D}} \mathbb{E}_{z|\boldsymbol{x},\boldsymbol{\theta}} \log P(\boldsymbol{x}, z|\boldsymbol{\theta})$$

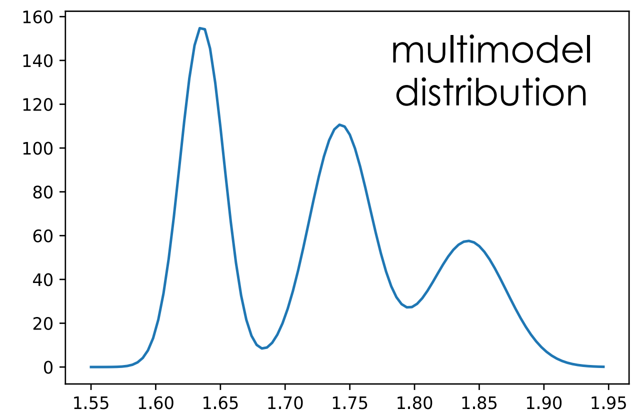
- *Initialization:* $\boldsymbol{\theta}^{(0)}, t = 0$
- *At iteration* t*:*
  - ***E step:*** *compute the expectation* $Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right) = LB\left(\boldsymbol{\theta}^{(t-1)}\right)$
    (tính hàm kỳ vọng Q khi cố định giá trị $\boldsymbol{\theta}^{(t)}$ đã biết ở bước trước)
  - ***M step:*** *find* $\boldsymbol{\theta}^{(t+1)} = \operatorname{argmax}_{\boldsymbol{\theta}} Q\left(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}\right)$
    (tìm điểm $\boldsymbol{\theta}^{(t+1)}$ mà làm cho hàm Q đạt cực đại)
- *If not convergence, go to iteration* $t + 1$.

EM: covergence condition

- Different conditions can be used to check convergence
  - $LB(\boldsymbol{\theta})$ does not change much between two consecutive iterations
  - $\boldsymbol{\theta}$ does not change much between two consecutive iterations
- In practice, we sometimes need to limit the maximum number of iterations

EM: some properties

- The EM algorithm is guaranteed to return a stationary point of the lower bound $LB(\boldsymbol{\theta})$
  (thuật toán EM đảm bảo sẽ hội tụ về một điểm dừng của hàm cận dưới)
  - It may be the local maximum
- Due to maximizing the lower bound, EM does not necessarily returns the maximizer of the log-likelihood function
  (EM chưa chắc trả về điểm cực đại của hàm log-likelihood)
  - No guarantee exists
  - It can be seen in cases of multimodel,
    where the log-likelihood function is non-concave
- The Baum-Welch algorithm is the a special case of EM for hidden Markov models

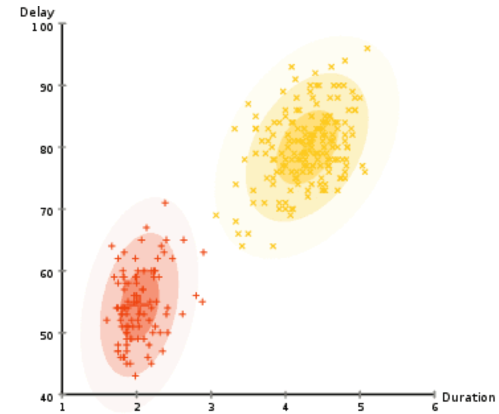


EM, mixture model, and clustering

- *Mixture model:* we assume the data population is composed of K different components (distributions), and each data point is generated from one of those components
  - E.g., Gaussian mixture model, categorical mixture model, Bernoulli mixture model,…
  - The mixture density function can be written as

$$f(\boldsymbol{x}; \boldsymbol{\theta}, \boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k f_k(\boldsymbol{x} \,|\boldsymbol{\theta}_k)$$

  where $f_k(\boldsymbol{x} \,|\boldsymbol{\theta}_k)$ is the density of the *k*-th component



- We can interpret that a mixture distribution partitions the data space into different regions, each associates with a component
  (Một phân bố hỗn hợp tạo ra một cách chia không gian dữ liệu ra thành các vùng khác nhau, mà mỗi vùng tương ứng với 1 thành phần trong hỗn hợp đó)
- Hence, mixture models provide solutions for clustering
- The EM algorithm provides a natural way to learn mixture models

EM: limitation

- When the lower bound $LB(\boldsymbol{\theta})$ does not admit easy computation of the expectation or maximization steps
  - Admixture models, Bayesian mixture models
  - Hierarchical probabilistic models
  - Nonparametric models
- EM finds a point estimate, hence easily gets stuck at a local maximum
- In practice, EM is sensitive with initialization
  - Is it good to use the idea of K-means++ for initialization?
- Sometimes EM converges slowly in practice

Further?

- Variational inference
  - Inference for more general models
- Deep generative models
  - Neural networks + probability theory
- Bayesian neural networks
  - Neural networks + Bayesian inference
- Amortized inference
  - Neural networks for doing Bayesian inference
  - Learning to do inference

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