Introduction to

Machine Learning and Data Mining

(Học máy và Khai phá dữ liệu)

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Content

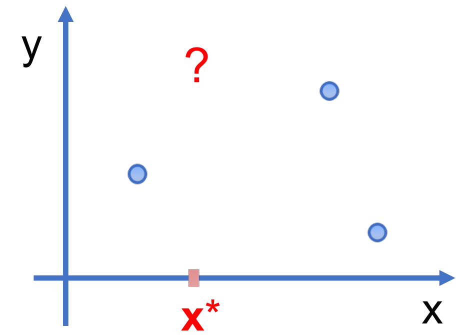
- Introduction to Machine Learning & Data Mining
- Unsupervised learning
- Supervised learning
- **Probabilistic modeling**
- Practical advice

Why probabilistic modeling?

- Inferences from data are intrinsically uncertain.
  (suy diễn từ dữ liệu thường không chắc chắn)
- Probability theory: *model uncertainty* instead of ignoring it!
- Inference or prediction can be done by using probabilities.
- Applications: Machine Learning, Data Mining, Computer Vision, NLP, Bioinformatics, …
- The goal of this lecture
  - Overview about probabilistic modeling
  - Key concepts
  - Application to classification & clustering

Data

- Let **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_M$, y_M)} be a dataset with *M* instances.
  - Each $\mathbf{x}_i$ is a vector in an *n*-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$. Each dimension represents an attribute.
  - y is the output (response), univariate
- **Prediction:** given data **D**, what can we say about *y** at an unseen input ***x****?



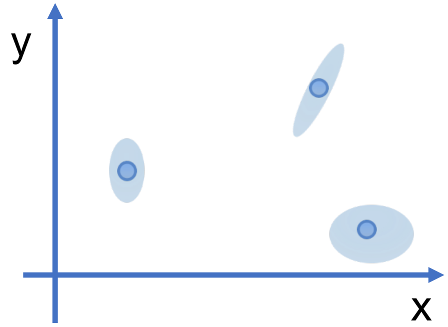
- To make predictions, we need to make **assumptions**
- A **model H** (mô hình) encodes these assumptions, and often depends on some parameters $\boldsymbol{\theta}$, e.g.,

$$y = f(\boldsymbol{x}|\boldsymbol{\theta})$$

- **Learning** (estimation) is to find an $h \in \boldsymbol{H}$ from a given **D**.

Uncertainty

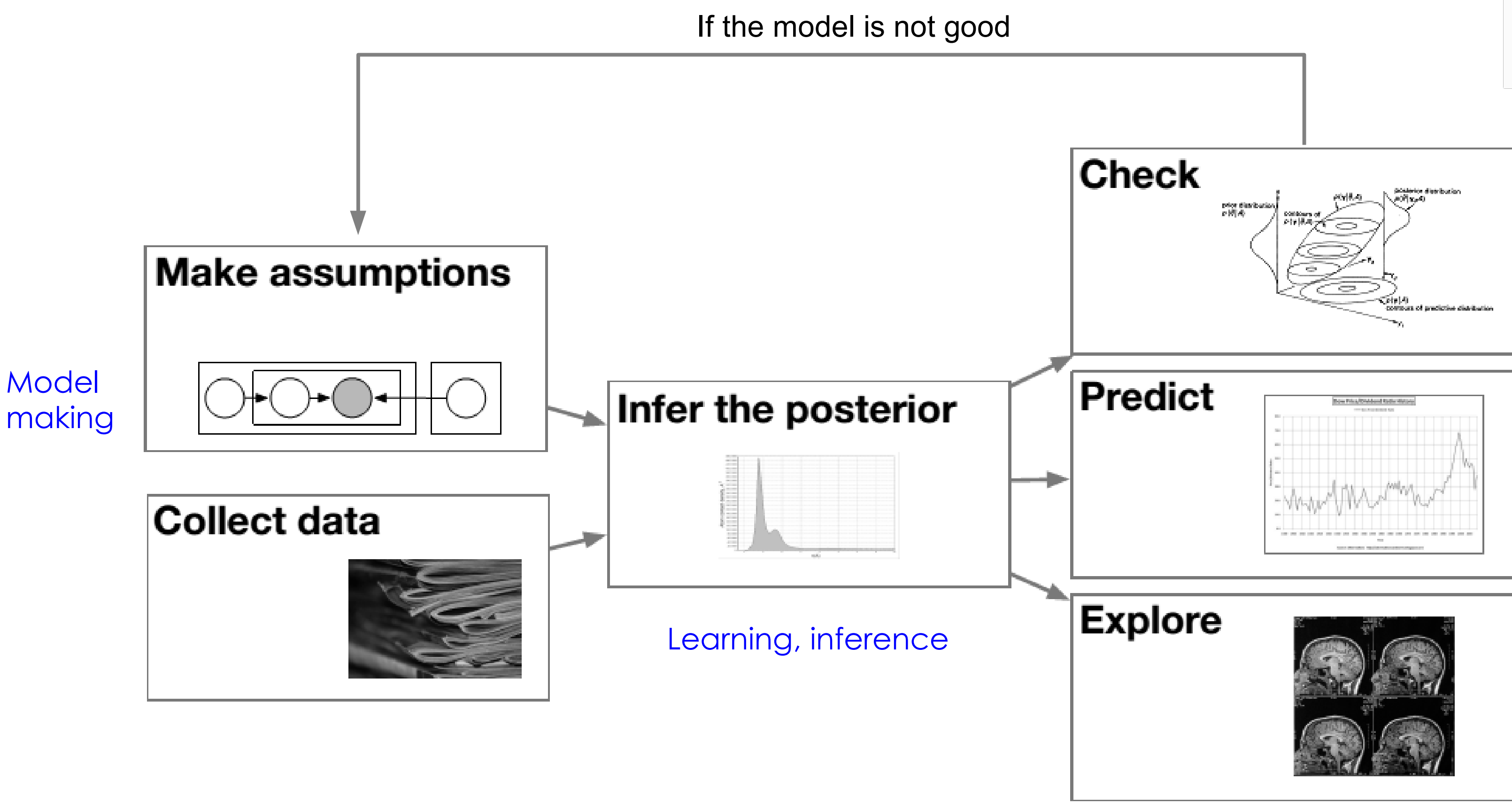
- Uncertainty apprears in any step
  - Measurement uncertainty (**D**)
  - Parameter uncertainty (**θ**)
  - Uncertainty regarding the correct model (**H**)
- Measurement uncertainty
  - Uncertainty can occur in both inputs and outputs.



- How to represent uncertainty?

→ **Probability theory**

The modeling process



[Blei, 2012]

Basics of Probability Theory

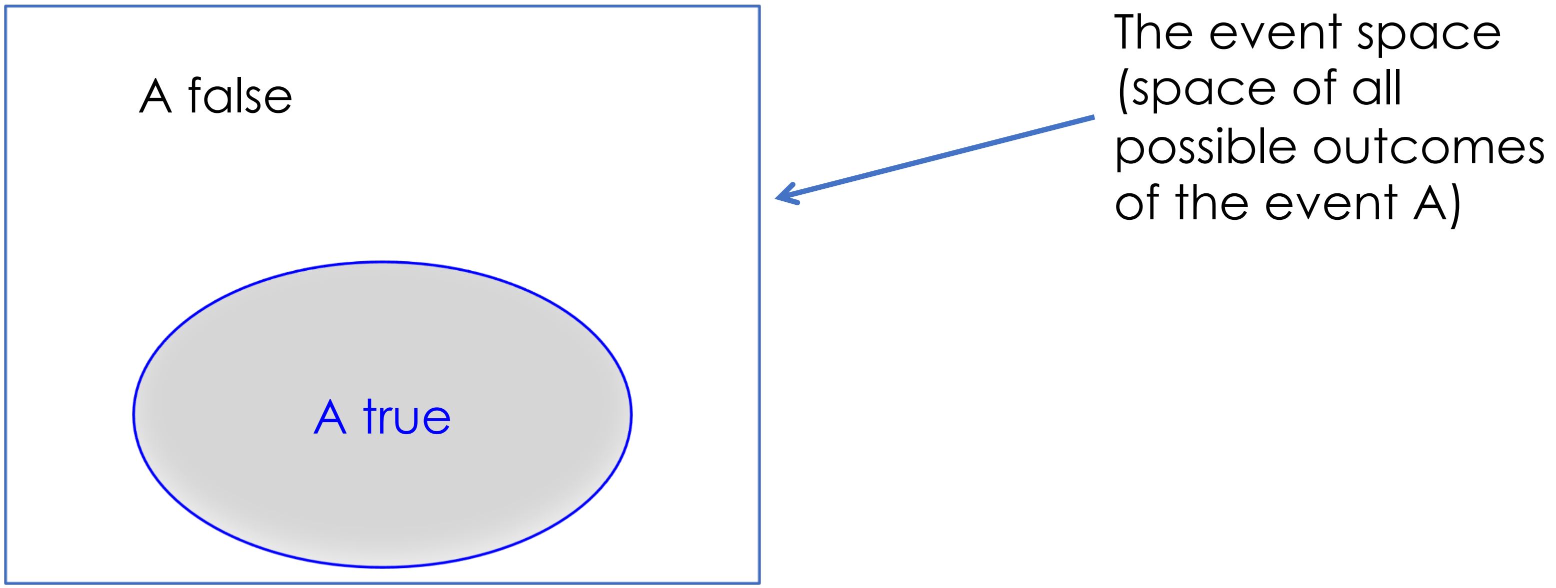
Basic concepts in Probability Theory

- Assume we do an experiment with random outcomes, e.g., tossing a die.
- *Space S of outcomes:* the set of all possible outcomes of an experiment
  - Ex: S = {1, 2, 3, 4, 5, 6} for tossing a die

- *Event E:* a subset of the outcome space S.
  - Ex: E = {1} the event that the die appears 1.
  - Ex: E = {1, 3, 5} the event that the die appears odd.
- *Space W of events:* the space of all possible events
  - Ex: W contains all possible tosses
- *Random variable:* represents a random event, and has an associated probability of occurrence of that event.

Probability visualization

- Probability represents the likelihood/possibility that an event A occurs.
  - Denoted by P(A).
- P(A) is the proportion of the subspace that A is true.



Binary random variables

- A binary (boolean) random variable can receive only value of either *True* or *False*.
- Some axioms:
  - $0 \leq P(A) \leq 1$
  - P(true)= 1
  - P(false)= 0
  - $P(A \text{ or } B) = P(A) + P(B) - P(A, B)$
- Some consequences:
  - P(not A) = P(~A)= 1 - P(A)
  - P(A)= P(A, B) + P(A, ~B)

Multinomial random variables

- A multinomial random variable can receive one from K possible values of $\{v_1, v_2, \ldots, v_k\}$.

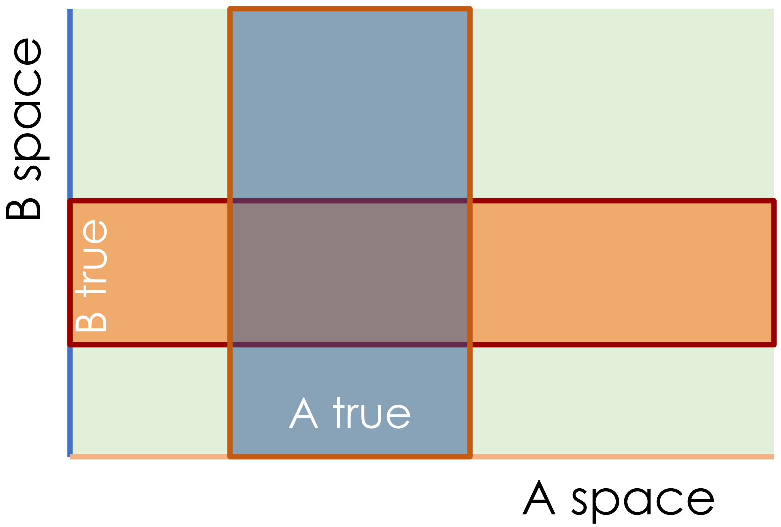
$$P(A = v_i, A = v_j) = 0 \text{ if } i \neq j$$

$$P\left(\bigcup_{n=1}^{m} (A = v_n)\right) = \sum_{n=1}^{m} P(A = v_n)$$

$$P\left(\bigcup_{n=1}^{k} (A = v_n)\right) = \sum_{n=1}^{k} P(A = v_n) = 1$$

Joint probability (1)

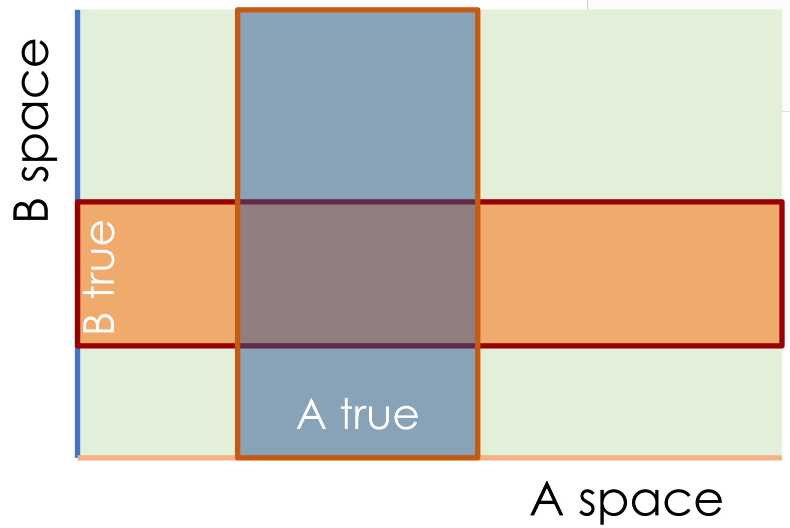
- Joint probability:
  - The possibility of A and B that occur simutaneously.
  - P(A,B) is the proportion of the space in which both A and B are true.
- Ex:
  - A: I will play football tomorrow.
  - B: John will not play football.
  - P(A,B): the probability that I will but John will not play football tomorrow.



Joint probability (2)

- Denote S_A the space of A.
- Denote S_B the space of B.
- Denote S_{AB} the space of (A, B).

$$S_{AB} = S_A \times S_B$$



- Then:

$$P(A,B) = |T_{AB}| \, / \, |S_{AB}|$$

  - T_{AB} is the space in which both A and B are true.
  - $|X|$ denotes the volumn of the set X.

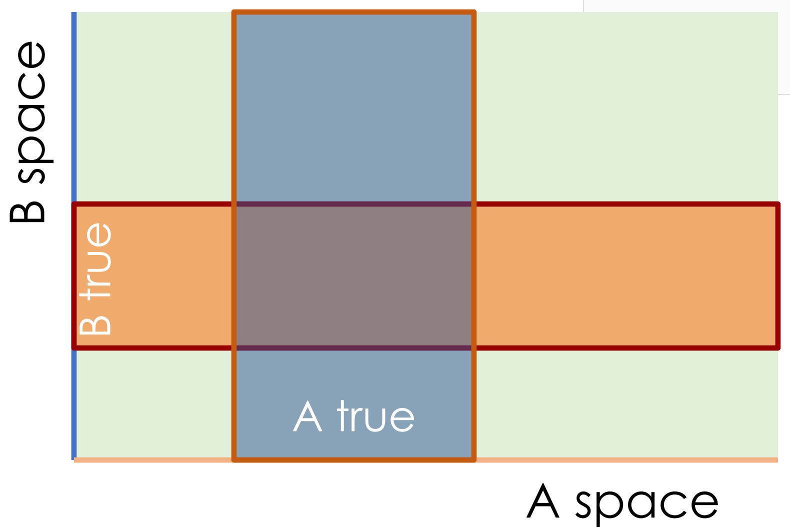
Conditional probability (1)

- Conditional probability:
  - P(A|B): the possibility that A happens given that B has already occurred.
  - P(A|B) is the proportion of the space in which A occurs, knowing that B is true.
- Ex:
  - A: I will play football tomorrow.
  - B: it will not rain tomorrow.
  - P(A|B): the probability that I will play football, provided that it will not rain tomorrow.
- What is different between joint and conditional probabilities?

Conditional probability (2)

- We have:

$$P(A \mid B) = \frac{P(A,B)}{P(B)}$$



- Some consequences:

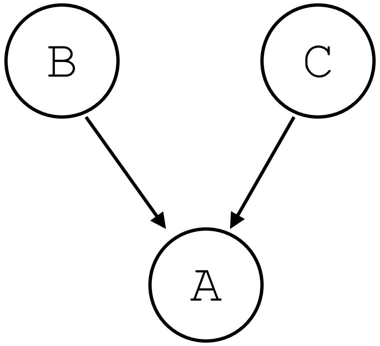
P(A,B) = P(A | B) . P(B)

P(A | B) + P(~A | B) = 1

$$\sum_{i=1}^{k} P(A = v_i \mid B) = 1$$

Conditional probability (3)

- P(A|B, C) shows the probability of A given that B and C already has occurred.
- Ex:
  - A: I will wander over the near river tomorrow morning.
  - B: it will be very nice tomorrow morning.
  - C: I will wake up early tomorrow morning.
  - P(A|B, C): the probability that wander over the near river, provided that it will be very nice and I will wake up early tomorrow morning.



P(A|B,C)

Statistical independence (1)

- Two events A and B are called ***Statistically Independent*** if the the probability that A occurs does not change with respect to the occurrence of B.
  - $P(A|B) = P(A)$.
- Ex:
  - A: I will play football tomorrow.
  - B: the pacific ocean contains many fishes.
  - $P(A|B) = P(A)$: the fact that the pacific ocean contains many fishes does not affect my decision to play football tomorrow.

Statistical independence (2)

- Assume P(A | B) = P(A), we have:
  - P(~A | B) = P(~A)
  - P(B | A) = P(B)
  - P(A,B) = P(A). P(B)
  - P(~A,B) = P(~A). P(B)
  - P(A,~B) = P(A). P(~B)
  - P(~A,~B) = P(~A). P(~B).

Conditional independence

- Two events A and C are called ***Conditionally Independent*** given B if P(A | B, C) = P(A | B).
- Ex:
  - A: I will play football tomorrow.
  - B: the football match will happen in-house tomorrow.
  - C: it will not rain tomorrow.
  - P(A | B, C) = P(A | B).

Some rules in probability theory

- Chain rules:
  - $P(A,B) = P(A|B).P(B) = P(B|A).P(A)= P(B,A)$
  - $P(A|B) = P(A,B)/P(B) = P(B|A).P(A)/P(B)$
  - $P(A,B|C) = P(A,B,C)/P(C) = P(A|B,C).P(B,C)/P(C)$
    $= P(A|B,C).P(B|C).$
- Independence:
  - $P(A|B) = P(A)$
    if A and B are statistically independent.
  - $P(A,B|C) = P(A|C).P(B|C)$
    if A and B are statistically independent, conditioned on C.
  - $P(A_1,\ldots,A_n|C) = P(A_1|C)\ldots P(A_n|C)$
    if $A_1,\ldots,A_n$ are statistically independent, conditioned on C.

Product and sum rules

- Consider x and y are discrete random variables. Their domains are X and Y respectively
- **Product rule:**

$$P(x, y) = P(x|y)P(y)$$

- **Sum rule**

$$P(x) = \sum_{y \in Y} P(x, y)$$

- The summation (tổng) should be integration (tích phân) if y is continuous
  (tổng sẽ được thay bằng tích phân nếu biến y liên tục)

Bayes' rule

$$P(\boldsymbol{\theta}|\boldsymbol{D}) = \frac{P(\boldsymbol{D}|\boldsymbol{\theta})P(\boldsymbol{\theta})}{P(\boldsymbol{D})}$$

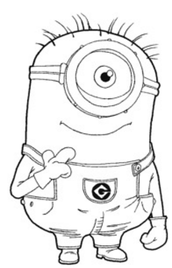
- P($\boldsymbol{\theta}$): *prior probability* (xác suất tiên nghiệm) of the variable $\boldsymbol{\theta}$.
  - Our uncertainty about $\boldsymbol{\theta}$ before observing data.
- P(**D**): prior probability that we can observe data **D**.
- P(**D** | $\boldsymbol{\theta}$): probability (*likelihood*) that we can observe data **D** provided that $\boldsymbol{\theta}$ is known.
- P($\boldsymbol{\theta}$ | **D**): *posterior probability* (xác suất hậu nghiệm) of $\boldsymbol{\theta}$ if we already have observed data **D**.
  - Bayesian approach bases on this quatity.

Probabilistic models

Model, inference, learning

Probabilistic model

- Our assumption on how the data were generated
  (giả thuyết của chúng ta về quá trình dữ liệu đã được sinh ra như thế nào)
- Example: how a sentence is generated?
  - We assume our brain does as follow:
  - *First choose the topic of the sentence*
  - *Generate the words one-by-one to form the sentence*
- How will TIM be drawn?



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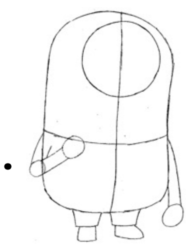

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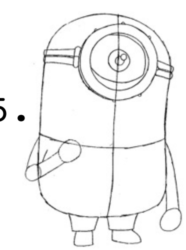
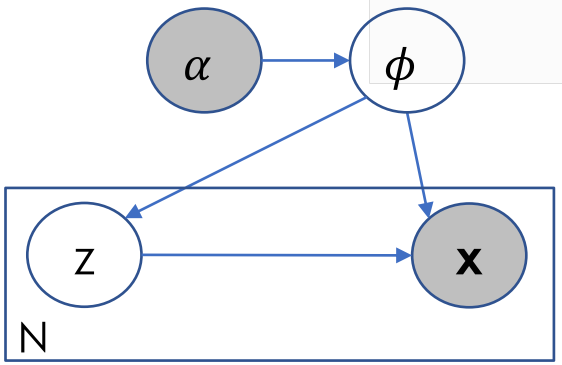


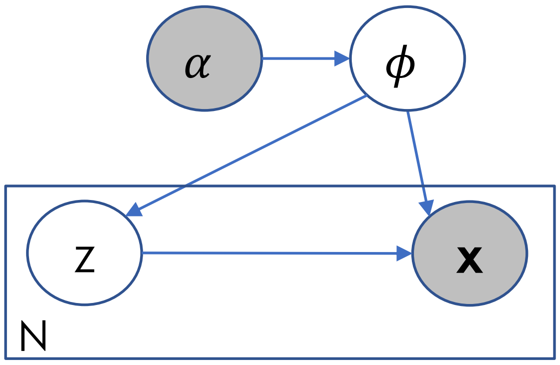
Probabilistic model

- A model sometimes consists of
  - **Observed variable** (e.g., $\boldsymbol{x}$) which models the observation (data instance) (biến quan sát được)
  - **Hidden variable** which describes the hidden things (e.g., z, ϕ) (biến ẩn)
  - **Local variable** (e.g., $z, \boldsymbol{x}$) which associates with one data instance
  - **Global variable** (e.g., ϕ) which is shared across the data instances, and is the representative of the model
  - **Relations** between the variables
- Each variable follows some probability distribution (mỗi biến tuân theo một phân bố xác suất nào đó)



Different types of models

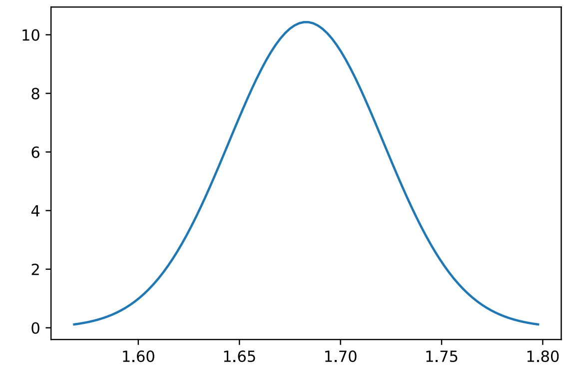
- **Probabilistic graphical model (PGM):** Graph + Probability Theory (mô hình đồ thị xác suất)
  - Each vertex represents a random variable, grey circle means “observed”, white circle means “latent”
  - Each edge represents the conditional dependence between two variables
  - *Directed graphical model:* each edge has a direction
  - *Undirected graphical model:* no direction in the edges



- Latent variable model: a PGM which has at least one latent variable
- Bayesian model: a PGM which has a prior distribution on its parameter

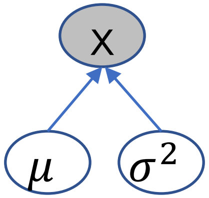
Univariate normal distribution

- We wish to model the height of a person
  - We had collected a dataset from 10 people in Hanoi:
    D={1.6, 1.7, 1.65, 1.63, 1.75, 1.71, 1.68, 1.72, 1.77, 1.62}
- Let x denote the random variable that represents the height of a person
- **Assumption:** x follows a Normal distribution (Gaussian) with the following *probability density function* (PDF)



$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

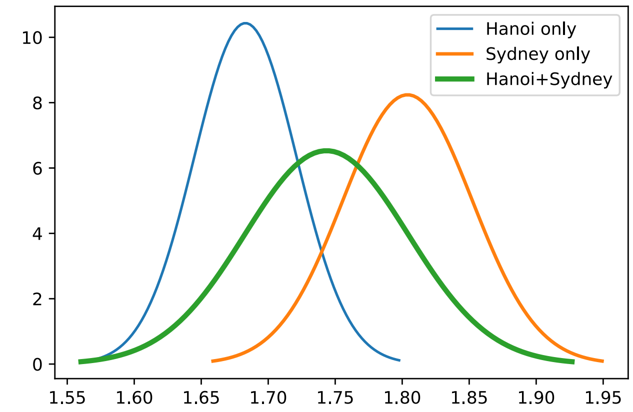
  - where $\{\mu, \sigma^2\}$ are the mean and variance
- Note:
  - $\mathcal{N}(x|\mu,\sigma^2)$ represents the class of normal distributions
  - This class is parameterized by $\boldsymbol{\theta} = (\mu, \sigma^2)$



- **Learning:** we need to know specific values of $\{\mu, \sigma^2\}$

Univariate Gaussian mixture model (1)

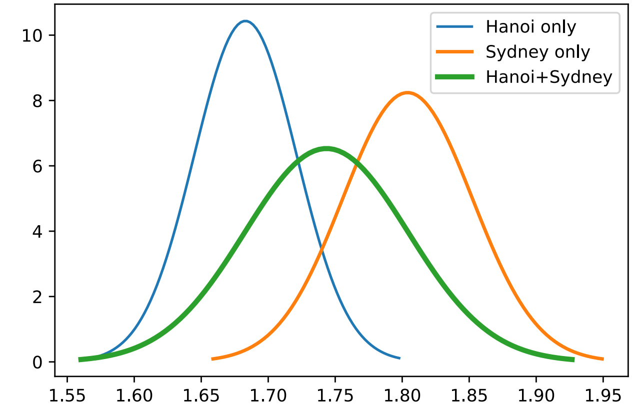
- We wish to model the height of a person
  - We had collected a dataset from 10 people in Hanoi + 10 people in Sydney **D**={1.6, 1.7, 1.65, 1.63, 1.75, 1.71, 1.68, 1.72, 1.77, 1.62, 1.75, 1.80, 1.85, 1.65, 1.91, 1.78, 1.88, 1.79, 1.82, 1.81}
- Let x denote the random variable that represents the height
- If we use Normal distribution:
  - Blue curve models the height in Hanoi
  - Orange curve models the height in Sydney
  - Green curve models the whole **D**



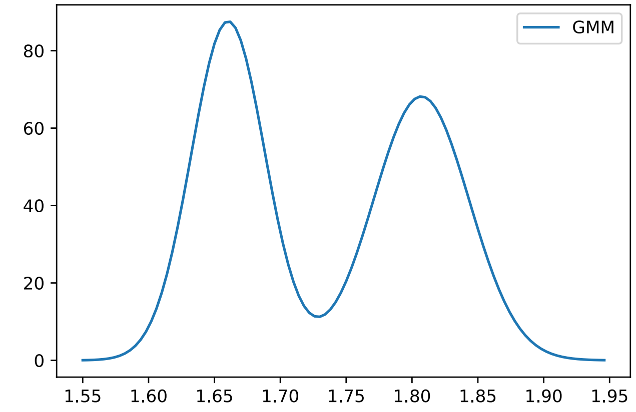
- Univariate Gaussian does not model well the underlying distribution
  - Mixture model?
    (mô hình hỗn hợp)

Univariate Gaussian mixture model (2)

- **Assumption**: the data are generated from two different Gaussians, and each instance is generated from one of those two Gaussians.
  Generative process:
  - *Pick the component index:* $z \sim Multinomial(z|\phi)$
  - *Generate sample:* $x \sim Normal(x \mid \mu_z, \sigma_z^2)$



- This is **Gaussian mixture model** (GMM) (mô hình hỗn hợp Gauss)
  - (μ_1, σ_1^2) represents the first Gaussian
  - (μ_2, σ_2^2) represents the second Gaussian
  - $\phi \in [0,1]$ is the parameter of the Multinomial distribution, $P(z = 1 | \phi) = \phi = 1 - P(z = 2 | \phi)$



- Density function of the GMM:

$$\phi \mathcal{N}(x|\mu_1, \sigma_1^2) + (1 - \phi)\mathcal{N}(x|\mu_2, \sigma_2^2)$$

Note: "~" means "follows" (tuân theo)

GMM: Multivariate case

- Consider the case each **x** belongs to the *n*-dimensional space $\mathbb{R}^n$.
- GMM: we assume that the data are samples from *K* Gaussian distributions.
- Each instance **x** is generated from one of those K Gaussians by the following ***generative process***:
  - *Take the component index* $z \sim Multinomial(z|\boldsymbol{\phi})$
  - *Generate* $\boldsymbol{x} \sim Normal(\boldsymbol{x} \mid \boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- The density function is

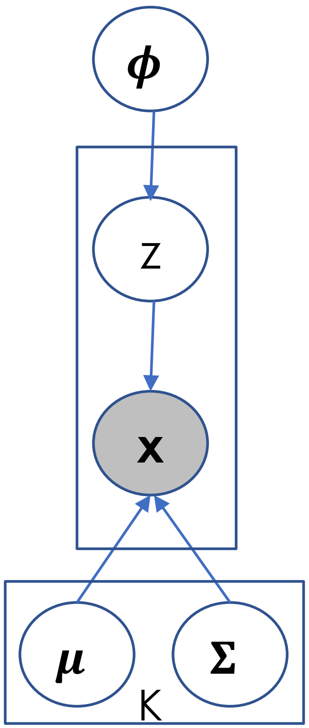
$$p(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

  - $\boldsymbol{\phi} = (\phi_1, \dots, \phi_K)$ represents the weights of the Gaussians

$$\sum_{k=1}^{K} \phi_k = 1, \qquad \phi_j \geq 0, \qquad \forall j$$

  - Each multivariate Gaussian has density

$$\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right]$$

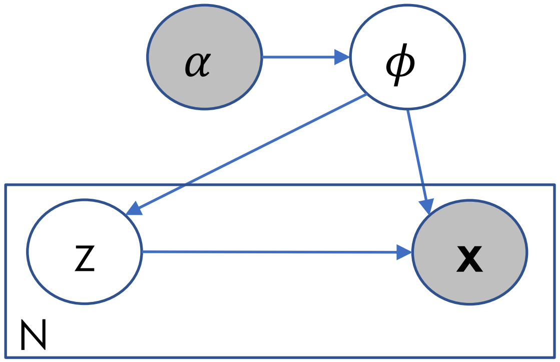


PGM: some well-known models

- Gaussian mixture model (GMM)
  - Modeling real-valued data
- Latent Dirichlet allocation (LDA)
  - Modeling the topics hidden in textual data
- Hidden Markov model (HMM)
  - Modeling time-series, i.e., data with time stamps or sequential nature
- Conditional Random Field (CRF)
  - for structured prediction
- Deep generative models
  - Modeling the hidden structures, generating artificial data

Probabilistic model: two problems

- **Inference** for a given instance $\boldsymbol{x}_n$
  - Recovery of the local variable (e.g., z_n), or
  - The distribution of the local variables (e.g., $P(z_n, \boldsymbol{x}_n | \phi)$)
  - Example: for GMM, we want to know z_n indicating which Gaussian did generate $\boldsymbol{x}_n$



- **Learning (estimation)**
  - Given a training dataset, estimate the joint distribution of the variables
    - E.g., estimate $P(\phi, z_1, \dots, z_n, \boldsymbol{x}_1, \dots, \boldsymbol{x}_n | \alpha)$
    - E.g., estimate $P(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n | \alpha)$
    - E.g., estimate α
    - Inference of local variables is often needed

Inference and Learning

MLE, MAP

Some inference approaches (1)

- Let D be the data, and *h* be a hypothesis
  - hypothesis: unknown parameter, hidden variables, …
- **Maximum Likelihood Estimation (MLE, cực đại hoá khả năng)**

$$h^* = \arg\max_{h \in \boldsymbol{H}} P(D|h)$$

  - Finds h* (in the hypothesis space **H**) that maximizes the likelihood of the data.
  - *Other words: MLE makes inference about the model that is most likely to have generated the data.*
- **Bayesian inference** (suy diễn Bayes) considers the transformation of our prior knowledge $P(h)$, through the data D, into the posterior knowledge $P(h|D)$.
  - Remember the Bayes'rule: $P(h|D) = P(D|h)P(h)/P(D)$. So

$$P(h|D) \propto P(D|h) * P(h)$$

(Posterior ∝ Likelihood * Prior)

Some inference approaches (2)

- In some cases, we may know the prior distribution of *h*.
- **Maximum a Posterior Estimation (MAP, cực đại hoá hậu nghiệm)**

$$h^* = \arg\max_{h \in \boldsymbol{H}} P(h|\boldsymbol{D}) = \arg\max_{h \in \boldsymbol{H}} P(\boldsymbol{D}|h)\, P(h)/P(\boldsymbol{D})$$

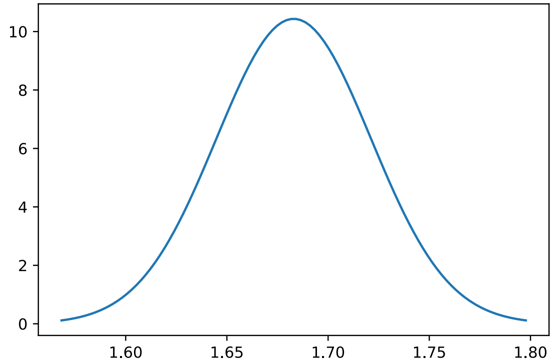
$$= \arg\max_{h \in \boldsymbol{H}} P(\boldsymbol{D}|h)\, P(h)$$

  - Finds h* that maximizes the posterior probability of h.
  - MAP finds a point (posterior mode), not a distribution → point estimation
- MLE is a special case of MAP, when using uniform prior over *h*.
- *Full Bayesian inference* tries to estimate the full posterior distribution $P(h|\boldsymbol{D})$, not just a point *h**.
- Note:
  - MLE, MAP, or full Bayesian approaches can be applied to both learning and inference.

MLE: Gaussian example (1)

- We wish to model the height of a person, using the dataset **D** = {1.6, 1.7, 1.65, 1.63, 1.75, 1.71, 1.68, 1.72, 1.77, 1.62}
  - Let x be the random variable representing the height of a person.
  - Model: assume that x follows a Gaussian distribution with ***unknown*** mean μ and variance σ^2
  - **Learning:** estimate (μ, σ) from the given data $\boldsymbol{D} = \{x_1, \dots, x_{10}\}$.
- Let $f(x|\mu, \sigma)$ be the density function of the Gaussian family, parameterized by (μ, σ).
  - $f(x_n|\mu, \sigma)$ is the likelihood of instance x_n.
  - $f(\boldsymbol{D}|\mu, \sigma)$ is the likelihood function of **D**.
- Using MLE, we will find

$$(\mu_*, \sigma_*) = \arg\max_{\mu,\sigma} f(\boldsymbol{D}|\mu, \sigma)$$



MLE: Gaussian example (2)

- **i.i.d assumption:** we assume that the data are independent and identically distributed (dữ liệu được sinh ra một cách độc lập)
  - As a result, we have $P(\boldsymbol{D}|\mu,\sigma) = P(x_1,\ldots,x_{10}|\mu,\sigma) = \prod_{i=1}^{10} P(x_i|\mu,\sigma)$
- Using this assumption, MLE will be

$$(\mu_*,\sigma_*) = \arg\max_{\mu,\sigma} \prod_{i=1}^{10} f(x_i|\mu,\sigma) = \arg\max_{\mu,\sigma} \prod_{i=1}^{10} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

$$= \arg\max_{\mu,\sigma} \log \prod_{i=1}^{10} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

Log trick, $\log \stackrel{\text{def}}{=} \ln$

$$= \arg\max_{\mu,\sigma} \sum_{i=1}^{10} \left(-\frac{1}{2\sigma^2}(x_i-\mu)^2 - \log\sqrt{2\pi\sigma^2}\right)$$

- Using gradients (w.r.t μ, σ), we can find

$$\mu_* = \frac{1}{10}\sum_{i=1}^{10} x_i = 1.683, \qquad \sigma_*^2 = \frac{1}{10}\sum_{i=1}^{10}(x_i-\mu_*)^2 \approx 0.0015$$

MAP: Gaussian Naïve Bayes (1)

- Consider the **classification problem**
  - Training data **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_M$, y_M)} with *M* instances, *C* classes.
  - Each $\mathbf{x}_i$ is a vector in the *n*-dimensional space $\mathbb{R}^n$, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$.
- *Model assumption:* we assume there are *C* different Gaussian distributions that generate the data in **D**, and the data with label *c* are generated from a Gaussian distribution parameterized by $(\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$
  - $\boldsymbol{\mu}_c$ is the mean vector, $\boldsymbol{\Sigma}_c$ is the covariance matrix of size $n \times n$.
- *Learning:* we consider $P(\boldsymbol{\mu}, \boldsymbol{\Sigma}, c|\boldsymbol{D})$, where $(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\mu}_C, \boldsymbol{\Sigma}_C)$

$$(\boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \stackrel{\text{def}}{=} \arg\max_{\boldsymbol{\mu},\boldsymbol{\Sigma},c} P(\boldsymbol{\mu}, \boldsymbol{\Sigma}, c|\boldsymbol{D}) = \arg\max_{\boldsymbol{\mu},\boldsymbol{\Sigma},c} P(\boldsymbol{D}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, c)P(c)$$

Bayes' rule, removing P(**D**), assuming uniform prior over $\boldsymbol{\mu}, \boldsymbol{\Sigma}$

  - We estimate P(c) to be the proportion of class *c* in **D**: $P(c) = |\boldsymbol{D}_c|/|\boldsymbol{D}|$ where $\boldsymbol{D}_c$ contains all instances with label *c* in **D**.
  - Since the C classes are independent, we can do learning for each class

$$(\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}) \stackrel{\text{def}}{=} \arg\max_{\boldsymbol{\mu}_c,\boldsymbol{\Sigma}_c} P(\boldsymbol{D}_c|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)P(c) = \arg\max_{\boldsymbol{\mu}_c,\boldsymbol{\Sigma}_c} P(\boldsymbol{D}_c|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

MAP: Gaussian Naïve Bayes (2)

- Assuming the samples are i.i.d, we have

$$(\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}) = \arg\max_{\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c} \prod_{\boldsymbol{x} \in \boldsymbol{D}_c} P(\boldsymbol{x} | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c) = \arg\max_{\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c} \sum_{\boldsymbol{x} \in \boldsymbol{D}_c} \log P(\boldsymbol{x} | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)$$

$$= \arg\max_{\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c} \sum_{\boldsymbol{x} \in \boldsymbol{D}_c} \log \left[\frac{1}{\sqrt{\det(2\pi \boldsymbol{\Sigma}_c)}} \exp\left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}_c)^T \boldsymbol{\Sigma}_c^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_c) \right) \right]$$

$$= \arg\max_{\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c} \sum_{\boldsymbol{x} \in \boldsymbol{D}_c} -\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}_c)^T \boldsymbol{\Sigma}_c^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_c) - \log \sqrt{\det(2\pi \boldsymbol{\Sigma}_c)}$$

- Using gradients (w.r.t $\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c$), we can arrive at

$$\boldsymbol{\mu}_{c*} = \frac{1}{|\boldsymbol{D}_c|} \sum_{\boldsymbol{x} \in \boldsymbol{D}_c} \boldsymbol{x}, \qquad \boldsymbol{\Sigma}_{c*} = \frac{1}{|\boldsymbol{D}_c|} \sum_{\boldsymbol{x} \in \boldsymbol{D}_c} (\boldsymbol{x} - \boldsymbol{\mu}_{c*})(\boldsymbol{x} - \boldsymbol{\mu}_{c*})^T$$

- So, after training we obtain the $(\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}, P(c))$ for each class *c*.

MAP: Gaussian Naïve Bayes (3)

- Trained model: $(\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}, P(c))$ for each class *c*
- Prediction for a new instance **z** by finding the class label that has the highest posterior probability:

Bayes' rule

$$c_z = \arg\max_{c\in\{1,\dots,C\}} P(c|\boldsymbol{z}, \boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}) = \arg\max_{c\in\{1,\dots,C\}} P(\boldsymbol{z}|\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}, c)P(c)$$

$$= \arg\max_{c\in\{1,\dots,C\}} \log P(\boldsymbol{z}|\boldsymbol{\mu}_{c*}, \boldsymbol{\Sigma}_{c*}, c) + \log P(c)$$

$$= \arg\max_{c\in\{1,\dots,C\}} -\frac{1}{2}(\boldsymbol{z}-\boldsymbol{\mu}_{c*})^T \boldsymbol{\Sigma}_{c*}^{-1}(\boldsymbol{z}-\boldsymbol{\mu}_{c*}) - \log\sqrt{\det(2\pi\boldsymbol{\Sigma}_{c*})} + \log P(c)$$

- If using MLE, we do not need to use/estimate the prior P(c).

MAP: Multinomial Naïve Bayes (1)

- Consider the text classification problem (dữ liệu có thuộc tính rời rạc)
  - Training data **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_M$, y_M)} with *M* documents, *C* classes.
  - TF: each document $\mathbf{x}_i$ is represented by a vector of *V* dimensions, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$, each x_{ij} is the *frequency* of term *j* in document $\mathbf{x}_i$
- *Model assumption:* we assume there are *C* different **multinomial distributions** that generate the data in **D**, and the data with label *c* are generated from a multinomial distribution which is parameterized by $\boldsymbol{\theta}_c$ and has probability mass function

$$f(x_1, \ldots, x_V | \theta_{c1}, \ldots, \theta_{cV}) = \frac{\Gamma(\sum_{j=1}^{V} x_j + 1)}{\prod_{j=1}^{V} \Gamma(x_j + 1)} \prod_{k=1}^{V} \theta_{ck}^{x_k}$$

  - $\theta_{cj} = P(x = j | \theta_{cj})$ is the probability that term $j \in \{1, \ldots, V\}$ appears, satisfying $\sum_{k=1}^{V} \theta_{ck} = 1$. Γ is the gamma function.
- *Learning:* we can do similarly with Gaussian Naïve Bayes to estimate $\boldsymbol{\theta}_c = (\theta_{c1}, \ldots, \theta_{cV})$ and P(c) for each class c.

Homework?

MAP: Multinomial Naïve Bayes (2)

- Trained model: $(\boldsymbol{\theta}_{c*}, P(c))$ for each class *c*
- Prediction for a new instance $\boldsymbol{z} = (z_1, \ldots, z_V)^T$ by

$$c_z = \arg\max_{c\in\{1,\ldots,C\}} P(c|\boldsymbol{z}, \boldsymbol{\theta}_{c*}) = \arg\max_{c\in\{1,\ldots,C\}} P(\boldsymbol{z}|\boldsymbol{\theta}_{c*}, c)P(c)$$

$$= \arg\max_{c\in\{1,\ldots,C\}} \log P(\boldsymbol{z}|\boldsymbol{\theta}_{c*}) + \log P(c) \quad \text{(MNB.1)}$$

$$= \arg\max_{c\in\{1,\ldots,C\}} \log \frac{\Gamma(\sum_{j=1}^{V} z_j + 1)}{\prod_{j=1}^{V} \Gamma(z_j + 1)} \prod_{k=1}^{V} \theta_{ck*}^{z_k} + \log P(c)$$

$$= \arg\max_{c\in\{1,\ldots,C\}} \log \prod_{k=1}^{V} \theta_{ck*}^{z_k} + \log P(c)$$

$$= \arg\max_{c\in\{1,\ldots,C\}} \log \prod_{k=1}^{V} P(z_k|\theta_{ck*}) + \log P(c) \quad \text{(MNB.2)}$$

  - The label that gives the highest posterior probability
- Note: we implicitly assume that *the attributes are conditionally independent*, as shown in equations (MNB.1) and (MNB.2).
(ta ngầm giả thuyết rằng các thuộc tính độc lập với nhau)

A revisit to GMM

- Consider learning GMM, with *K* Gaussian distributions, from the training data **D** = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_M$}.
- 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
  - 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

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

- We cannot find a closed-form solution!
  - Approximation and iterative algorithms are needed.

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 suy diễn không khả thi)
  - Inference in many probabilistic models is NP-hard. [Sontag & Roy, 2011; Tosh & Dasgupta, 2019]

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