NỀN TẢNG AI TẠO SINH

(IT5410 – Foundation of Generative AI)

MÔ HÌNH SINH SÂU
VAE

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Nội dung

- Mở đầu
- Một số vấn đề của Học sâu
- Một số kiến trúc mạng nơron
- **Mô hình sinh sâu**
- Đánh giá chất lượng
- Học tăng cường

Some successes: Image + Video generation

Midjourney

Imagen
Imagen
Imagen

An extremely angry bird.

A cute corgi lives in a house made out of sushi.

Generative Models

- Probabilistic models of data

- Sample: lấy mẫu dữ liệu (sinh/tạo ra dữ liệu)

- Evaluate likelihood: tính likelihood của mẫu dữ liệu cho trước

- Train: huấn luyện

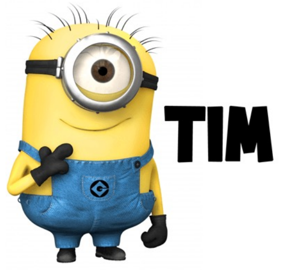
- Representation: biểu diễn mới
- What if all we care about is sampling?
  - *Not in the training data, but the novel samples.*

Probabilistic models

Introduction

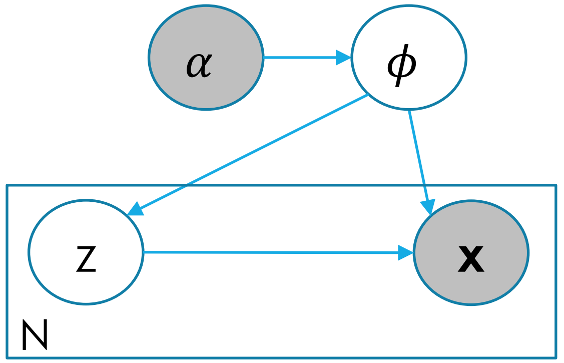
Probabilistic model

- Our assumption on how the data samples were generated
  (giả thuyết của chúng ta về quá trình mà các mẫu 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?



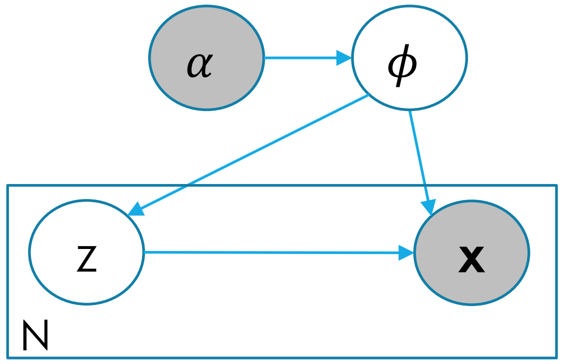
Probabilistic model

- 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 which is used to model only one data instance
  - **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

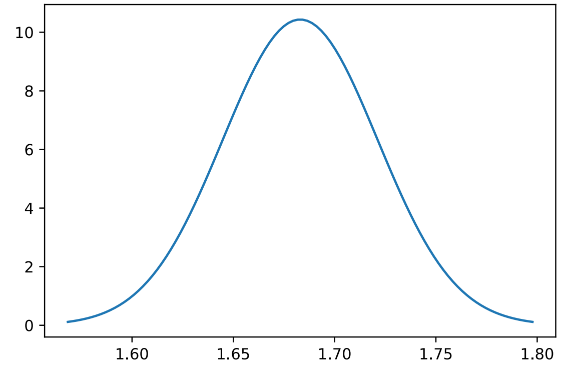


- Latent variable model: a PGM which has at least one latent variable
- **Generative model:** a model that enables us to generate data instances

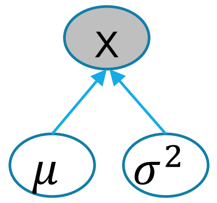
Univariate normal distribution

- We wish to know the average 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 $\boldsymbol{\theta} = (\mu,\sigma^2)$



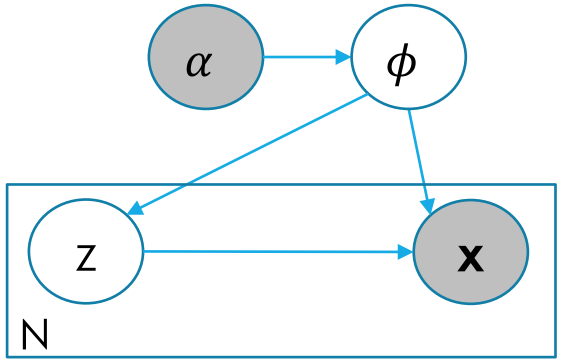
- **Learning:** we need to know specific values of $\{\mu,\sigma^2\}$

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: inference & learning

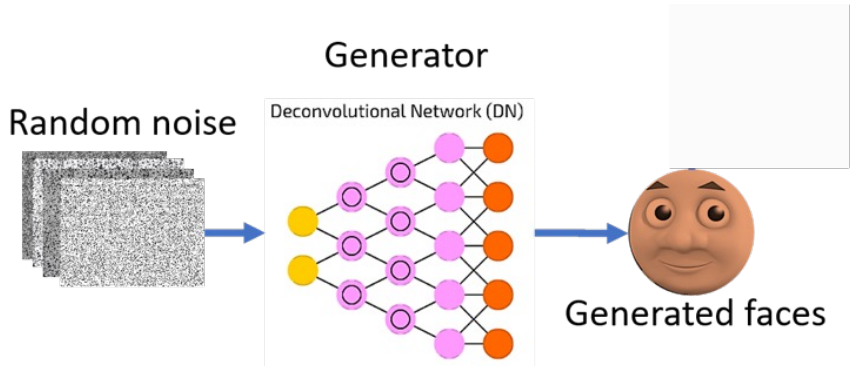
- **Inference** for a given instance $\boldsymbol{x}_n$
  (Suy diễn/phán đoán đối với một quan sát cho trước)
  - Recovery of the local variable (e.g., z_n), or
  - The distribution of the local variables (e.g., $P(z_n|\phi, \boldsymbol{x}_n)$)
  - Example: for GMM, we want to know z_n indicating which Gaussian did generate $\boldsymbol{x}_n$



- **Learning (estimation)**
  (Học/ước lượng mô hình)
  - Given a training dataset, estimate the joint distribution of the variables
    - E.g., estimate the density function $p(\phi, z_1, \ldots, z_n, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_n|\alpha)$
    - E.g., estimate $P(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n|\alpha)$
    - E.g., estimate α
    - Inference of local variables is often needed

Generative model: sampling

- **Sampling** data
  - Make novel data samples, given a trained model
    (tạo ra dữ liệu mới từ mô hình đã có)



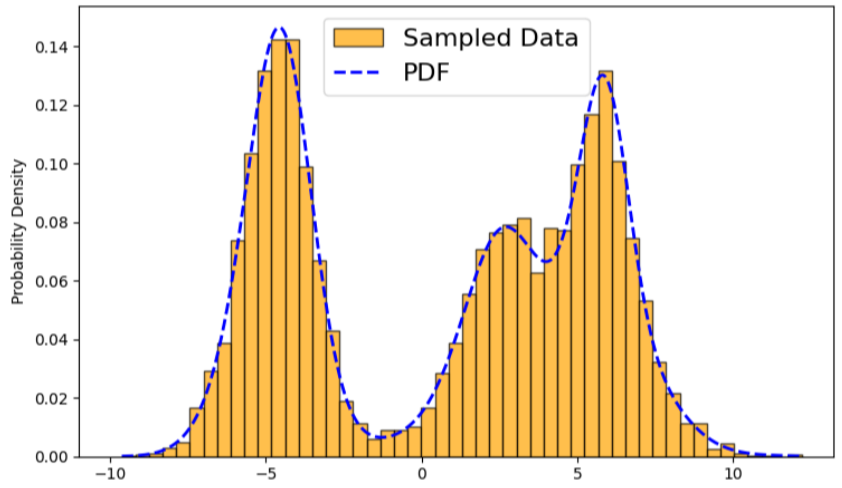
- Application:
  - Entertainment (ngành giải trí): videos, images, musics, …
  - Limited resources: khi khả năng thu thập được ít mẫu dữ liệu
  - Fashion: tạo mẫu quần/áo thời trang
  - Design: tạo mẫu trang thiết bị mới
  - Materials: tạo các vật liệu mới
  - …

Generative models

Learning

Learning a generative model

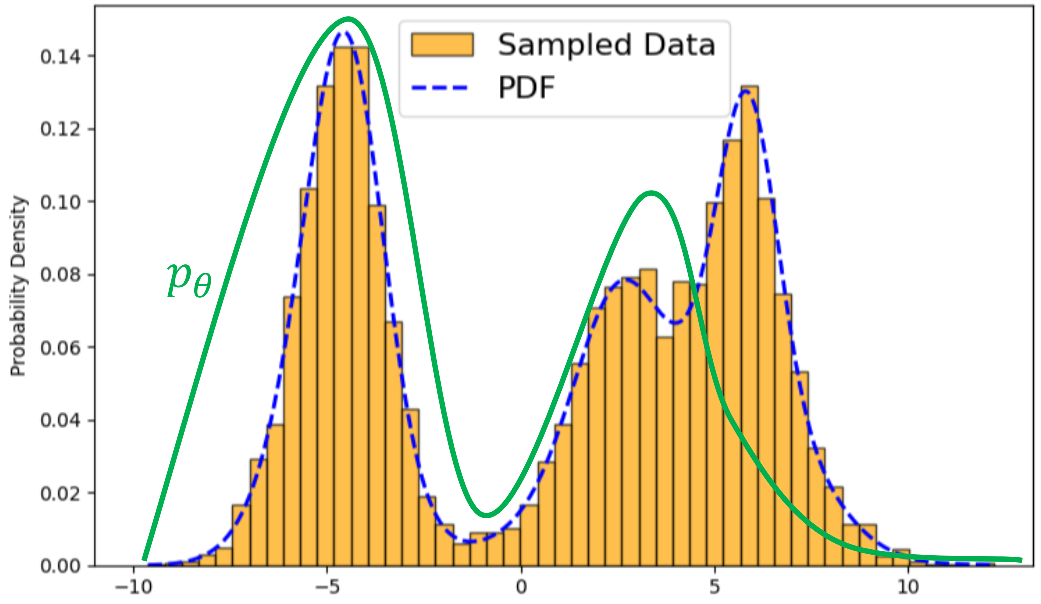
- Given a training set of examples, e.g., images of dogs
- We want to learn a probability distribution P(**x**) over images **x** such that
  - **Generation:** If we sample $\boldsymbol{x}_{new} \sim P(\boldsymbol{x})$, $\boldsymbol{x}_{new}$ should look like a dog (*sampling*)
  - **Density estimation:** P(**x**)
  - **Unsupervised representation learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc. (*features*)



The sampling distribution

- Dataset **D** = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_m$}
- **Hardness** of the learning problem:
  - P(**x**) in the space of all probability distributions
- In practice, we often find a $P_\theta(\boldsymbol{x})$ to **approximate** $P(\boldsymbol{x})$

Impossible

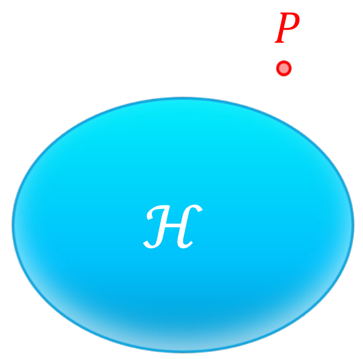


Hypothesis space

- Ussually, we can choose a restricted set $\mathcal{H}$ of distributions
  - Parameterized by $\theta \in \Theta$
  - A learner must find one $P_\theta \in \mathcal{H}$
- Hypothesis space *(model family)*:

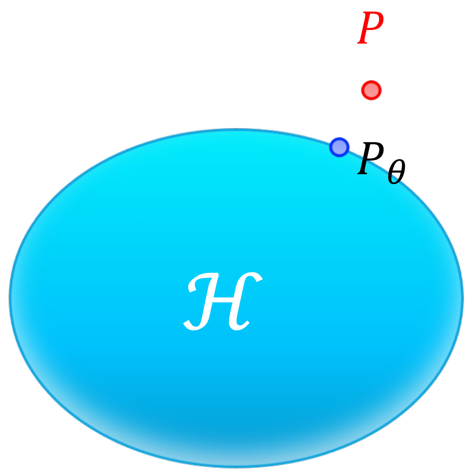
  a set $\mathcal{H}$ of distributions, providing candidates for a learner
  - Represents prior knowledge about a task
  - Represents our ***inductive bias*** or *preference*
- Each P_θ is often called a "**model**"
- Gaussian family:

$$\mathcal{H} = \{P_\theta : P_\theta \text{ is the normal distribution with } \theta = (\mu, \sigma), \mu \in \mathbb{R}, \sigma \in \mathbb{R}_+\}$$



Learning goal

- *Find a model P_θ that precisely captures the distribution P from which our data was sampled*
- Intractability:
  - P(**x**) is in the space of all probability distributions
  - The sampled data set is limited
  - Computational reasons
- We want to select P_θ to be the "best" approximation to the underlying distribution P
  - **What is "best"?**
  - Depends on specific task of interest



Learning as density estimation

- We want to learn the full distribution so that later we can answer any probabilistic inference query
  (ta muốn tìm phân bố đầy đủ của các biến để về sau có thể dễ thực hiện các suy luận)
- In this setting we can view the learning problem as **density estimation**
  (có thể coi bài toán học là bài toán ước lượng hàm mật độ)
- We want to construct P_θ as "**close**" as possible to P
  (recall we assume we are given a dataset **D** of samples from P)

How do we evaluate "closeness"?

KL-divergence

- How should we measure distance between distributions?
  (ta nên đo khoảng cách giữa hai phân bố thế nào?)
- The **Kullback-Leibler divergence** (KL-divergence) between two distributions P and Q is defined as

$$KL(P||Q) = \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}\left(\log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}\right)$$

  - where $\mathrm{p}(\boldsymbol{x})$ and $\mathrm{q}(\boldsymbol{x})$ represents the densities of P and Q, respectively
- Note that:
  - $KL(P||Q) \geq 0$ for any P and Q, and $KL(P||P) = 0$
  - $KL(P||Q) \neq KL(Q||P)$
- It measures the loss (in bits) when describing distribution P by Q.

Learning: a revisit

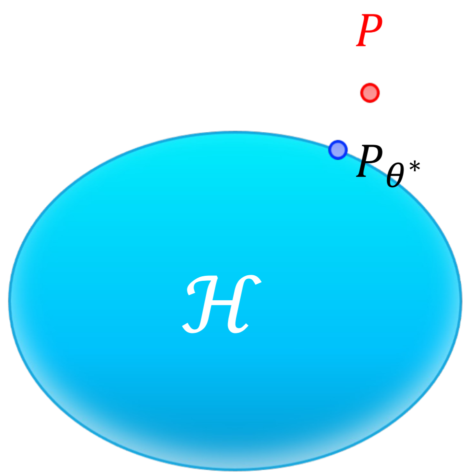
- We want to construct P$_\theta$ as **"close"** as possible to P
  (Given a dataset **D** of samples from P)
- Closeness by KL:

$$KL(P||P_\theta) = \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}\left(\log \frac{p(\boldsymbol{x})}{p_\theta(\boldsymbol{x})}\right)$$

- Learning by minimizing $KL(P||P_\theta)$

$$\theta^* = \underset{\theta\in\Theta}{\operatorname{argmin}}\, KL(P||P_\theta)$$

  - Find the parameter θ^* that minimizes $KL(P||P_\theta)$
  - θ^* provides the minimal loss when compressing P by P_{θ^*}
    (θ^* sẽ có mất mát bé nhất nếu ta nén P bằng P_{θ^*})



Expected log-likelihood

- We can rewrite

$$KL(P||P_\theta) = \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}\left(\log \frac{p(\boldsymbol{x})}{p_\theta(\boldsymbol{x})}\right) = \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}(\log p(\boldsymbol{x})) - \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}(\log p_\theta(\boldsymbol{x}))$$

  - The first term does not depend on θ
- Minimizing KL is equivalent to maximizing the *Expected log-likelihood* $\mathbb{E}_{\boldsymbol{x}}(\log p_\theta(\boldsymbol{x}))$
- Learning can be done by **Maximum Likelihood Estimation (MLE)** (việc học có thể thực hiện bằng cách ước lượng hợp lý cực đại)

$$\theta^* = \underset{\theta\in\Theta}{\operatorname{argmax}}\, \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}(\log p_\theta(\boldsymbol{x}))$$

  - In general, we do not know P
  - So, we cannot access to the objective

Maximum likelihood

- We approximate the *expected log-likelihood* $\mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}(\log p_\theta(\boldsymbol{x}))$ by
  (ta có thể xấp xỉ hàm log-likelihood trung bình)

$$\mathbb{E}_{\boldsymbol{x}\in \boldsymbol{D}}(\log p_\theta(\boldsymbol{x})) = \frac{1}{m}\sum_{\boldsymbol{x}\in \boldsymbol{D}} \log p_\theta(\boldsymbol{x})$$

  - Sometimes known as *Empirical log-likelihood*
    (note the similarity with empirical loss in ML)

- MLE is the formulated as (phương pháp MLE có thể viết lại)

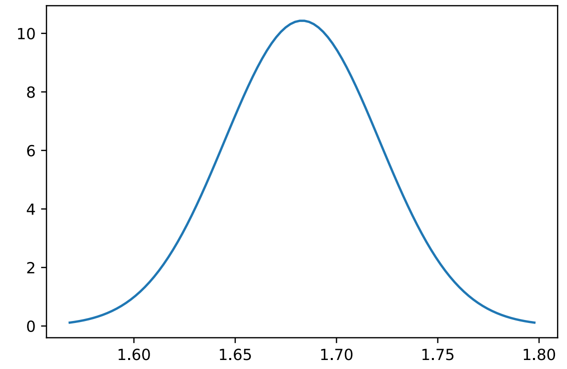
$$\theta^* = \operatorname*{argmax}_{\theta\in\Theta} \frac{1}{m}\sum_{\boldsymbol{x}\in \boldsymbol{D}} \log p_\theta(\boldsymbol{x})$$

  - This is equivalent to maximizing the likelihood $P(\boldsymbol{x}_1, \dots, \boldsymbol{x}_m) = \prod_{i=1}^{m} P(\boldsymbol{x}_i)$ for i.i.d. samples

MLE: Gaussian example (1)

- We wish to estimate the height of a person in the world.
- Use a 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 $P(\boldsymbol{D}|\mu,\sigma) = P(x_1,\dots,x_{10}|\mu,\sigma) = \prod_{i=1}^{10} P(x_i|\mu,\sigma)$
- 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

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

Generative models

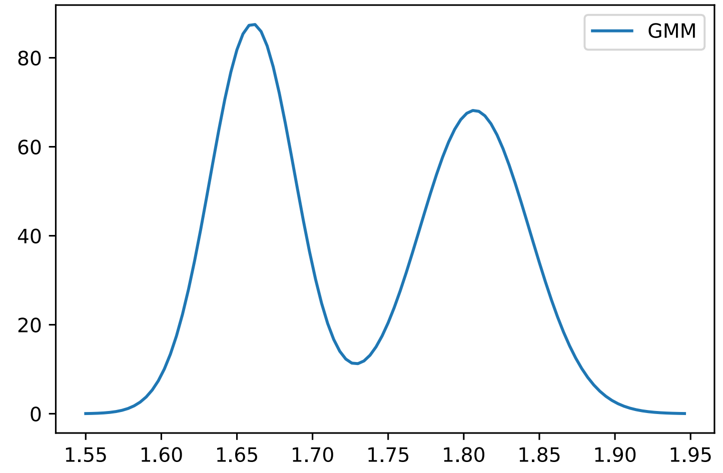
Approximation by mixture models

Learning the data distribution

- Dataset **D** = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_m$}
  - Images about dogs
- **Hardness** of the learning problem:
  - P(**x**) is in the space of all probability distributions
- In practice
  - We often find a $P_\theta(\boldsymbol{x})$ to **approximate** $P(\boldsymbol{x})$
- How to choose a good model family?
  - Gaussian family? => too simple

Gaussian mixture model (GMM)

- 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* $z \sim Categorical(\boldsymbol{\phi})$
    - *Generate* $\boldsymbol{x} \sim Normal(\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- The density function is



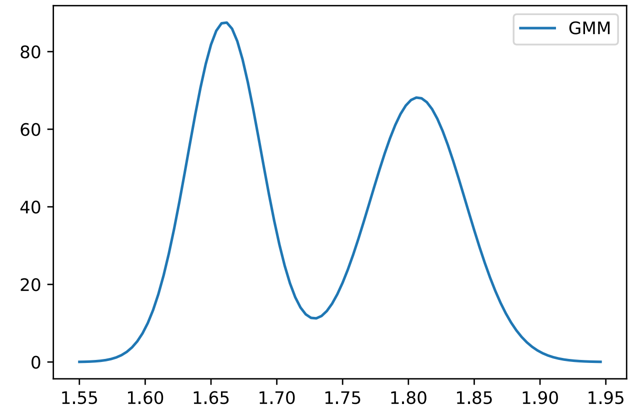
$$q(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

  - $\boldsymbol{\phi} = (\phi_1, \dots, \phi_K)$ represents the weights of the Gaussians: $\sum_{k=1}^{K} \phi_k = 1, \quad \phi_j \geq 0, \ \forall j$
  - Each Gaussian has density $\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right]$

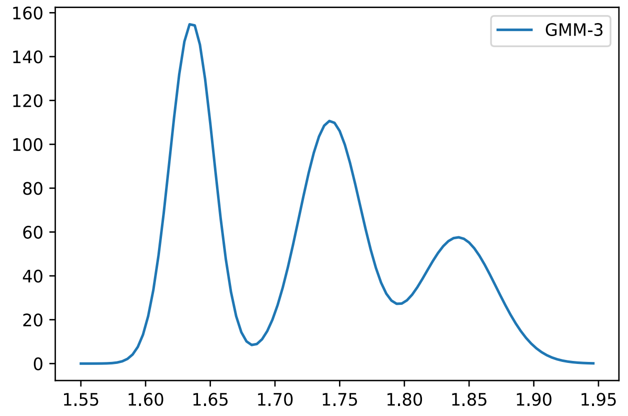
- Note: z is an unobserved (latent) variable, x is observable

GMM: approximation ability

- The density $q(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
  - Gaussian model: $K = 1$ component
- A larger K produces a more complex model Q
- **GMMs are universal approximators**
  - Any smooth density can be approximated arbitrarily well by a GMM with enough components
    (bất kỳ hàm mật độ trơn nào đều có thể được xấp xỉ tốt bằng một GMM với số lượng thành phần đủ lớn)



GMM with 2 components



GMM with 3 components

Dalal, S. R., and W. J. Hall. "Approximating Priors by Mixtures of Natural Conjugate Priors." J. of the Royal Statistical Society. Series B (Methodological), vol. 45, no. 2, 1983, pp. 278–286.

Infinite GMM

- *Mixture of an infinite number of Gaussians:* we assume that the data are samples from an infinite number of Gaussians
  - Each instance **x** is generated from one of those Gaussians by the following ***generative process***:
    - *Choose* $\boldsymbol{z} \sim Normal(0, \boldsymbol{I})$ P(**z**)
    - *Generate* $\boldsymbol{x} \sim Normal(\boldsymbol{\mu}_\theta(\boldsymbol{z}), \boldsymbol{\Sigma}_\theta(\boldsymbol{z}))$ P(**x** | **z**)
      - Where $\boldsymbol{\mu}_\theta, \boldsymbol{\Sigma}_\theta$ are neural networks, parameterized by θ
- **Universal approximator?**
- Each component is simple, but the marginal P(**x**) is very complex

Variational auto-encoder

Variational inference,
Amortized inference,
Sampling

Learning for GMM

- Learning by MLE:

$$\theta^* = \underset{\theta}{\operatorname{argmax}} \frac{1}{m} \sum_{\boldsymbol{x} \in \boldsymbol{D}} \log p_\theta(\boldsymbol{x})$$

  - where $p_\theta(\boldsymbol{x}) = \sum_{k=1}^{K} \phi_k \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma}_k)}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)\right]$, $\theta = (\boldsymbol{\phi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$

- Evaluation of $\log p_\theta(\boldsymbol{x})$ is **hard** in general, since

$$\log p_\theta(\boldsymbol{x}) = \log \sum_{\text{All possible values of } \boldsymbol{z}} p_\theta(\boldsymbol{x}, \boldsymbol{z})$$

  - E.g., for $\boldsymbol{z} \in \{0,1\}^{100}$, the sum has 2^{100} terms

- It is even harder for more complex models

→Approximation is needed

Evidence Lower Bound

- Note

$$\log p_\theta(\boldsymbol{x}) = \log \sum_{\boldsymbol{z}\in\mathcal{Z}} p_\theta(\boldsymbol{x},\boldsymbol{z}) = \log \sum_{\boldsymbol{z}\in\mathcal{Z}} \frac{q(\boldsymbol{z})}{q(\boldsymbol{z})} p_\theta(\boldsymbol{x},\boldsymbol{z}) = \log \mathbb{E}_{q(\boldsymbol{z})} \frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})}$$

- Since log is concave, Jensen Inequality suggests

$$\log \mathbb{E}_{q(\boldsymbol{z})} \frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})} \geq \mathbb{E}_{q(\boldsymbol{z})} \log \frac{p_\theta(\boldsymbol{x},\boldsymbol{z})}{q(\boldsymbol{z})} = \mathbb{E}_{q(\boldsymbol{z})} \log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \mathbb{E}_{q(\boldsymbol{z})} \log q(\boldsymbol{z})$$

- This is called the Evidence Lower Bound (**ELBO**)
- For any $q(\boldsymbol{z})$:

$$\log p_\theta(\boldsymbol{x}) \geq ELBO$$

  - For $\mathrm{ELBO} = \mathbb{E}_{q(\boldsymbol{z})} \log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \mathbb{E}_{q(\boldsymbol{z})} \log q(\boldsymbol{z})$
- When $q(\boldsymbol{z}) = p_\theta(\boldsymbol{z}|\boldsymbol{x})$*:*

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

Variational inference (suy diễn biến phân)

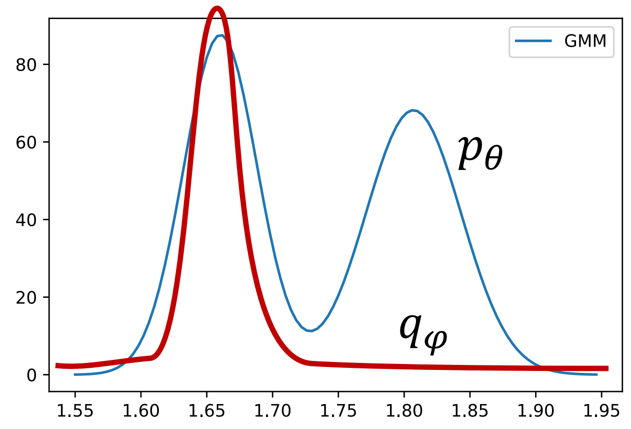
- When the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$ is easy to compute, we can learn the model by maximizing

$$\frac{1}{m}\sum_{\boldsymbol{x}\in\boldsymbol{D}} \log p_\theta(\boldsymbol{x}) = \frac{1}{m}\sum_{\boldsymbol{x}\in\boldsymbol{D}} \left[\mathbb{E}_{p_\theta(\boldsymbol{z}|\boldsymbol{x})} \log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \mathbb{E}_{p_\theta(\boldsymbol{z}|\boldsymbol{x})} \log p_\theta(\boldsymbol{z}|\boldsymbol{x})\right]$$

  - E.g., for the case of GMM

- What if the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$ is intractable to compute?
  (nếu phân bố hậu nghiệm không tính toán được thì sao?)

- **Variational inference (VI):**
  - choose a family of *simple* distributions $q_\varphi(\boldsymbol{z})$, parameterized by φ (variational parameters)
  - then find φ^* so that $q_{\varphi^*}(\boldsymbol{z})$ is as close as possible to $p_\theta(\boldsymbol{z}|\boldsymbol{x})$



VI and KL

- Maximize the ELBO

$$\frac{1}{m}\sum_{i=1}^{m}\left[\mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})}\log p_\theta(\boldsymbol{x}_i,\boldsymbol{z}) - \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})}\log q_{\varphi_i}(\boldsymbol{z})\right]$$

  - given a training set **D** = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_m$}

- Maximizing ELBO is equivalent to Minimizing KL, due to

$$\log p_\theta(\boldsymbol{x}) = ELBO + KL(q_\varphi(\boldsymbol{z})||p_\theta(\boldsymbol{z}|\boldsymbol{x}))$$

- Jointly optimize over
  - $\varphi_1, \ldots, \varphi_m$ (variational parameters)
  - θ (model parameters)

VI: some properties

- **Variational inference (VI):**
  - choose a family of *simple* distributions $q_\varphi(\boldsymbol{z})$, parameterized by φ
  - find φ^* so that $q_{\varphi^*}(\boldsymbol{z})$ is as close as possible to $p_\theta(\boldsymbol{z}|\boldsymbol{x})$

- Pros:
  - Easy to be used in a large class of models
  - Efficient in practice
- Cons:
  - Hard to choose a good variational family
    - When we do not know the explicit form for the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$
  - For *inference*, given model param θ and instance $\boldsymbol{x}$, we estimate the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$ *by solving an optimization problem:*

$$\max_{\varphi} \mathbb{E}_{q_\varphi(\boldsymbol{z})} \log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \mathbb{E}_{q_\varphi(\boldsymbol{z})} \log q_\varphi(\boldsymbol{z})$$

Expensive

  - Require too many variational parameters
    - Each instance **x**$_i$ requires one specific φ_i ➔ O(m) parameters
    - GMM needs O(mKn^2) params, where K is #components, n is #dims

Amortized inference

$$\max_{\theta} \frac{1}{m} \sum_{\boldsymbol{x} \in \boldsymbol{D}} \log p_\theta(\boldsymbol{x}) \quad \geq \quad \max_{\theta, \varphi_1, \dots, \varphi_m} \frac{1}{m} \sum_{\boldsymbol{x}_i \in \boldsymbol{D}} \mathrm{L}(\boldsymbol{x}_i; \theta, \varphi)$$

- Where $\mathrm{L}(\boldsymbol{x}_i; \theta, \varphi) = \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log p_\theta(\boldsymbol{x}_i, \boldsymbol{z}) - \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log q_{\varphi_i}(\boldsymbol{z})$

- VI uses φ_i for each point **x**$_i$.
  - May not scale well with large datasets; prone to overfitting
- **Amortization:** *we learn a* ***single*** *neural network $f_w: \boldsymbol{x} \longmapsto \varphi$ that maps each input* ***x*** *to a set of (good) variational parameters*
  - f_w has a *trainable* parameter w
  - For a given input **x**$_i$, f_w will produce the parameter $\varphi_i = f_w(\boldsymbol{x}_i)$ of the variational distribution $q_{\varphi_i}(\boldsymbol{z})$
- *Amortized inference:* feed instance **x** to the trained network to get the variational parameter $\varphi = f_w(\boldsymbol{x})$
  - No optimization ➔ cheap

Kingma, D. P. & Welling, M. (2014). Auto-Encoding Variational Bayes. *ICLR*.

Learning with amortized inference

- We can use using stochastic gradient descent to solve

$$\max_{\theta,\varphi_1,\dots,\varphi_m} \sum_{\boldsymbol{x}_i \in \boldsymbol{D}} \mathrm{L}(\boldsymbol{x}_i; \theta, \varphi)$$

- *Initialize* $\theta^{(0)}, \varphi^{(0)}$
- *At iteration* $j \geq 1$*:*
  - *Randomly sample a data point* $\boldsymbol{x}_i$ *from* ***D***
  - *Compute* $\nabla_\theta L\left(\boldsymbol{x}_i; \theta^{(j-1)}, \varphi^{(j-1)}\right)$ *and* $\nabla_\varphi L\left(\boldsymbol{x}_i; \theta^{(j-1)}, \varphi^{(j-1)}\right)$
  - *Update* $\theta^{(j)}, \varphi^{(j)}$ *in the gradient direction*

- How to compute the gradients?
  - $\mathrm{L}(\boldsymbol{x}_i; \theta, \varphi) = \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log p_\theta(\boldsymbol{x}_i, \boldsymbol{z}) - \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log q_{\varphi_i}(\boldsymbol{z})$
  - The expectation complicates gradient computation for φ

Reparameterization trick (mẹo đổi biến)

- Consider **z** being **continuous**, and we want to compute a gradient with respect to φ of

$$\mathbb{E}_{q_\varphi(\boldsymbol{z})}[r(\boldsymbol{z})] = \int q_\varphi(\boldsymbol{z}) r(\boldsymbol{z}) d\boldsymbol{z}$$

- Suppose $q_\varphi(\boldsymbol{z}) = \mathcal{N}(\boldsymbol{\mu}, \sigma^2 \boldsymbol{I})$ is Gaussian with parameters $\varphi = (\boldsymbol{\mu}, \sigma)$
  - Since $\boldsymbol{z} \sim q_\varphi(\boldsymbol{z})$, there exists representation $\boldsymbol{z} = \boldsymbol{\mu} + \sigma \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})$
- We can write

$$\mathbb{E}_{\boldsymbol{z} \sim q_\varphi(\boldsymbol{z})}[r(\boldsymbol{z})] = \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})}[r(\boldsymbol{\mu} + \sigma \boldsymbol{\epsilon})]$$

$$\nabla_\varphi \mathbb{E}_{q_\varphi(\boldsymbol{z})}[r(\boldsymbol{z})] = \nabla_\varphi \mathbb{E}_{\boldsymbol{\epsilon}}[r(\boldsymbol{\mu} + \sigma \boldsymbol{\epsilon})] = \mathbb{E}_{\boldsymbol{\epsilon}}\left[\nabla_\varphi r(\boldsymbol{\mu} + \sigma \boldsymbol{\epsilon})\right]$$

- Easy to estimate via Monte Carlo if r is differentiable w.r.t. φ, since $\boldsymbol{\epsilon}$ is easy to sample
  - $\mathbb{E}_{\boldsymbol{\epsilon}}\left[\nabla_\varphi r(\boldsymbol{\mu} + \sigma \boldsymbol{\epsilon})\right] \approx \frac{1}{K} \sum_{j=1}^{K} \nabla_\varphi r\left(\boldsymbol{\mu} + \sigma \boldsymbol{\epsilon}_j\right)$, where $\boldsymbol{\epsilon}_1, \ldots, \boldsymbol{\epsilon}_K \sim \mathcal{N}(0, \boldsymbol{I})$

(dùng Monte Carlo để xấp xỉ, nếu hàm r có đạo hàm, vì ta dễ lấy mẫu $\boldsymbol{\epsilon}$)

Variational auto-encoder (VAE)

- Since $q_\varphi(\boldsymbol{z})$ approximates the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$, we can write it as $q_\varphi(\boldsymbol{z}|\boldsymbol{x})$ and

$$\begin{aligned} \mathrm{L}(\boldsymbol{x};\theta,\varphi) &= \mathbb{E}_{q_\varphi(\boldsymbol{z}|\boldsymbol{x})} \log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \mathbb{E}_{q_\varphi(\boldsymbol{z}|\boldsymbol{x})} \log q_\varphi(\boldsymbol{z}|\boldsymbol{x}) \\ &= \mathbb{E}_{q_\varphi(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x},\boldsymbol{z}) - \log p_\theta(\boldsymbol{z}) + \log p_\theta(\boldsymbol{z}) - \log q_\varphi(\boldsymbol{z}|\boldsymbol{x})\right] \\ &= \mathbb{E}_{q_\varphi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - KL(q_\varphi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p_\theta(\boldsymbol{z})) \end{aligned}$$

- Maximize L: maximize $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ and push $q_\varphi(\boldsymbol{z}|\boldsymbol{x})$ close to $p_\theta(\boldsymbol{z})$
- **Encoder (bộ mã hoá):**
  - Maps each data point $\boldsymbol{x}$ to a latent vector $\hat{\boldsymbol{z}}$, a sample from a Gaussian ($q_\varphi(\boldsymbol{z}|\boldsymbol{x})$) with parameter $(\mu,\sigma) = Encoder_\varphi(\boldsymbol{x})$
- **Decoder (bộ giải mã):**
  - Reconstruct $\hat{\boldsymbol{x}}$ from a latent vector $\hat{\boldsymbol{z}}$, i.e., pick a sample from a Gaussian ($p_\theta(\boldsymbol{x}|\hat{\boldsymbol{z}})$) with parameter $Decoder_\theta(\hat{\boldsymbol{z}})$

Kingma, D. P. & Welling, M. (2014). Auto-Encoding Variational Bayes. *ICLR*.

VAE

$$L(\boldsymbol{x};\theta,\varphi) = \mathbb{E}_{q_\varphi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - KL(q_\varphi(\boldsymbol{z}|\boldsymbol{x})\,||p_\theta(\boldsymbol{z}))$$

- Maximizing L:
  - The first term encourages accurate reconstruction $\hat{\boldsymbol{x}} \approx \boldsymbol{x}$
    (đại lượng đầu muốn khôi phục chính xác mỗi mẫu x)
  - The KL term encourages $\hat{\boldsymbol{z}}$ to have a distribution similar to the prior $p_\theta(\boldsymbol{z})$
    (KL muốn phân bố của $\hat{\boldsymbol{z}}$ gần với $p_\theta(\boldsymbol{z})$)
- Training: SGD + reparameterization trick

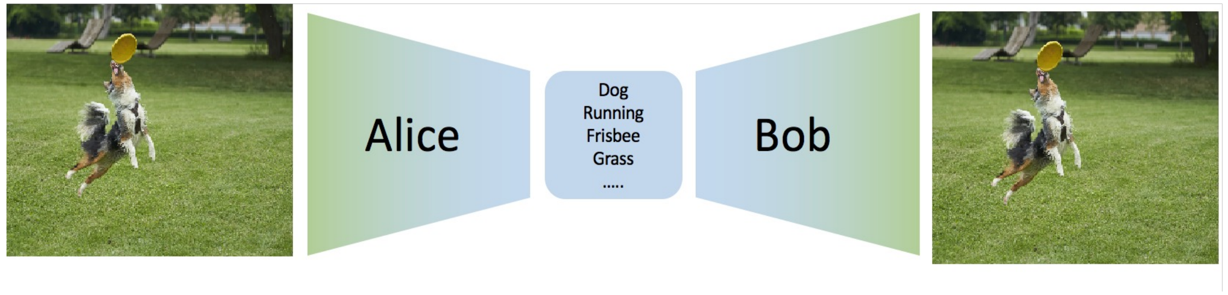


Image from Stefano Ermon

$$\begin{tikzcd} \boldsymbol{x} \arrow[r, "Encoder_\varphi"] & \hat{\boldsymbol{z}} \arrow[r, "Decoder_\theta"] & \hat{\boldsymbol{x}} \end{tikzcd}$$

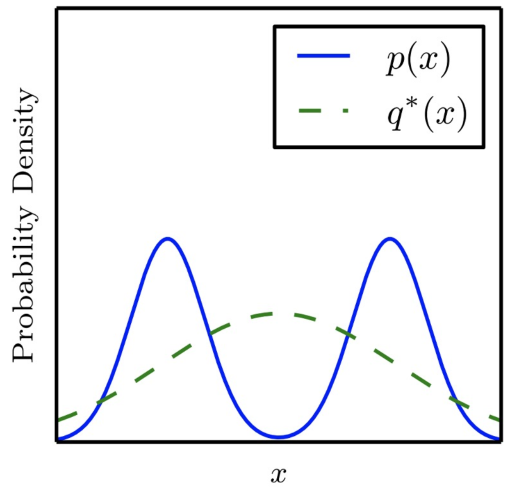
$p_\theta(\boldsymbol{x})$ $q_\varphi(\boldsymbol{z}|\boldsymbol{x})$ $p_\theta(\boldsymbol{x}|\boldsymbol{z})$

VAE: some properties

- Pros:
  - Efficient inference
  - Flexible and expressive (Universal approximator)
  - Good diversity of the synthetic samples
- Cons:
  - Blur images

VAE (2014)

$q^* = \text{argmin}_q D_{\text{KL}}(p\|q)$



Maximum likelihood

VQ-VAE (2017)