Introduction to

Deep Generative Models

(Mô hình tạo sinh sâu)

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SoICT summer school, August 2024

Contents

Some successes: Text-to-image (2022)

- Draw pictures by descriptions

A bowl of soup

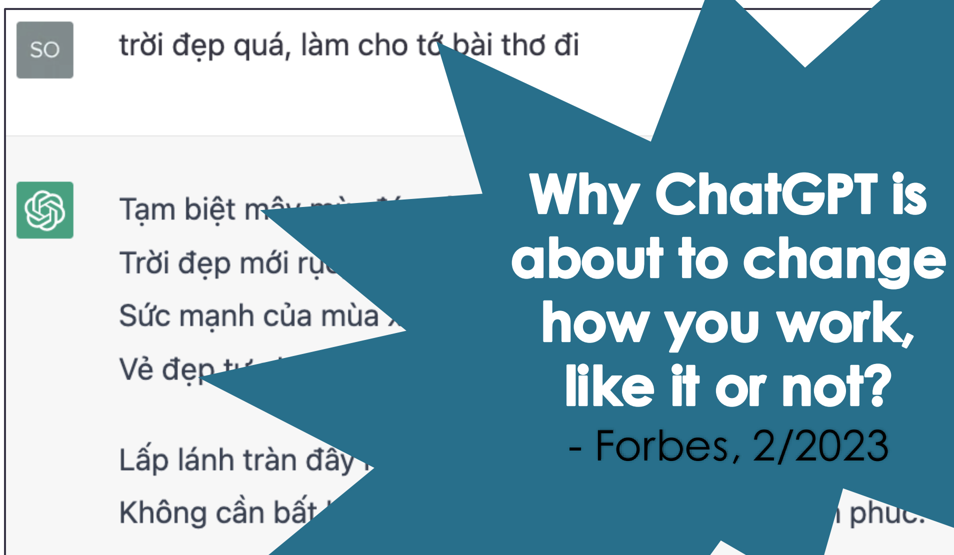
Google Imagen

An extremely angry bird.

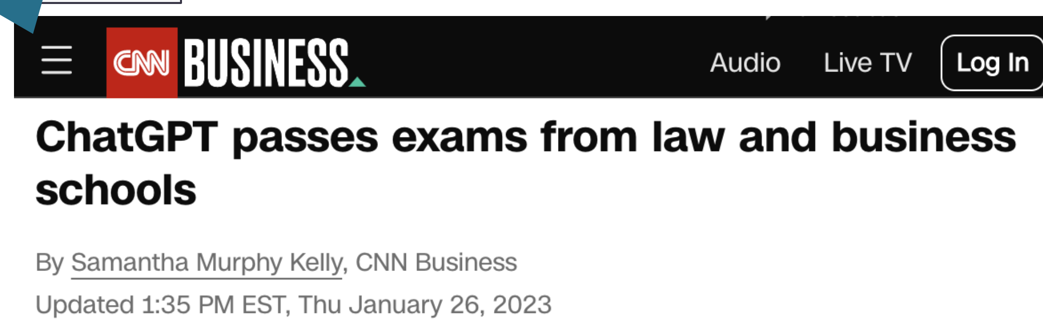
A cute corgi lives in a house made out of sushi.

Some successes: ChatGPT (2022)

- Human-level Chatting, Writing, QA,…



Why ChatGPT is about to change how you work, like it or not?
- Forbes, 2/2023


CNN BUSINESS Audio Live TV Log In

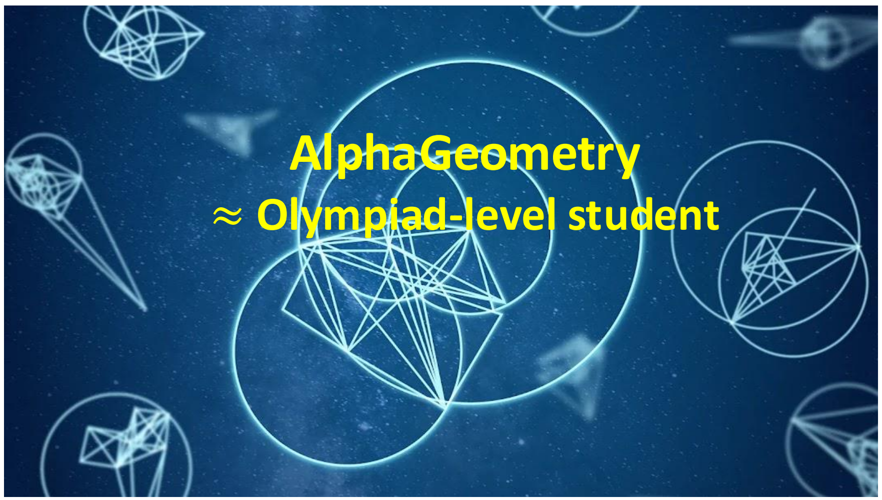
ChatGPT passes exams from law and business schools

By Samantha Murphy Kelly, CNN Business

Updated 1:35 PM EST, Thu January 26, 2023

OpenAI

Some successes: more



Gemini

Generative Models

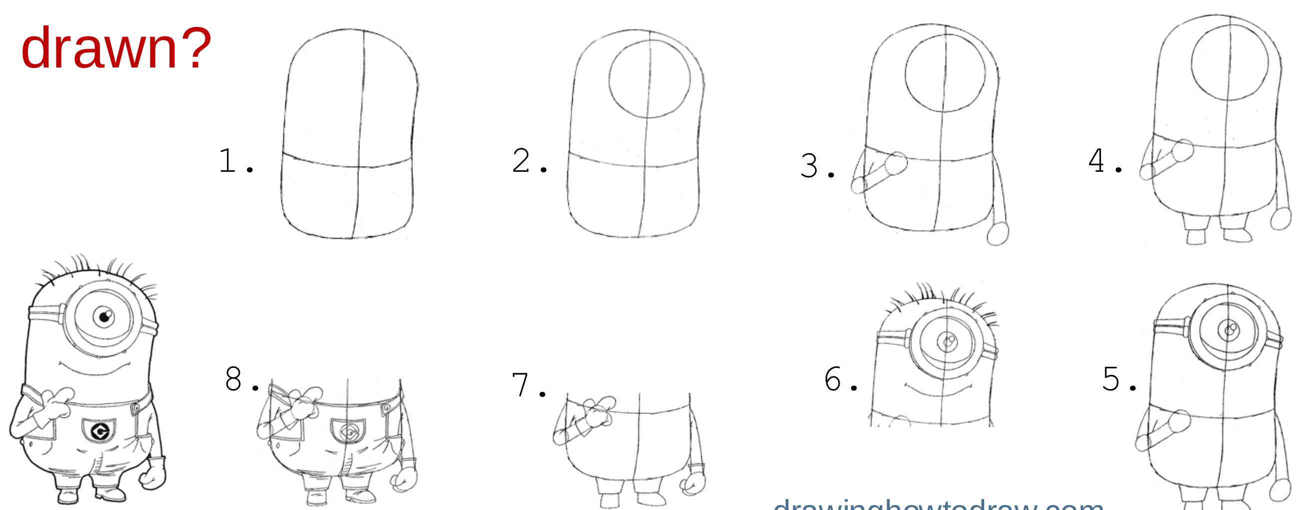
- Probabilistic models of data
- Sample: lấy mẫu dữ liệu (sinh/tạo ra dữ liệu)
- Evaluate likelihood: tính likelihood của dữ liệu cho trước
- Train: huấn luyện
- Representation: biểu diễn mới
- What if all we care about is sampling?
  - *Not in the training data, but the novel samples.*

Probabilistic models

Introduction

Probabilistic model

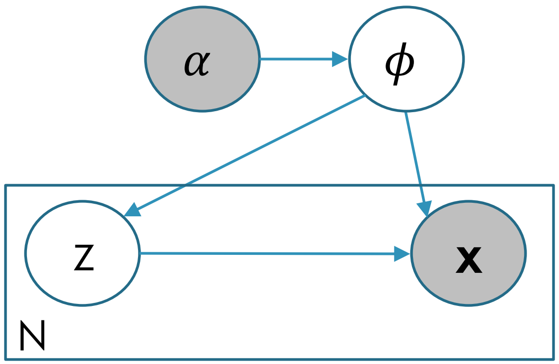
- Our assumption on how the data samples were generated
  (giả thuyết của chúng ta về quá trình mà các mẫu dữ liệu đã được sinh ra như thế nào)
- Example: how a sentence is generated?
  - We assume our brain does as follow:
  - *First choose the topic of the sentence*
  - *Generate the words one-by-one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



drawinghowtodraw.com

Probabilistic model

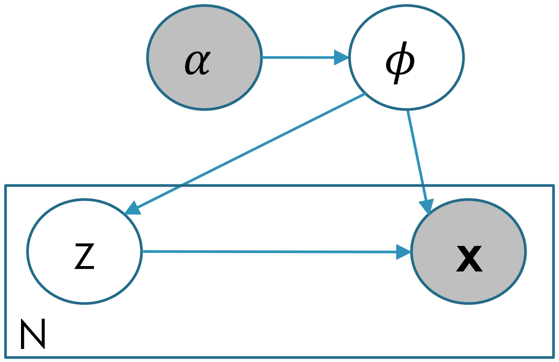
- A model sometimes consists of
  - **Observed variable** (e.g., $\boldsymbol{x}$) which models the observation (data instance)
    (biến quan sát được)
  - **Hidden variable** which describes the hidden things (e.g., z, ϕ)
    (biến ẩn)
  - **Relations** between the variables



- 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

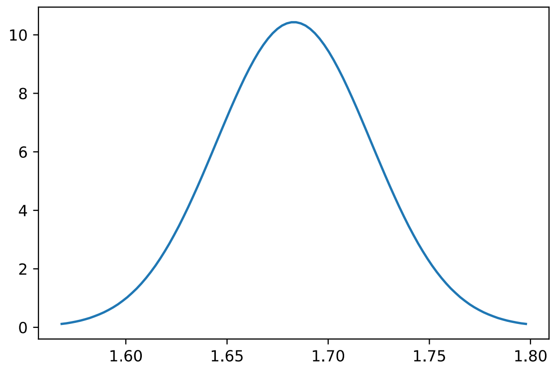


- Latent variable model: a PGM which has at least one latent variable
- **Generative model:** a model that enables us to generate data instances

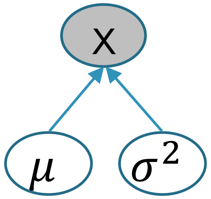
Univariate normal distribution

- 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 $\boldsymbol{\theta} = (\mu, \sigma^2)$



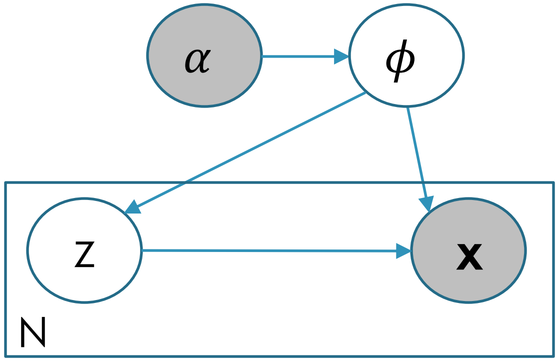
- **Learning:** we need to know specific values of $\{\mu, \sigma^2\}$

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

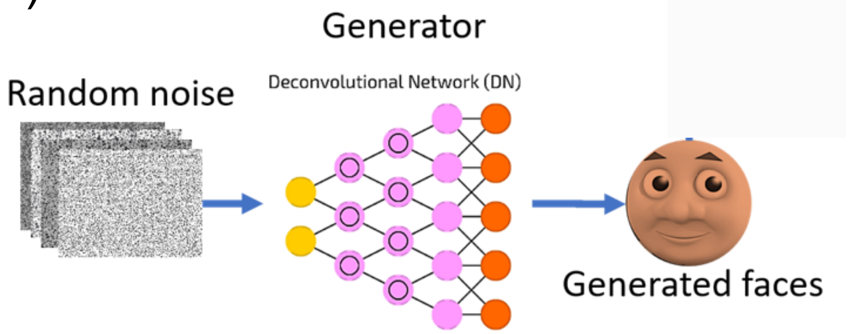
- **Inference** for a given instance $\boldsymbol{x}_n$
  (Suy diễn/phán đoán đối với một quan sát cho trước)
  - Recovery of the local variable (e.g., z_n), or
  - The distribution of the local variables (e.g., $P(z_n|\phi, \boldsymbol{x}_n)$)
  - Example: for GMM, we want to know z_n indicating which 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 $p(\phi, z_1, \dots, z_n, \boldsymbol{x}_1, \dots, \boldsymbol{x}_n|\alpha)$
    - E.g., estimate $P(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n|\alpha)$
    - E.g., estimate α
    - Inference of local variables is often needed

Generative model: sampling

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



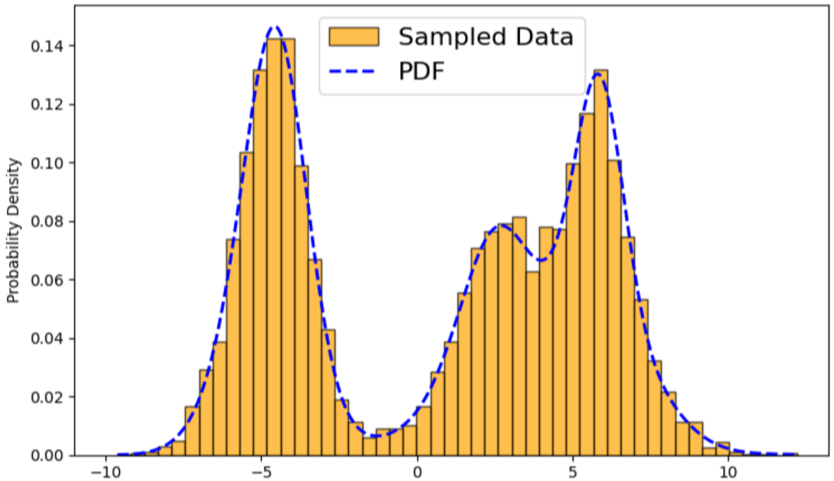
- Application:
  - Entertainment (ngành giải trí): videos, images, musics, …
  - Limited resources: khi khả năng thu thập được ít mẫu dữ liệu
  - Fashion: tạo mẫu quần/áo thời trang
  - Design: tạo mẫu trang thiết bị mới
  - Materials: tạo các vật liệu mới
  - …

Generative models

Learning

Learning a generative model

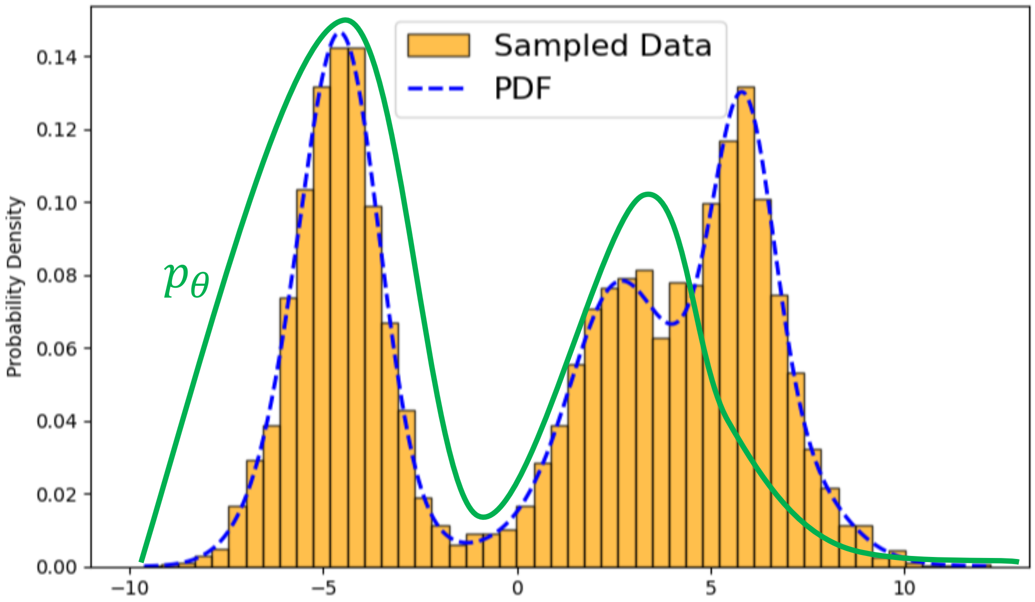
- Given a training set of examples, e.g., images of dogs
- We want to learn a probability distribution P(**x**) over images **x** such that
  - **Generation:** If we sample $\boldsymbol{x}_{new} \sim P(\boldsymbol{x})$, $\boldsymbol{x}_{new}$ should look like a dog (*sampling*)
  - **Density estimation:** 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

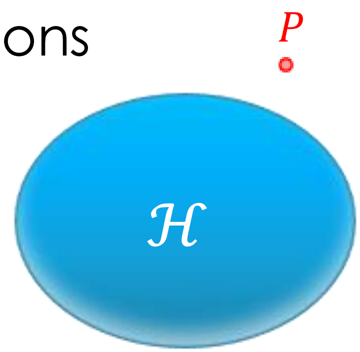
- Dataset **D** = {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_m$}
- **Hardness** of the learning problem:
  - P(**x**) in the space of all probability distributions

- In practice, we often find a $P_\theta(\boldsymbol{x})$ to **approximate** $P(\boldsymbol{x})$



Hypothesis space

- Usually, we can choose a restricted set $\mathcal{H}$ of distributions
  - Parameterized by $\theta \in \Theta$
  - A learner must find one $P_\theta \in \mathcal{H}$



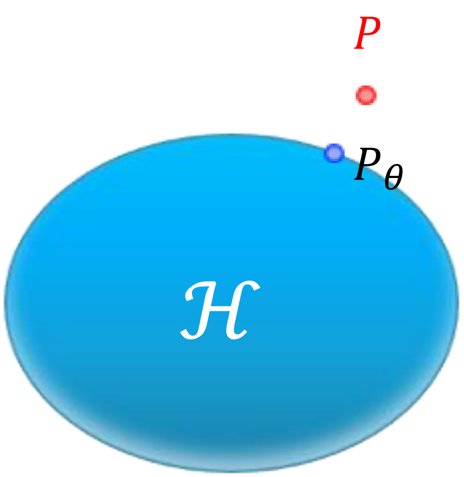
- Hypothesis space *(model family)*:

  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
- In this setting we can view the learning problem as **density estimation**
- 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?
- The **Kullback-Leibler divergence** (KL-divergence) between two distributions P and Q is defined as

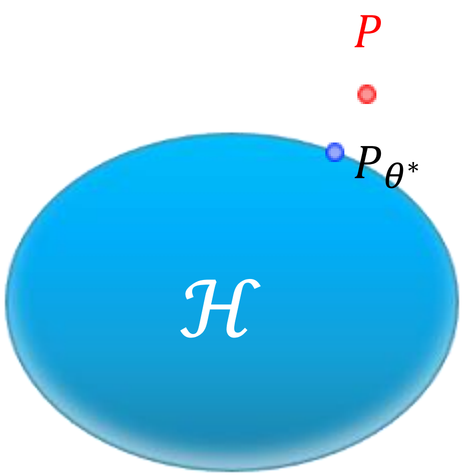
$$KL(P||Q) = \mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}\left(\log\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}\right)$$

  - 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_θ 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^*}

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* $\mathbb{E}_{\boldsymbol{x}\sim P(\boldsymbol{x})}(\log p_\theta(\boldsymbol{x}))$
- Learning can be done by **Maximum Likelihood Estimation (MLE)**

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

  - 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

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

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

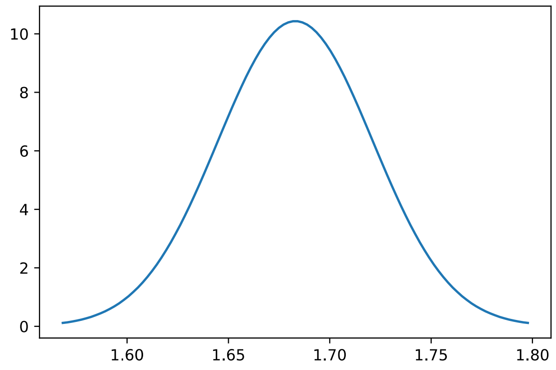
- MLE is the formulated as

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

  - 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

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

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

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

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

- 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

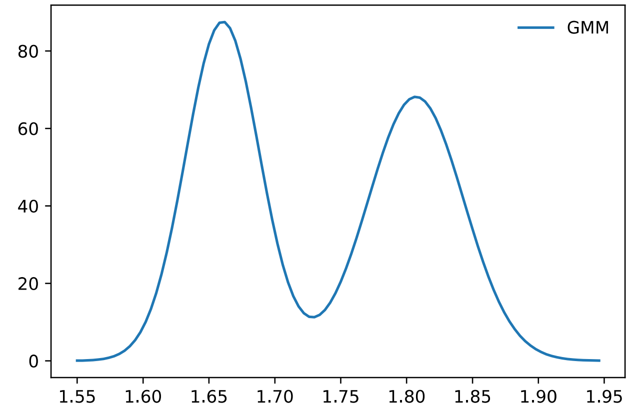
Learning the data distribution

- 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

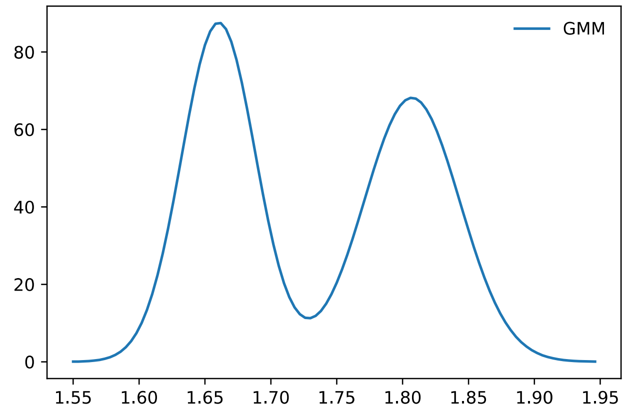
$$q(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\phi}) = \sum_{k=1}^{K} \phi_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



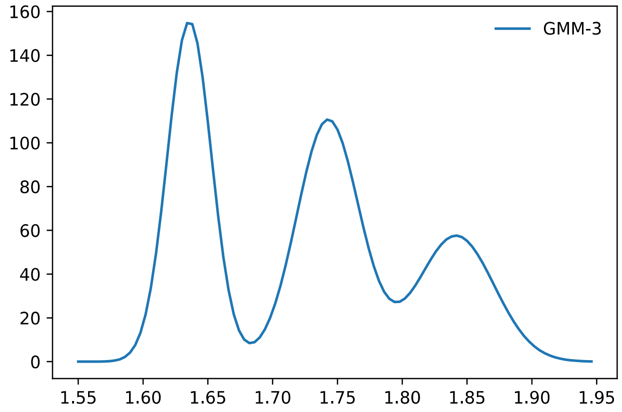
  - $\boldsymbol{\phi} = (\phi_1, \dots, \phi_K)$ represents the weights of the Gaussians: $\sum_{k=1}^{K} \phi_k = 1, \quad \phi_j \geq 0, \ \forall j$
  - Each Gaussian has density $\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{\det(2\pi\boldsymbol{\Sigma})}}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



GMM with 2 components



GMM with 3 components

- **GMMs are universal approximators**
  - Any smooth density can be approximated arbitrarily well by a GMM with enough 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 $q(\boldsymbol{z}) = p_\theta(\boldsymbol{z}|\boldsymbol{x})$:

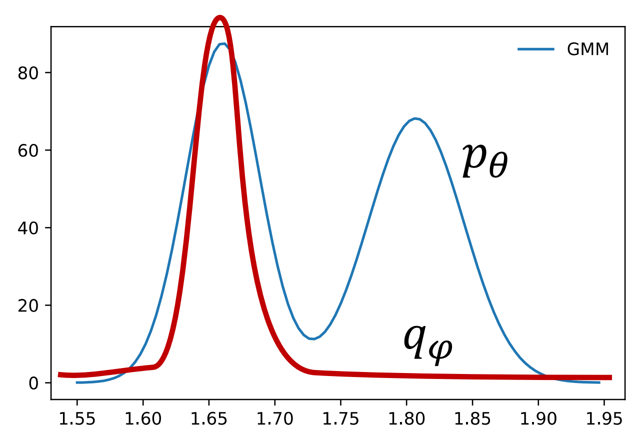
$$\log p_\theta(\boldsymbol{x}|\boldsymbol{\theta}) = \mathbb{E}_{p_\theta(\boldsymbol{z}|\boldsymbol{x})} \log p_\theta(\boldsymbol{x},\boldsymbol{z}|\boldsymbol{\theta}) - \mathbb{E}_{p_\theta(\boldsymbol{z}|\boldsymbol{x})} \log p_\theta(\boldsymbol{z}|\boldsymbol{x}) = \boldsymbol{ELBO}$$

Variational inference

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

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

  - E.g., for the case of GMM
- What if the posterior $p_\theta(\boldsymbol{z}|\boldsymbol{x})$ is intractable to compute?
- **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

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

  - 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

- 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:*

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

Expensive

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

- **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 $p_\theta(\boldsymbol{z}|\boldsymbol{x})$

Amortized inference

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

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

- VI uses φ_i for each point $\mathbf{x}_i$.
  - May not scale well with large datasets; prone to overfitting
- **Amortization:** *we learn a **single** neural network $f_w: \boldsymbol{x} \mapsto \varphi$ that maps each input **x** to a set of (good) variational parameters*
  - f_w has a *trainable* parameter w
  - For a given input $\mathbf{x}_i$, 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

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

- *Initialize $\theta^{(0)}, \varphi^{(0)}$*
- *At iteration $j \geq 1$:*
  - *Randomly sample a data point $\mathbf{x}_i$ 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?
  - $\mathrm{L}(\boldsymbol{x}_i; \theta, \varphi) = \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log p_\theta(\boldsymbol{x}_i, \boldsymbol{z} | \boldsymbol{\theta}) - \mathbb{E}_{q_{\varphi_i}(\boldsymbol{z})} \log q_{\varphi_i}(\boldsymbol{z})$
  - The expectation complicates gradient computation for φ

Reparameterization trick

- 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 $\boldsymbol{\epsilon}_1, \ldots, \boldsymbol{\epsilon}_K \sim \mathcal{N}(0, \boldsymbol{I})$

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

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

- Maximize L: maximize $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ and push $q_\varphi(\boldsymbol{z}|\boldsymbol{x})$ close to $p_\theta(\boldsymbol{z})$
- **Encoder:**
  - 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:**
  - 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 $\hat{\boldsymbol{x}} \approx \boldsymbol{x}$
  - The KL term encourages $\hat{\boldsymbol{z}}$ to have a distribution similar to the prior $p_\theta(\boldsymbol{z})$
- Training: SGD + reparameterization trick

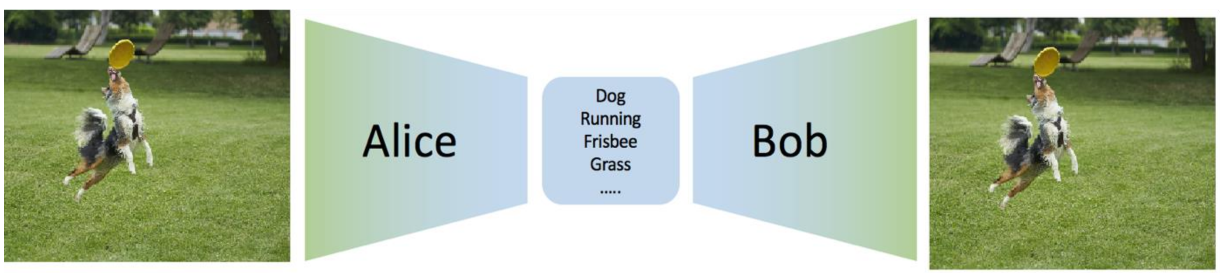


Image from Stefano Ermon

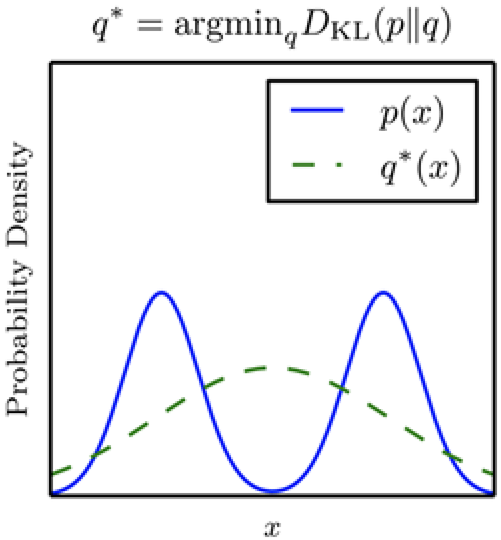
$$\boldsymbol{x} \xrightarrow{Encoder_\varphi} \hat{\boldsymbol{z}} \xrightarrow{Decoder_\theta} \hat{\boldsymbol{x}}$$

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

VAE: some properties

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

VAE (2014)



Maximum likelihood

VQ-VAE (2017)

Generative Adversarial Networks

Introduction

Generative Adversarial Networks

$$\min_G \max_D \mathbb{E}_{\boldsymbol{x}\sim p_{data}}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p(\boldsymbol{z})}\left[\log\left(1 - D(G(\boldsymbol{z}))\right)\right]$$

- Two player minimax game between generator (G) and discriminator (D)
- D tries to maximize the log-likehood for the binary classification problem (D cố gắng cực đại hoá hàm log-likehood của bài toán phân loại nhị phân)
  - Data: real (1)
  - Generated: fake (0)
- G tries to minimize the log-probability of its samples being classified as “fake” by the discriminator D
  (G cố gắng cực tiểu hoá xác suất để D phân loại chính xác các mẫu dữ liệu do G tạo ra)

Generative Adversarial Networks

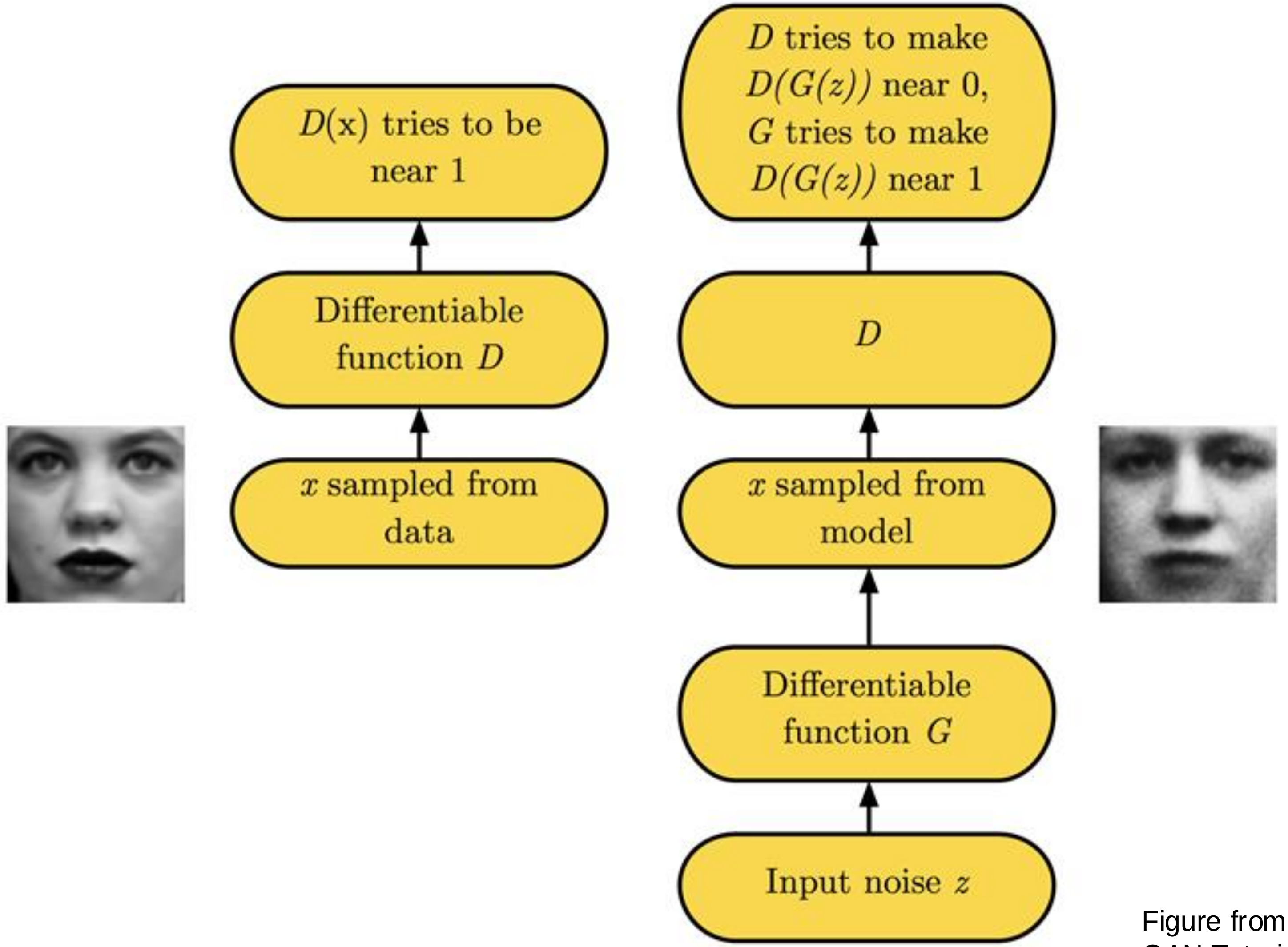


Figure from NeurIPS 2016 GAN Tutorial (Goodfellow)

Representation for the players

- D and G can be represented as two neural networks
- Discriminator:

$$D(\boldsymbol{x}) = NN(\boldsymbol{x}; \theta_d)$$

  - θ_d is the weight of the neural network which takes a sample ***x*** as input.
  - Output is a value in [0, 1].
    (biểu diễn D bằng một mạng nơron với trọng số θ_d, với đầu vào **x** thì trả về một giá trị thuộc [0, 1])
- Generator:

$$G(\boldsymbol{z}) = NN(\boldsymbol{z}; \theta_g)$$

  - θ_g is the weight of the neural network which takes a noise ***z*** as input.
  - ***z*** often follows a simple distribution, and is of low dimensionality.
  - Output is a fake sample $\boldsymbol{x} = G(\boldsymbol{z})$.
    (biểu diễn G bằng một mạng nơron với trọng số θ_g, với đầu vào **z** thì trả về một mẫu dữ liệu **x**)

GANs: pseudocode for training

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

  for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right) \right].$$

D

  end for

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

G

end for

The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

[Goodfellow et al., NeurIPS 2014]

GAN

- See it in action: http://poloclub.github.io/ganlab/

GAN samples from 2014

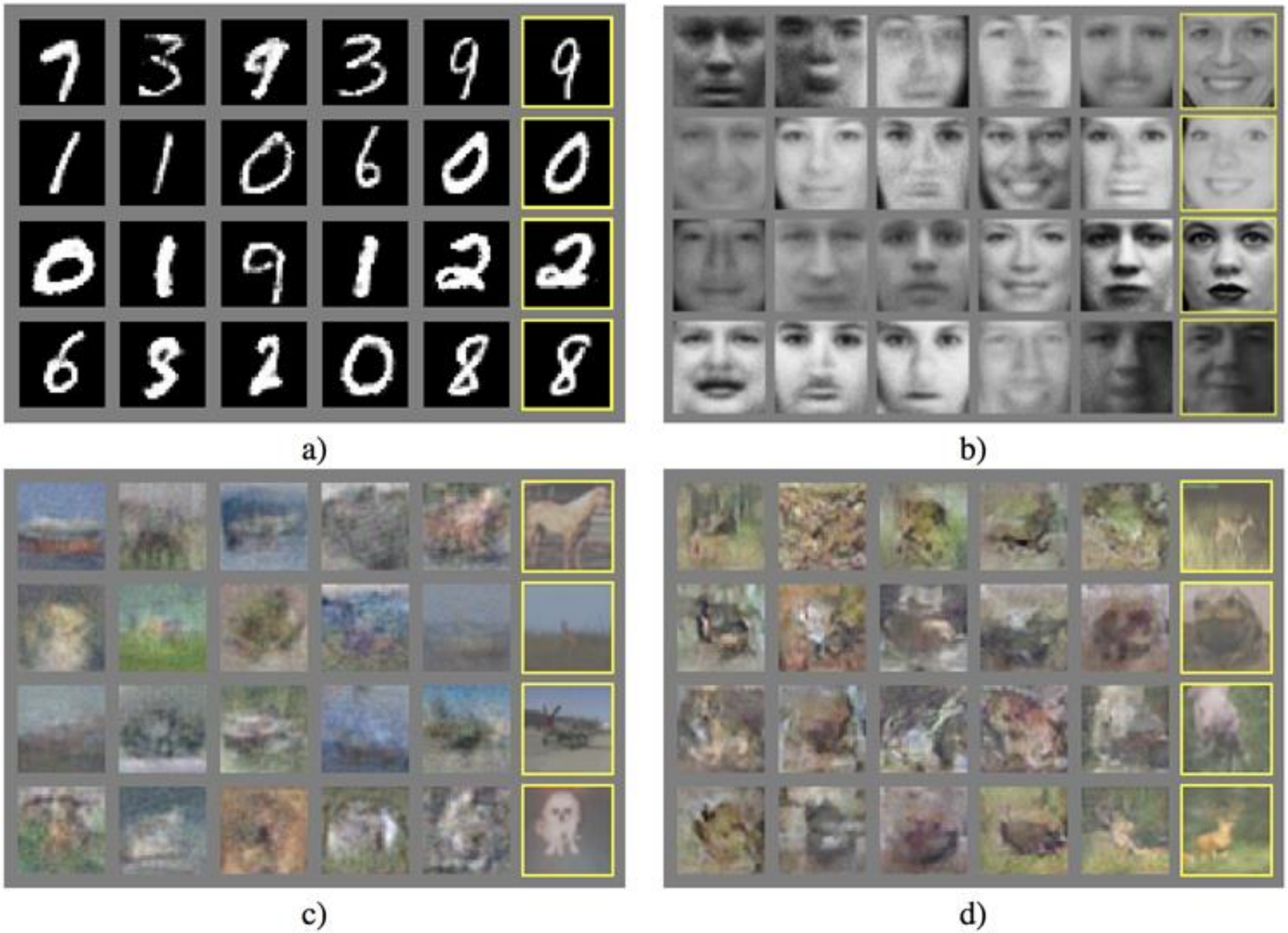


Figure from [Goodfellow et al., NeurIPS 2014]

Generative Adversarial Networks

- Key pieces of GAN
  - Fast sampling
  - No inference
  - Notion of optimizing directly for what you care about – perceptual samples

GAN: Bayes optimal discriminator

- What's the optimal discriminator given generated and true distributions?

$$V(G,D) = \mathbb{E}_{x \sim p_{data}}[\log D(x)] + \mathbb{E}_{z \sim p(z)}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

$$= \int_x p_{data}(x) \log D(x)\, dx + \int_z p(z) \log\left(1 - D\big(G(z)\big)\right) dz$$

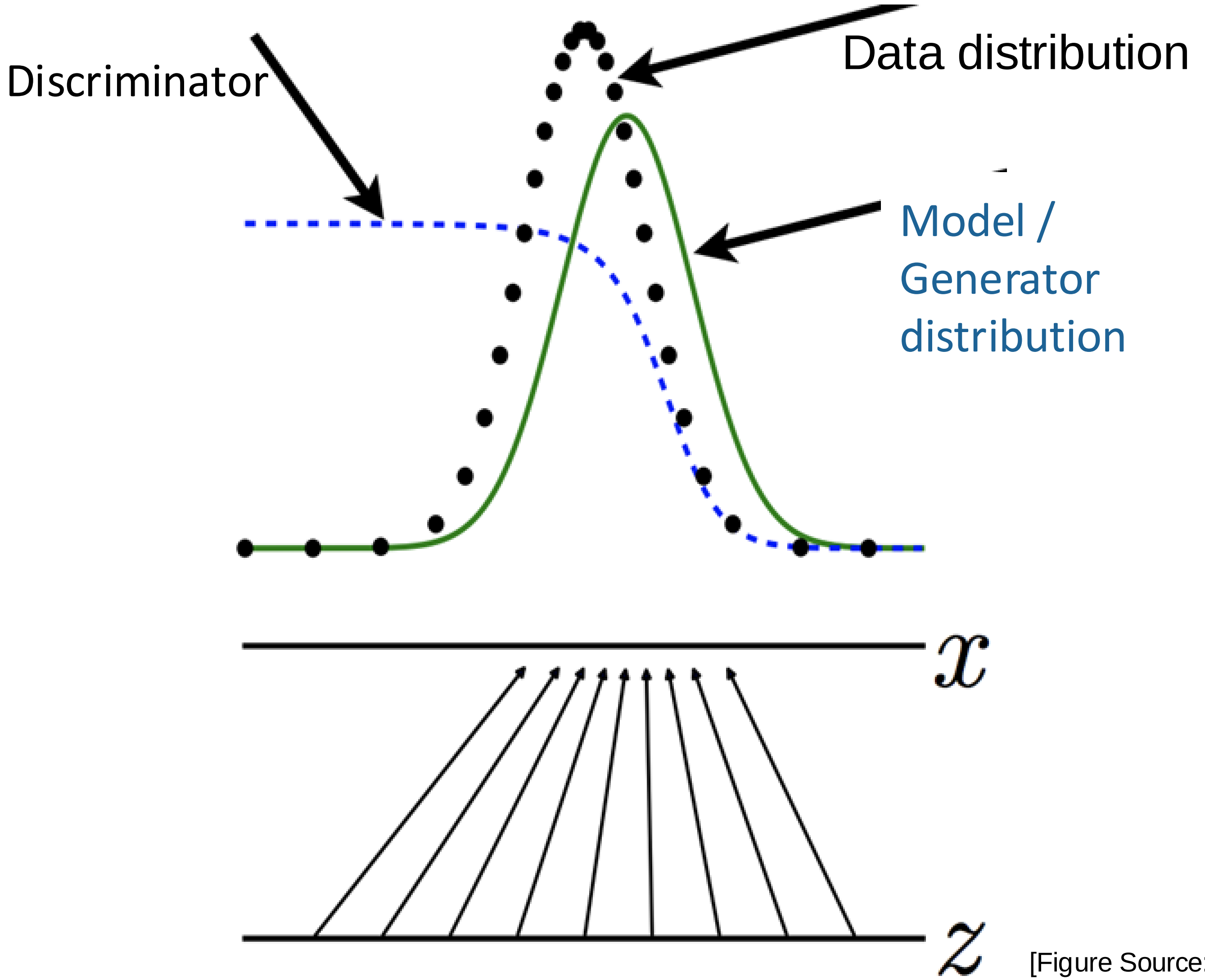
$$= \int_x p_{data}(x) \log D(x)\, dx + \int_x p_g(x) \log\big(1 - D(x)\big)\, dx$$

$$= \int_x \left[\, p_{data}(x) \log D(x) + p_g(x) \log\big(1 - D(x)\big)\right] dx$$

$$\nabla_y [a \log y + b \log(1-y)] = 0 \implies y^* = \frac{a}{a+b} \quad \forall\ (a,b) \in \mathbb{R}^2 \backslash (0,0)$$

$$\implies D^*(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

GAN: Bayes optimal discriminator



[Figure Source: Goodfellow NeurIPS 2016 Tutorial on GANs]

Generator Objective under Optimal Discriminator

$$V(G, D^*) = \mathbb{E}_{x \sim p_{data}}[\log D^*(x)] + \mathbb{E}_{z \sim p_g}\left[\log\left(1 - D^*(x)\right)\right]$$

$$= \mathbb{E}_{x \sim p_{data}}\left[\log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}\right] + \mathbb{E}_{z \sim p_g}\left[\log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}\right]$$

$$= -\log(4) + \underbrace{KL\left(p_{data} \parallel \frac{p_{data} + p_g}{2}\right) + KL\left(p_g \parallel \frac{p_{data} + p_g}{2}\right)}_{\left(\text{Jensen–Shannon Divergence (JSD) of } p_{data} \text{ and } p_g\right) \geq 0}$$

(KL(p||q) is the Kullback-Leibler divergence between p and q)

$$V(G^*, D^*) = -\log(4) \;\; \text{when} \;\; p_g = p_{data}$$

- Given the Bayes-optimal D*, solving for G is equivalent to minimizing the JSD divergence between p_{data} and p_g

Behaviors across divergence measures

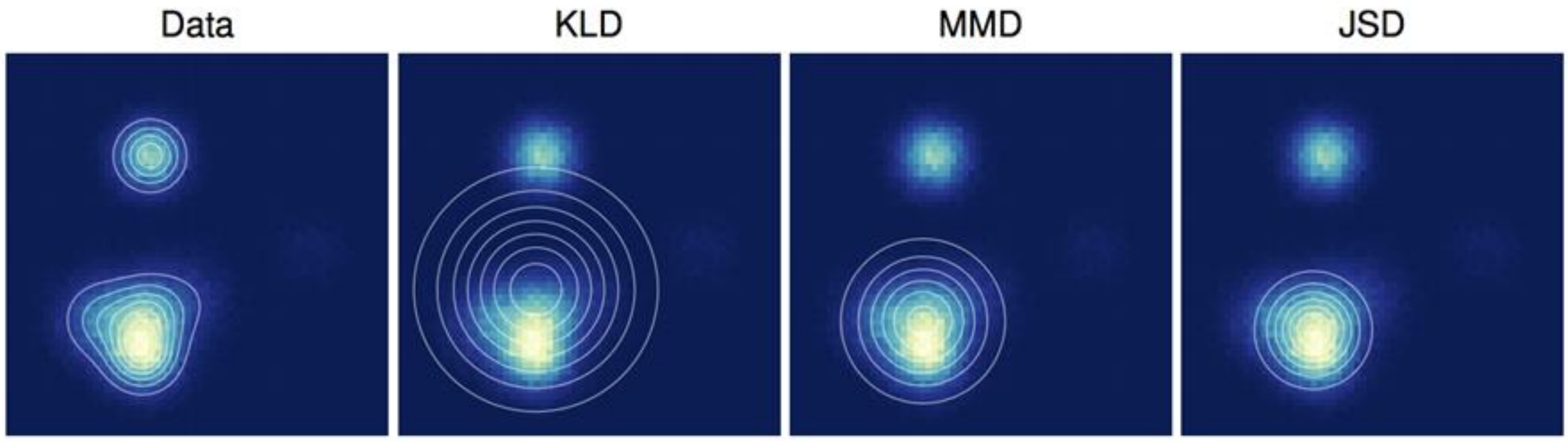
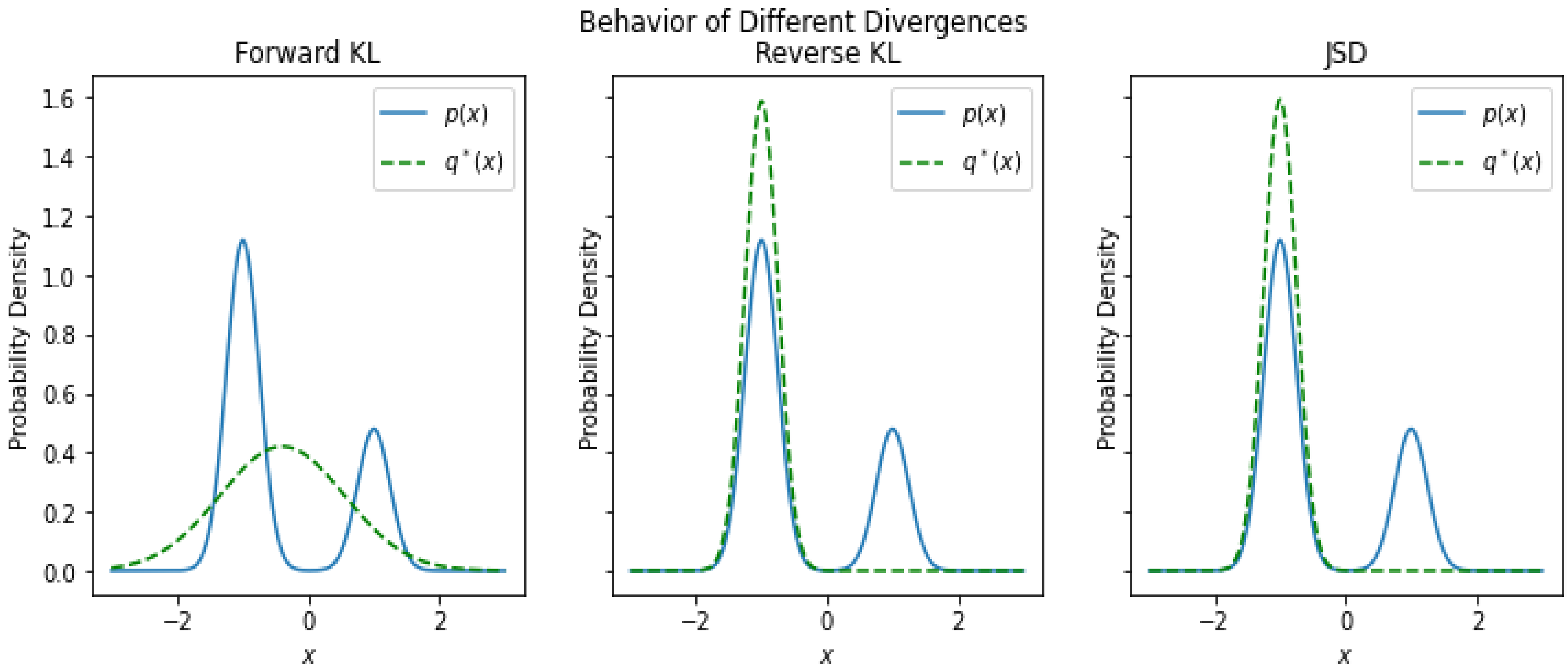


Figure 1: An isotropic Gaussian distribution was fit to data drawn from a mixture of Gaussians by either minimizing Kullback-Leibler divergence (KLD), maximum mean discrepancy (MMD), or Jensen-Shannon divergence (JSD). The different fits demonstrate different tradeoffs made by the three measures of distance between distributions.

[“A note on the evaluation of generative models” -- Theis, Van den Oord, Bethge 2015]

KL and JSD

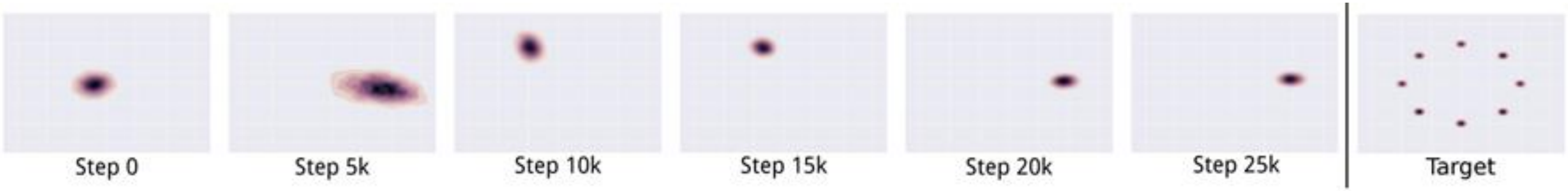


For given $p(x)$, find $q^*(x)$ that minimizes the divergence between them

Mode covering vs Mode seeking: Tradeoffs

- For compression, one would prefer to ensure all points in the data distribution are assigned probability mass.
- For generating good samples, blurring across modes spoils perceptual quality because regions outside the data manifold are assigned non-zero probability mass.
- Picking one mode without assigning probability mass on points outside can produce “better-looking” samples.
- Caveat: More expressive density models can place probability mass more accurately.

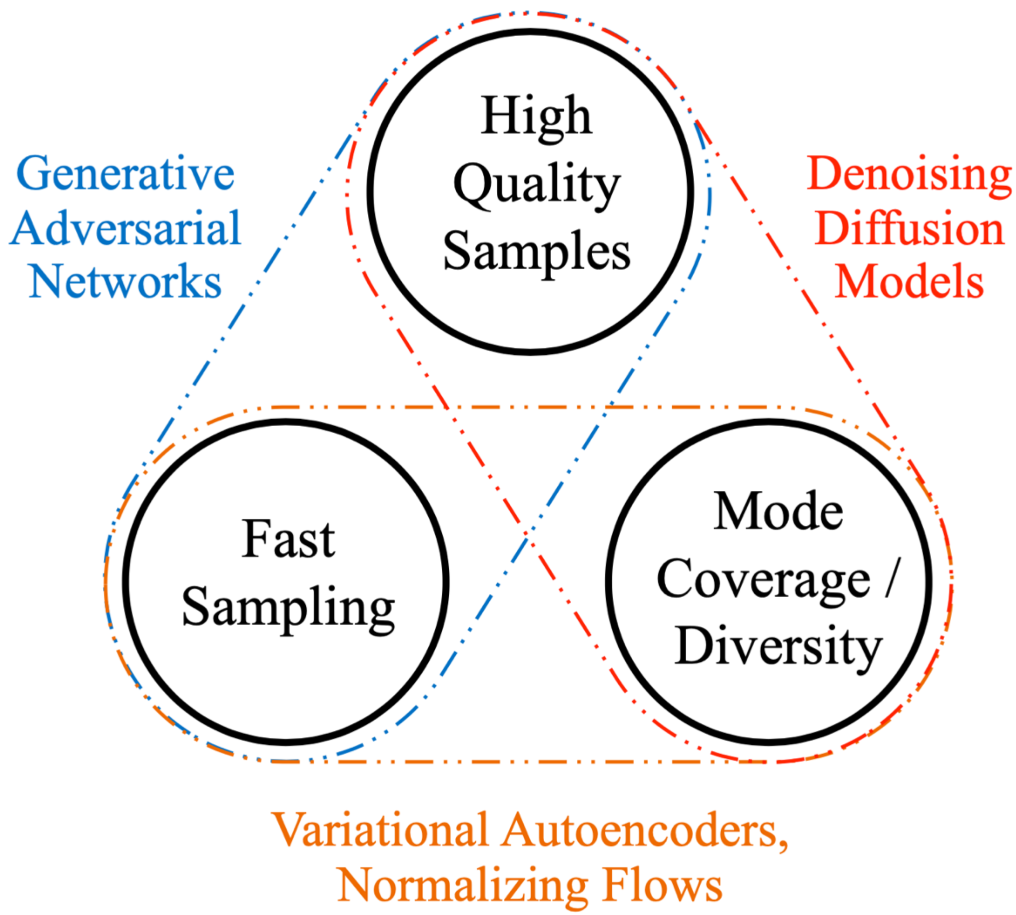
Mode Collapse



Standard GAN training collapses when the true distribution is a mixture of gaussians (Figure from Metz et al 2016)

More?

- Diffusion models
- …



Xiao, Z., Kreis, K., & Vahdat, A. Tackling the Generative Learning Trilemma with Denoising Diffusion GANs. In *ICLR, 2022*.

Thank you

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