

Deep Generative Models

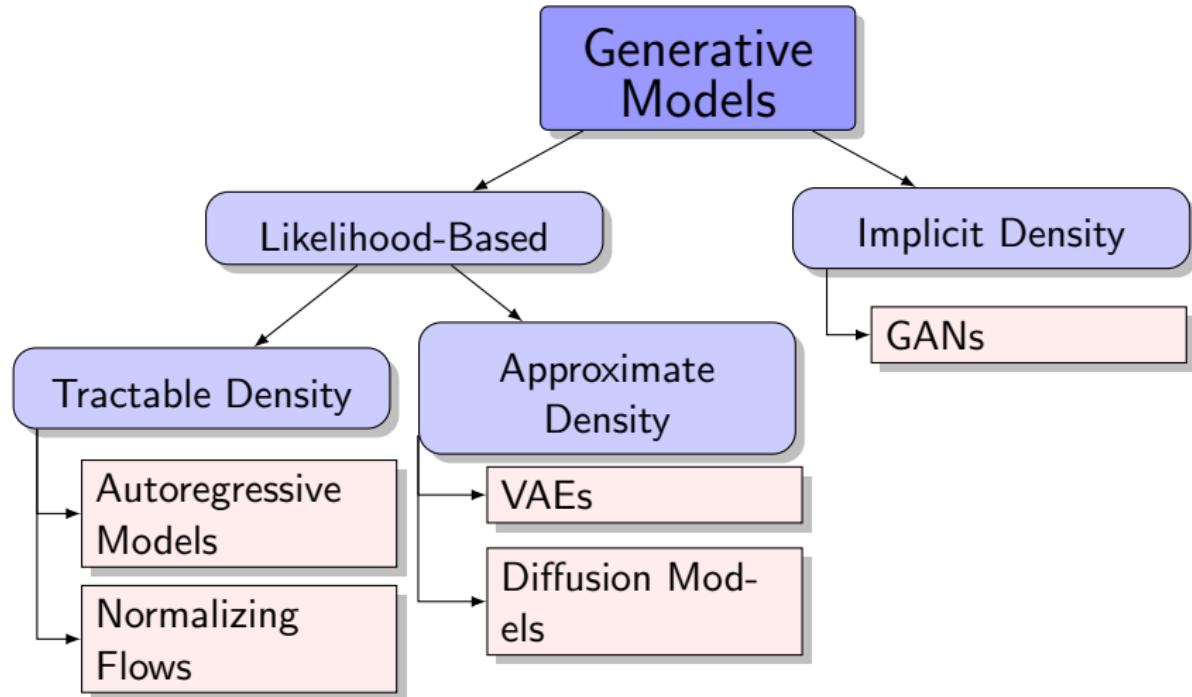
Lecture 1

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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Generative Models Zoo



Outline

1. Generative Models Overview
2. Course Tricks
3. Problem Statement
4. Divergence Minimization Framework
5. Autoregressive Modeling

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VAE – The First Scalable Approach for Image Generation



DCGAN – The First Convolutional GAN for Image Generation



Radford A., Metz L., Chintala S. *Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks*, 2015

StyleGAN – High-Quality Face Generation



Karras T., Laine S., Aila T. A Style-Based Generator Architecture for Generative Adversarial Networks, 2018

Language Modeling at Scale

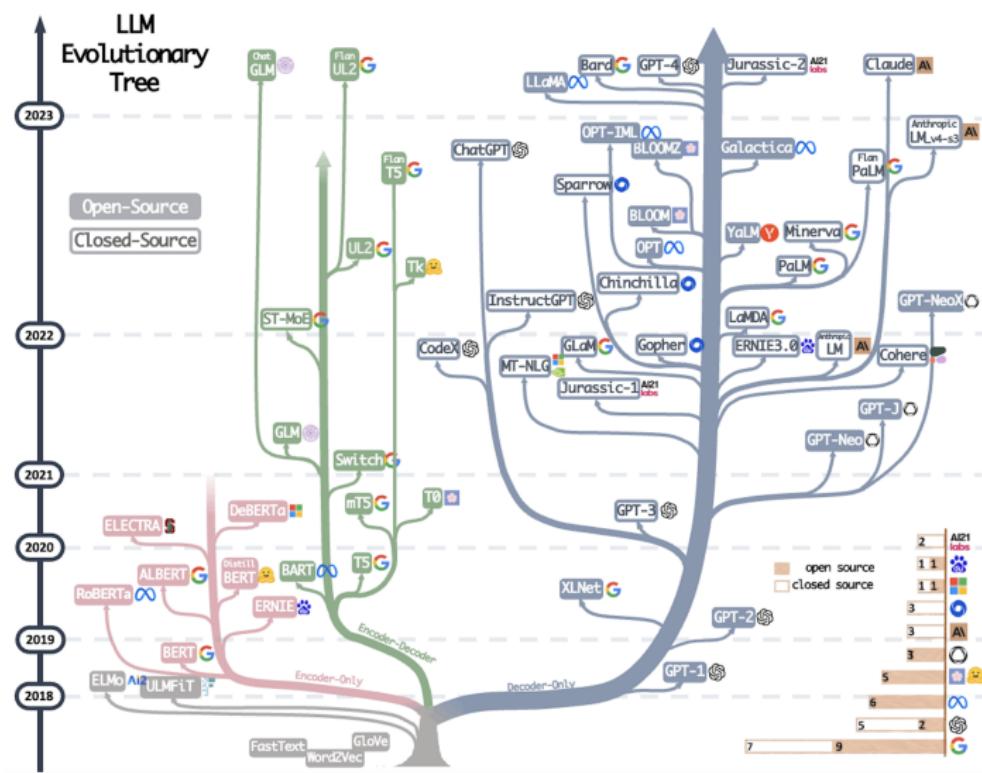
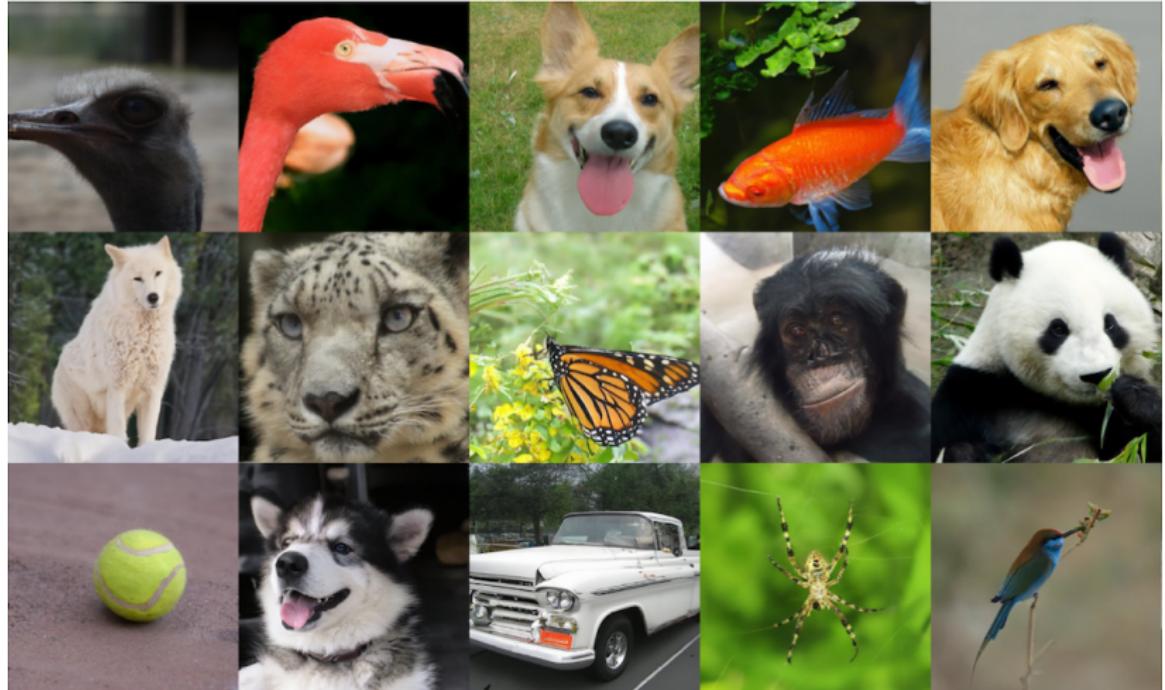


Image credit:

<https://blog.biocomm.ai/2023/05/14/open-source-proliferation-lm-evolutionary-tree/>

Denoising Diffusion Probabilistic Model



Midjourney – Impressive Text-to-Image Results



Image credit: <https://www.midjourney.com/explore>

Stable Diffusion 3 – Flow Matching



Sora – Video Generation



Image credit: <https://openai.com/index/sora>

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Course Tricks I

Log-Derivative Trick

Given a differentiable function $f : \mathbb{R}^m \rightarrow \mathbb{R}$,

$$\nabla \log f(\mathbf{x}) = \frac{1}{f(\mathbf{x})} \cdot \nabla f(\mathbf{x}).$$

Jensen's Inequality

If $\mathbf{x} \in \mathbb{R}^m$ is a continuous random variable with density $p(\mathbf{x})$ and $f : \mathbb{R}^m \rightarrow \mathbb{R}$ is convex, then

$$\mathbb{E}[f(\mathbf{x})] \geq f(\mathbb{E}[\mathbf{x}]).$$

Monte Carlo Estimation

Let $\mathbf{x} \in \mathbb{R}^m$ be a continuous random variable with density $p(\mathbf{x})$, and $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^d$ be any vector-valued function. Then,

$$\mathbb{E}_{p(\mathbf{x})}\mathbf{f}(\mathbf{x}) = \int p(\mathbf{x})\mathbf{f}(\mathbf{x})d\mathbf{x} \approx \frac{1}{n} \sum_{i=1}^n \mathbf{f}(\mathbf{x}_i), \quad \text{where } \mathbf{x}_i \sim p(\mathbf{x}).$$

Course Tricks II

Change of Variables Theorem (CoV)

Suppose \mathbf{x} is a continuous random variable with density $p(\mathbf{x})$, and $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ is differentiable and **invertible**. If $\mathbf{y} = \mathbf{f}(\mathbf{x})$, then

$$p(\mathbf{y}) = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}} \right) \right| = p(\mathbf{f}^{-1}(\mathbf{y})) \left| \det \left(\frac{\partial \mathbf{f}^{-1}(\mathbf{y})}{\partial \mathbf{y}} \right) \right|.$$

Proof (1D)

Assume f is monotonically increasing.

$$F_Y(y) = P(Y \leq y) = P(x \leq f^{-1}(y)) = F_X(f^{-1}(y))$$

$$p(y) = \frac{dF_Y(y)}{dy} = \frac{dF_X(f^{-1}(y))}{dy} = \frac{dF_X(x)}{dx} \frac{df^{-1}(y)}{dy} = p(x) \frac{df^{-1}(y)}{dy}$$

Course Tricks III

Law of the Unconscious Statistician (LOTUS)

Let $\mathbf{x} \in \mathbb{R}^m$ be a continuous random variable with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ be measurable. If $\mathbf{y} = \mathbf{f}(\mathbf{x})$, then

$$\mathbb{E}_{p(\mathbf{y})}\mathbf{g}(\mathbf{y}) = \int p(\mathbf{y})\mathbf{g}(\mathbf{y})d\mathbf{y} = \int p(\mathbf{x})\mathbf{g}(\mathbf{f}(\mathbf{x}))d\mathbf{x} = \mathbb{E}_{p(\mathbf{x})}\mathbf{g}(\mathbf{f}(\mathbf{x})).$$

Dirac Delta Function

Any deterministic variable \mathbf{x}_0 can be interpreted as a random variable with density $p(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0)$.

$$\delta(\mathbf{x}) = \begin{cases} +\infty, & \mathbf{x} = \mathbf{x}_0 \\ 0, & \mathbf{x} \neq \mathbf{x}_0 \end{cases} \quad \int \delta(\mathbf{x})d\mathbf{x} = 1$$

$$\mathbb{E}_{p(\mathbf{x})}\mathbf{f}(\mathbf{x}) = \int \delta(\mathbf{x} - \mathbf{x}_0)\mathbf{f}(\mathbf{x})d\mathbf{x} = \mathbf{f}(\mathbf{x}_0)$$

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Problem Statement

We're given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^m$ drawn from an **unknown** distribution $\pi(\mathbf{x})$.

Objective

Our aim is to learn a distribution $\pi(\mathbf{x})$ that allows us to:

- ▶ Evaluate $\pi(\mathbf{x})$ on novel data (answering “How likely is an object \mathbf{x} ?”) — **density estimation**;
- ▶ Generate new samples from $\pi(\mathbf{x})$ (sample $\mathbf{x} \sim \pi(\mathbf{x})$) — **generation**.

Challenge

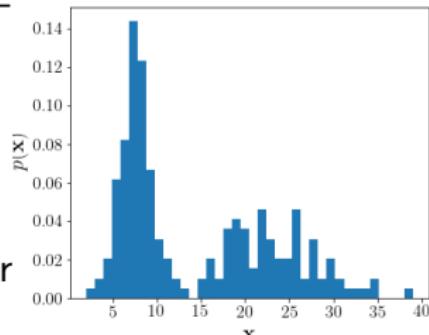
The data is high-dimensional and complex. For example, image datasets live in $\mathbb{R}^{\text{width} \times \text{height} \times \text{channels}}$. The curse of dimensionality makes accurately estimating $\pi(\mathbf{x})$ infeasible.

Histogram as a Generative Model

Assume $x \sim \text{Categorical}(\pi)$. The histogram model is fully characterized by

$$\hat{\pi}_k = \hat{\pi}(x = k) = \frac{\sum_{i=1}^n [x_i = k]}{n}.$$

Curse of dimensionality: The number of bins rises exponentially.



MNIST example: 28×28 grayscale images, with each image $\mathbf{x} = (x_1, \dots, x_{784})$, $x_i \in \{0, 1\}$:

$$\pi(\mathbf{x}) = \pi(x_1) \cdot \pi(x_2|x_1) \cdot \dots \cdot \pi(x_m|x_{m-1}, \dots, x_1).$$

A complete histogram would require $2^{28 \times 28} - 1$ parameters for $\pi(\mathbf{x})$.

Question: How many parameters are required in these cases?

$$\pi(\mathbf{x}) = \pi(x_1) \cdot \pi(x_2) \cdot \dots \cdot \pi(x_m);$$

$$\pi(\mathbf{x}) = \pi(x_1) \cdot \pi(x_2|x_1) \cdot \dots \cdot \pi(x_m|x_{m-1}).$$

Problem Statement: Conditional Models

Conditional Models

In practice, we're typically interested in learning conditional models $\pi(\mathbf{x}|\mathbf{y})$.

- ▶ $\mathbf{y} = \emptyset, \mathbf{x} = \text{image}$ \Rightarrow unconditional image model
- ▶ $\mathbf{y} = \text{class label}, \mathbf{x} = \text{image}$ \Rightarrow class-conditional image model
- ▶ $\mathbf{y} = \text{text prompt}, \mathbf{x} = \text{image}$ \Rightarrow text-to-image model
- ▶ $\mathbf{y} = \text{image}, \mathbf{x} = \text{image}$ \Rightarrow image-to-image model
- ▶ $\mathbf{y} = \text{image}, \mathbf{x} = \text{text}$ \Rightarrow image-to-text (image captioning) model
- ▶ $\mathbf{y} = \text{English text}, \mathbf{x} = \text{Russian text}$ \Rightarrow sequence-to-sequence model (machine translation) model
- ▶ $\mathbf{y} = \text{sound}, \mathbf{x} = \text{text}$ \Rightarrow speech-to-text (automatic speech recognition) model
- ▶ $\mathbf{y} = \text{text}, \mathbf{x} = \text{sound}$ \Rightarrow text-to-speech model

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Divergences

- ▶ Let us fix a probabilistic model $p(\mathbf{x}|\boldsymbol{\theta})$ —a parametric family of distributions.
- ▶ Instead of searching among all possible distributions for the true $\pi(\mathbf{x})$, we seek a functional approximation $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

What is a Divergence?

Let \mathcal{P} be the set of all probability distributions. A mapping $D : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R}$ is called a **divergence** if

- ▶ $D(\pi\|p) \geq 0$ for all $\pi, p \in \mathcal{P}$
- ▶ $D(\pi\|p) = 0$ if and only if $\pi \equiv p$

Divergence Minimization Problem

$$\min_{\boldsymbol{\theta}} D(\pi\|p)$$

where $\pi(\mathbf{x})$ is the true data distribution and $p(\mathbf{x}|\boldsymbol{\theta})$ is the model distribution.

Forward KL vs Reverse KL (Kullback-Leibler Divergence)

Forward KL

$$\text{KL}(\pi \| p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\theta)} d\mathbf{x} \rightarrow \min_{\theta}$$

Reverse KL

$$\text{KL}(p \| \pi) = \int p(\mathbf{x}|\theta) \log \frac{p(\mathbf{x}|\theta)}{\pi(\mathbf{x})} d\mathbf{x} \rightarrow \min_{\theta}$$

What's the practical distinction between these two objectives?

Maximum Likelihood Estimation (MLE)

Let $\{\mathbf{x}_i\}_{i=1}^n$ be i.i.d. observed samples.

$$\theta^* = \arg \max_{\theta} \prod_{i=1}^n p(\mathbf{x}_i|\theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta).$$

Forward KL vs Reverse KL: MLE as Forward KL

Forward KL

$$\begin{aligned}\text{KL}(\pi \| p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\theta)} d\mathbf{x} \\ &= \int \pi(\mathbf{x}) \log \pi(\mathbf{x}) d\mathbf{x} - \int \pi(\mathbf{x}) \log p(\mathbf{x}|\theta) d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} [\log p(\mathbf{x}|\theta)] + \text{const} \\ &\approx -\frac{1}{n} \sum_{i=1}^n \log p(\mathbf{x}_i|\theta) + \text{const} \rightarrow \min_{\theta}.\end{aligned}$$

Maximum likelihood estimation is thus equivalent to minimizing a Monte Carlo estimate of the forward KL divergence.

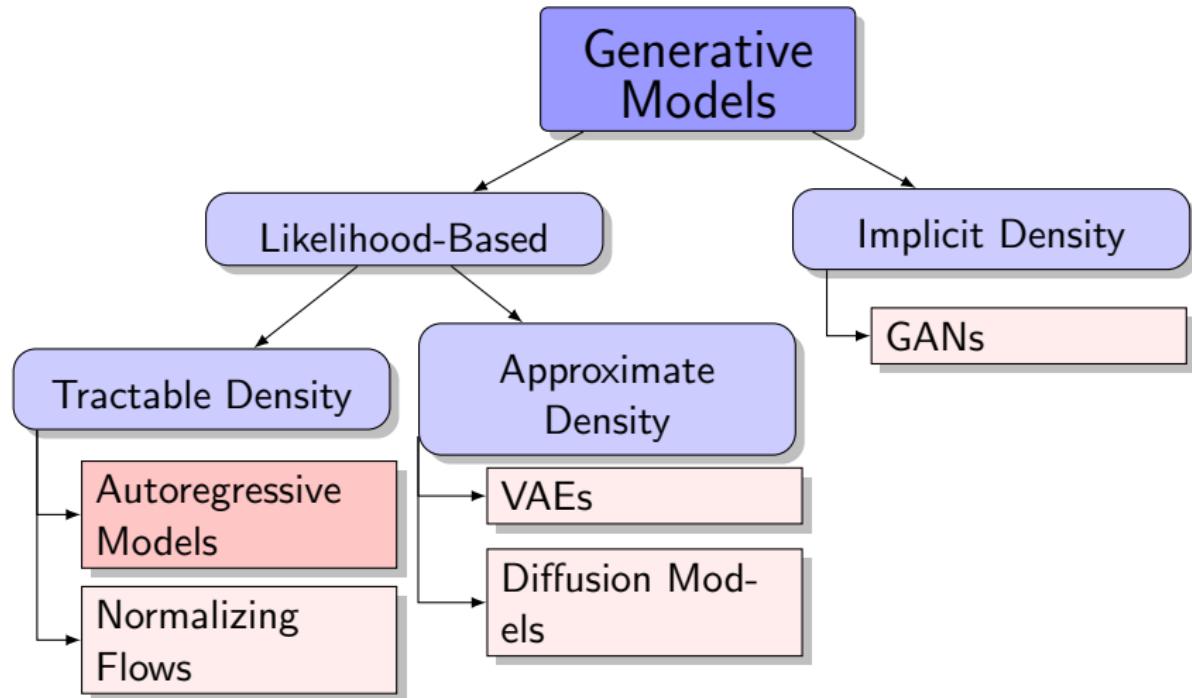
Reverse KL

$$\begin{aligned}\text{KL}(p \| \pi) &= \int p(\mathbf{x}|\theta) \log \frac{p(\mathbf{x}|\theta)}{\pi(\mathbf{x})} d\mathbf{x} \\ &= \mathbb{E}_{p(\mathbf{x}|\theta)} [\log p(\mathbf{x}|\theta) - \log \pi(\mathbf{x})] \rightarrow \min_{\theta}\end{aligned}$$

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Autoregressive Modeling

MLE Problem

$$\boldsymbol{\theta}^* = \arg \max_{\boldsymbol{\theta}} \prod_{i=1}^n p(\mathbf{x}_i | \boldsymbol{\theta}) = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \log p(\mathbf{x}_i | \boldsymbol{\theta})$$

- ▶ This maximization is typically solved via gradient-based optimization.
- ▶ Thus, efficient computation of both $\log p(\mathbf{x} | \boldsymbol{\theta})$ and its gradient $\frac{\partial \log p(\mathbf{x} | \boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$ is crucial.

Likelihood as a Product of Conditionals

For $\mathbf{x} = (x_1, \dots, x_m)$, $\mathbf{x}_{1:j} = (x_1, \dots, x_j)$,

$$p(\mathbf{x} | \boldsymbol{\theta}) = \prod_{j=1}^m p(x_j | \mathbf{x}_{1:j-1}, \boldsymbol{\theta}); \quad \log p(\mathbf{x} | \boldsymbol{\theta}) = \sum_{j=1}^m \log p(x_j | \mathbf{x}_{1:j-1}, \boldsymbol{\theta})$$
$$\boldsymbol{\theta}^* = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \left[\sum_{j=1}^m \log p(x_{ij} | \mathbf{x}_{i,1:j-1}, \boldsymbol{\theta}) \right]$$

Autoregressive Models

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{j=1}^m \log p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$$

- ▶ Sampling is performed sequentially:
 - ▶ Sample $\hat{x}_1 \sim p(x_1|\boldsymbol{\theta})$;
 - ▶ Sample $\hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta})$;
 - ▶ ...
 - ▶ Sample $\hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$;
 - ▶ The generated sample is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.
- ▶ Each conditional $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$ can be modeled using a neural network.
- ▶ Modeling all conditionals separately isn't feasible. To address this, we share parameters across all conditionals.

Autoregressive Models: MLP

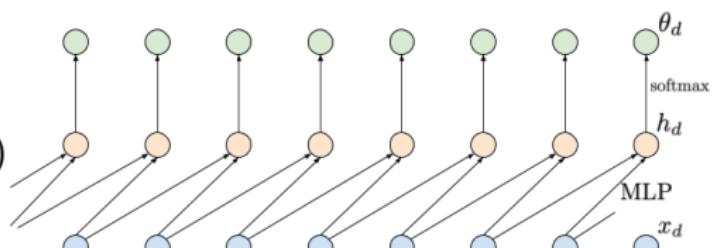
For large j , the conditional $p(x_j|\mathbf{x}_{1:j-1}, \theta)$ becomes intractable as the history $\mathbf{x}_{1:j-1}$ grows variable-length.

Markov Assumption

$$p(x_j|\mathbf{x}_{1:j-1}, \theta) = p(x_j|\mathbf{x}_{j-d:j-1}, \theta), \quad d \text{ is a fixed parameter.}$$

Example

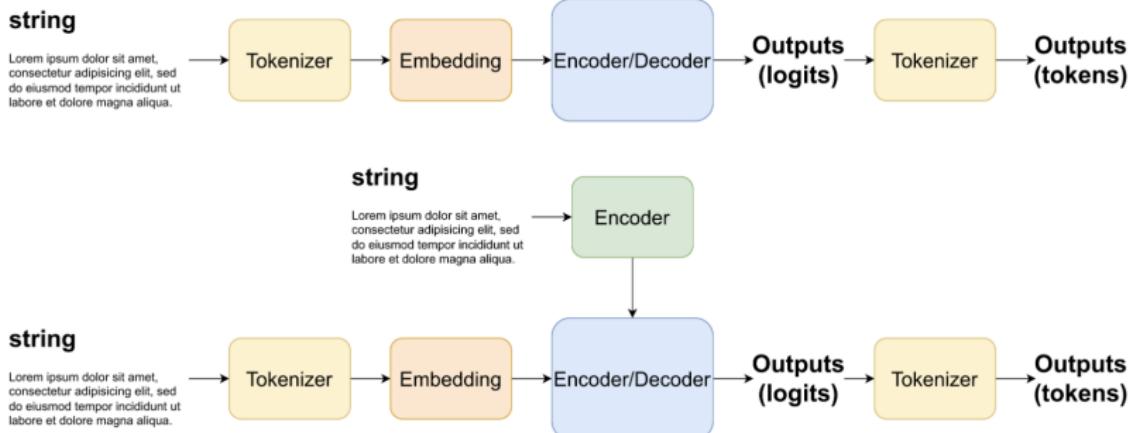
- ▶ $d = 2$
- ▶ $x_j \in \{0, 255\}$
- ▶ $\mathbf{h}_j = \text{MLP}_{\theta}(x_{j-1}, x_{j-2})$
- ▶ $\pi_j = \text{softmax}(\mathbf{h}_j)$
- ▶ $p(x_j|x_{j-1}, x_{j-2}, \theta) =$



Categorical(π_j) Can we also model continuous-valued data, not just the discrete case?

Autoregressive Models: LLM

$$p(x_j | \mathbf{x}_{1:j-1}, \theta) = p(x_j | \mathbf{x}_{j-d:j-1}, \theta), \quad d \text{ is the context window.}$$

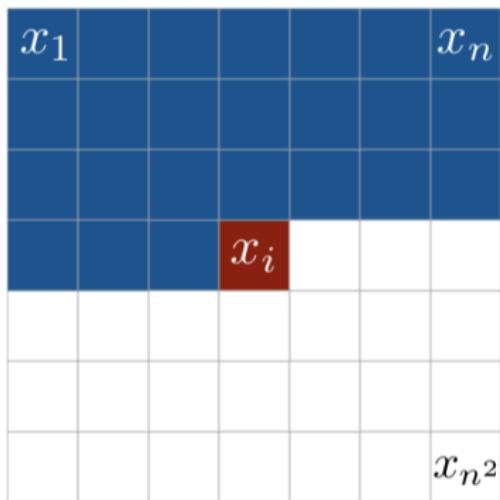


Autoregressive Models for Images

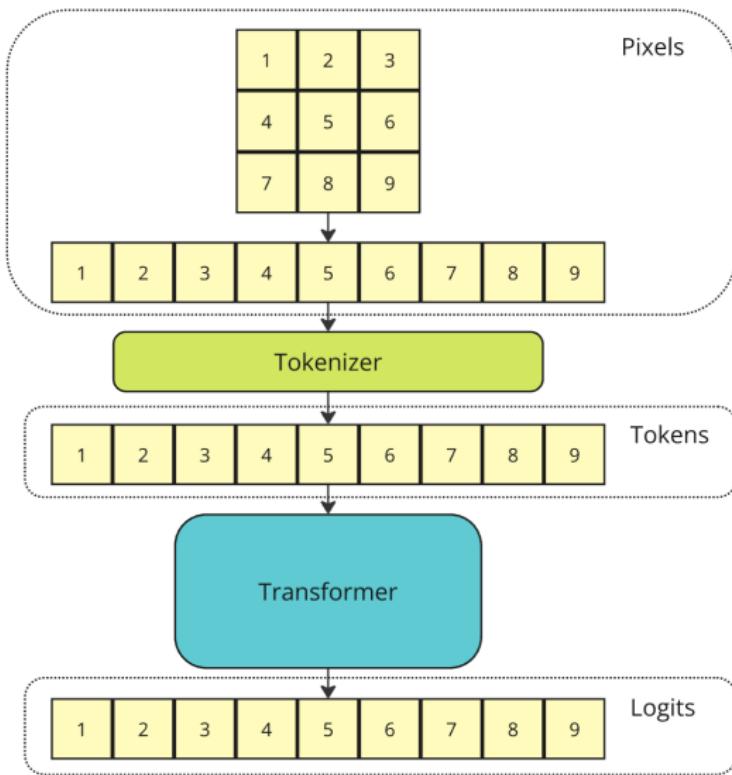
How do we model the distribution $\pi(\mathbf{x})$ of natural images?

$$p(\mathbf{x}|\theta) = \prod_{j=1}^{\text{width} \times \text{height}} p(x_j | \mathbf{x}_{1:j-1}, \theta)$$

- ▶ A pixel ordering must be selected; the raster scan is a standard choice.
- ▶ RGB channel dependencies can be modeled explicitly as well.



Autoregressive Models: ImageGPT



Summary

- ▶ Our target is to approximate the data distribution both for density estimation and for generation.
- ▶ The divergence minimization framework offers a principled way to learn distributions that match the data.
- ▶ Minimizing the forward KL divergence is equivalent to maximum likelihood estimation.
- ▶ Autoregressive models decompose the joint distribution as a product of conditionals.
- ▶ Autoregressive sampling is simple, but inherently sequential.
- ▶ Joint density evaluation multiplies all conditional probabilities $p(x_j | \mathbf{x}_{1:j-1}, \theta)$.
- ▶ ImageGPT applies a transformer architecture to sequences of raster-ordered image pixels.