

Deep Generative Models

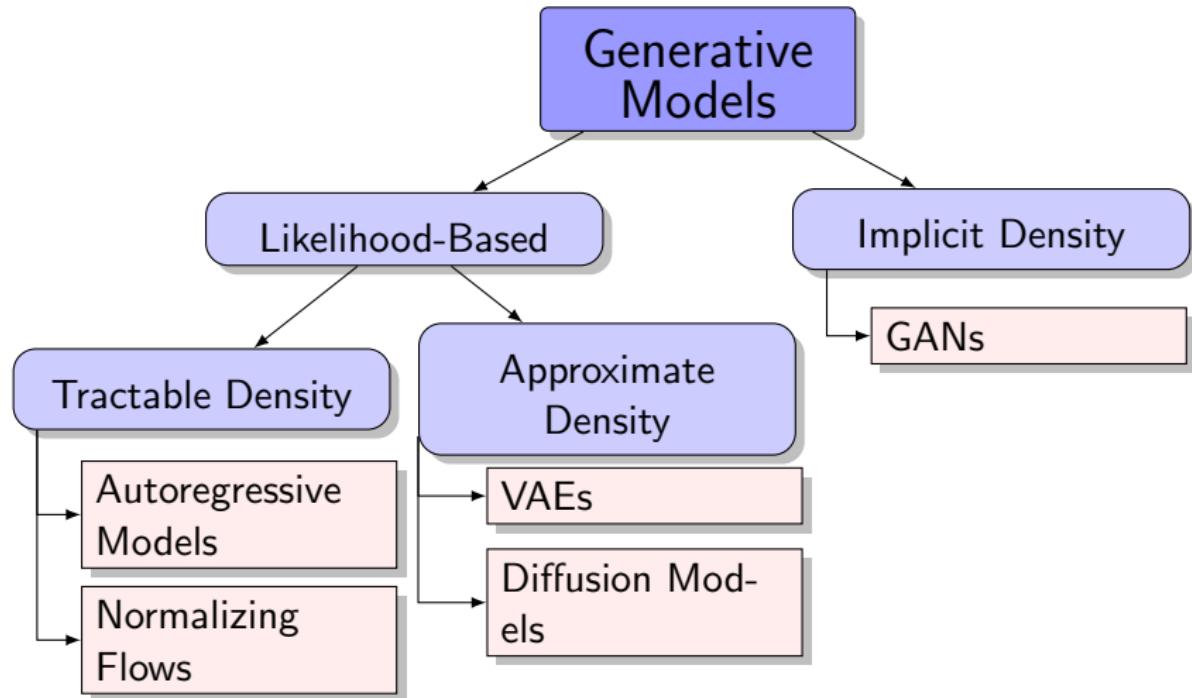
Lecture 1

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Moscow Institute of Physics and Technology
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2025, Autumn

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



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

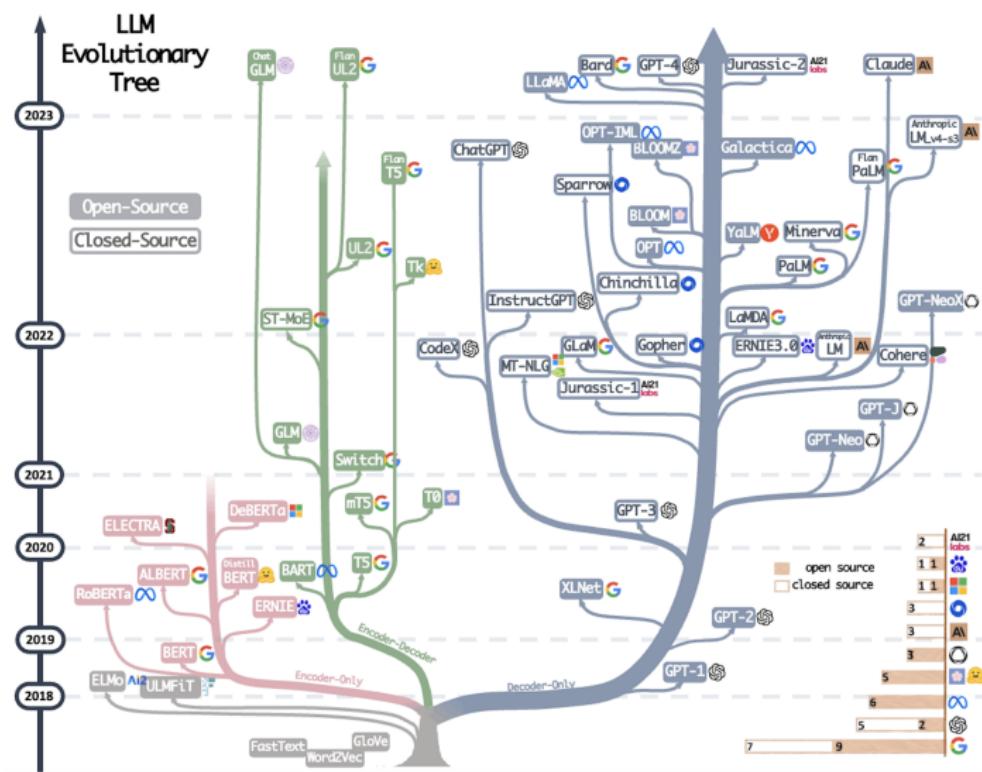
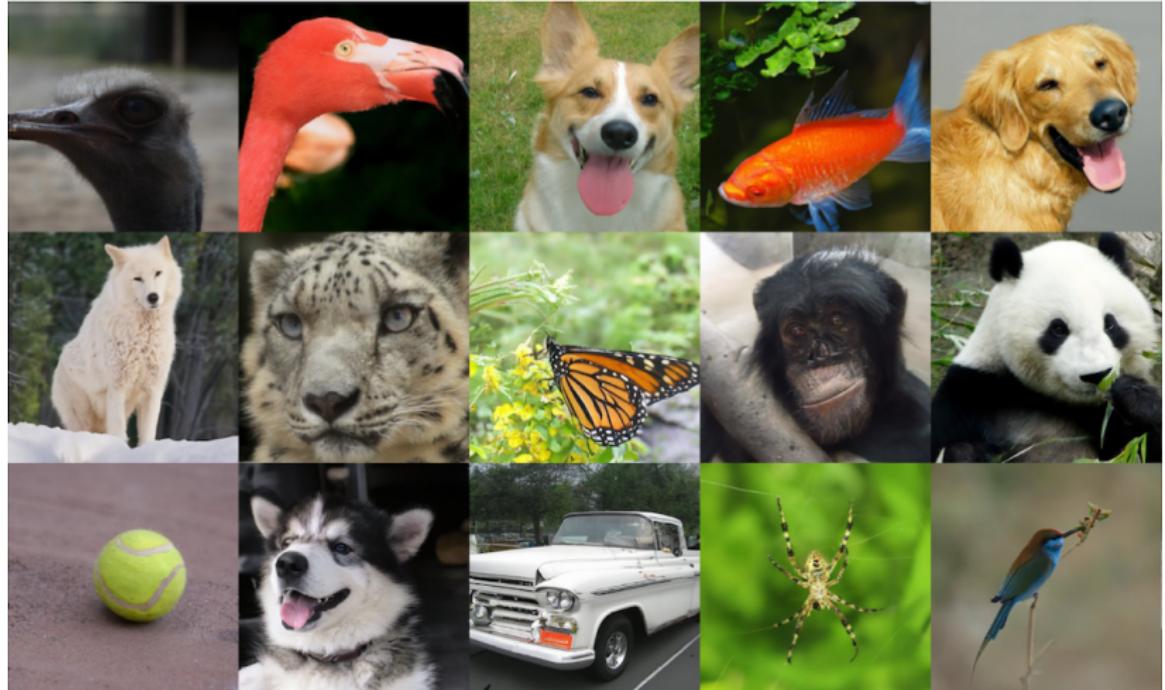


Image credit:

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

Denoising Diffusion Probabilistic Model



Midjourney – Impressive Text-to-Image Results



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

Sora – Video Generation



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

GPT4o Image Editing

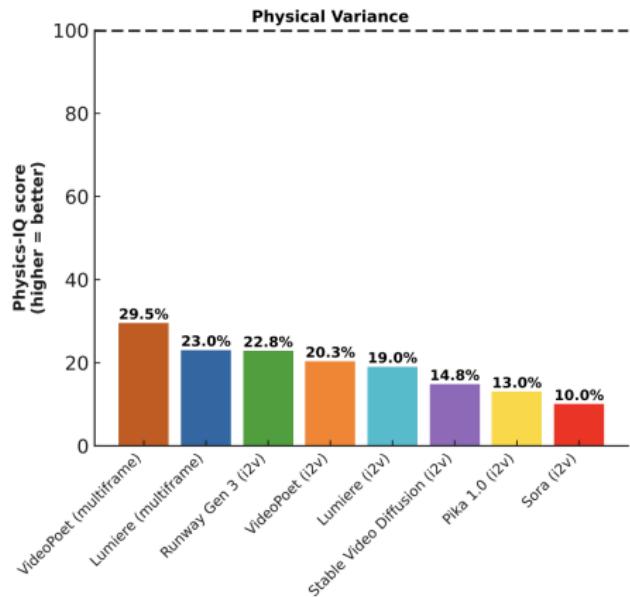
Prompt: Give this cat a detective hat and a monocle



Image credit: <https://openai.com/index/introducing-4o-image-generation/>

Open Problems in Generative Models

- ▶ Video generation
- ▶ 3D scene generation
- ▶ Understanding of physical processes
- ▶ Multimodal end-to-end models



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Course Tricks I

Log-Derivative Trick

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

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

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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

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

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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

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

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Proof (1D)

Assume f is monotonically increasing.

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

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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

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Dirac Delta Function

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

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

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Challenge

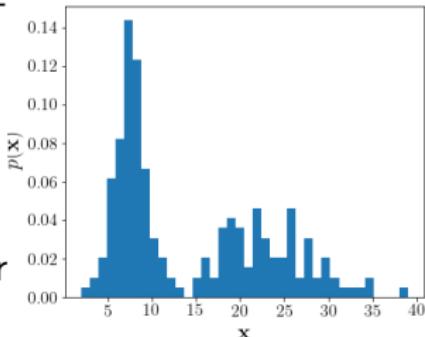
The data is high-dimensional and complex. For example, image datasets live in $\mathbb{R}^{\text{width} \times \text{height} \times \text{channels}}$. The curse of dimensionality makes accurately estimating $\pi(\mathbf{x})$ infeasible.

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.

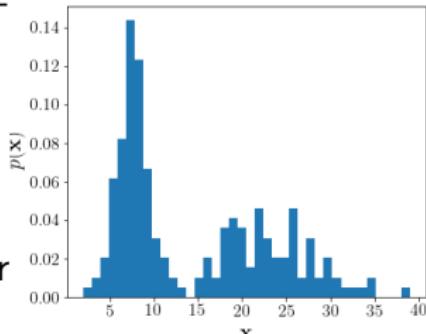


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MNIST example: 28×28 grayscale images, with each image $\mathbf{x} = (x_1, \dots, x_{784})$, $x_i \in \{0, 1\}$:

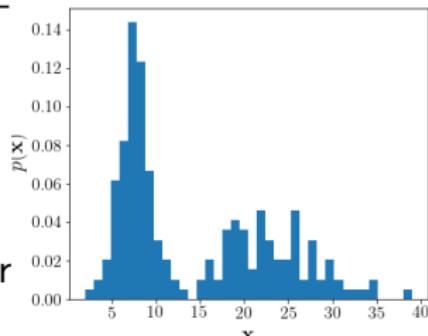
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A complete histogram would require $2^{28 \times 28} - 1$ parameters for $\pi(\mathbf{x})$.

Question: How many parameters are required in these cases?

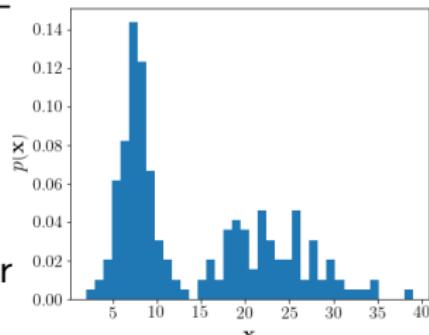
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- ▶ $\mathbf{y} = \emptyset, \mathbf{x} = \text{image}$ \Rightarrow unconditional image model
- ▶ $\mathbf{y} = \text{class label}, \mathbf{x} = \text{image}$ \Rightarrow class-conditional image model
- ▶ $\mathbf{y} = \text{text prompt}, \mathbf{x} = \text{image}$ \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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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

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Divergence Minimization Problem

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

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

Forward KL vs Reverse KL (Kullback-Leibler Divergence)

Forward KL

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

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Maximum Likelihood Estimation (MLE)

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

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

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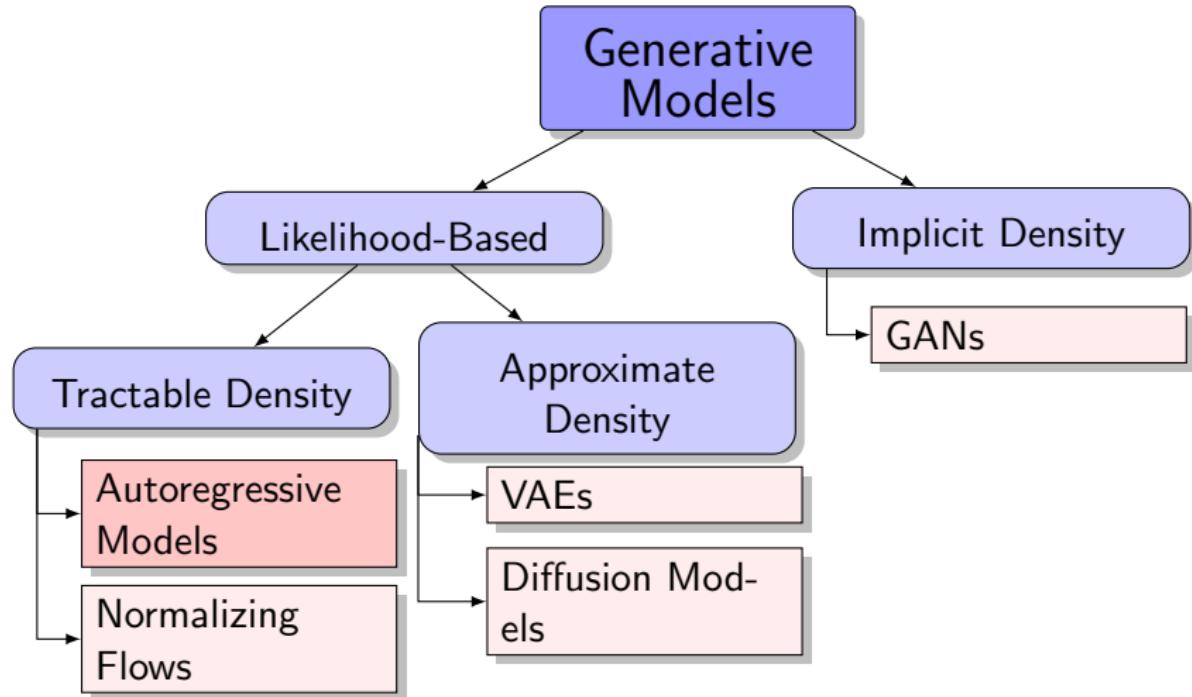
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Autoregressive Modeling

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- ▶ 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.

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

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- ▶ 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.

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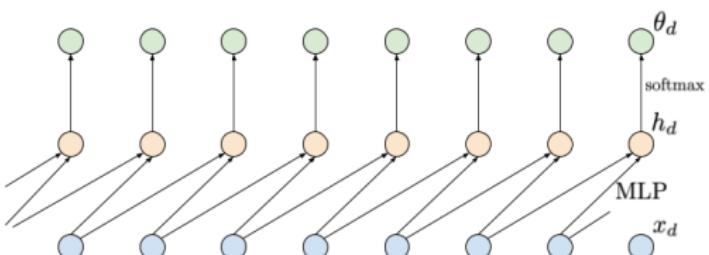
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Example

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



Autoregressive Models: MLP

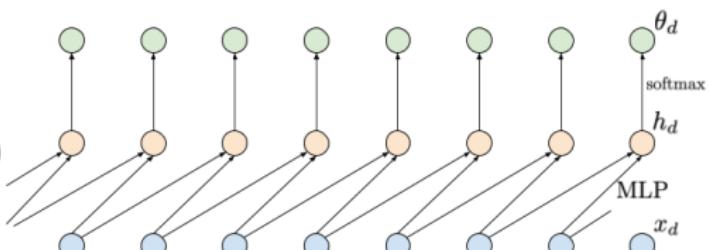
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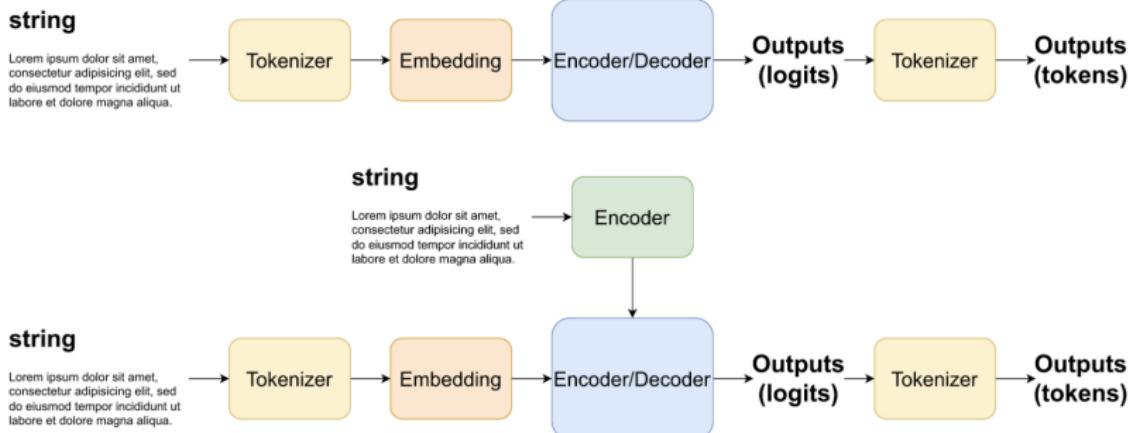
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Can we also model continuous-valued data, not just the discrete case?

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?

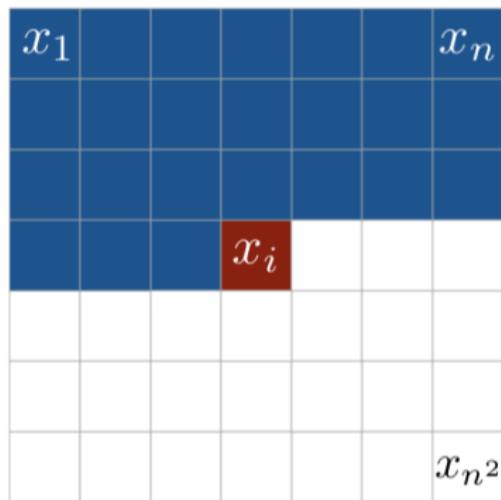
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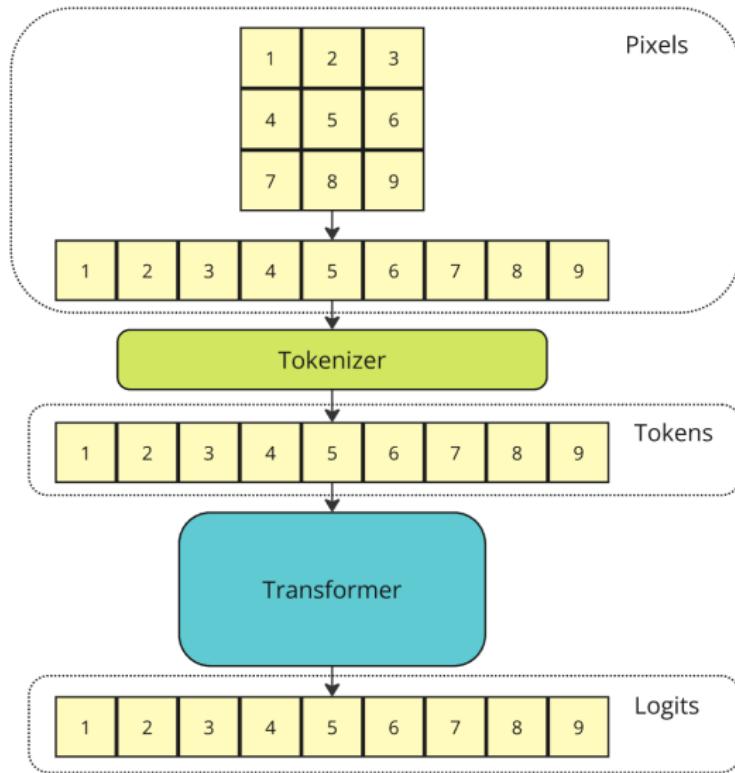
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$$p(\mathbf{x}|\theta) = \prod_{j=1}^{\text{width} \times \text{height}} p(x_j | \mathbf{x}_{1:j-1}, \theta)$$

- ▶ 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.