Deep Generative Models

Lecture 1

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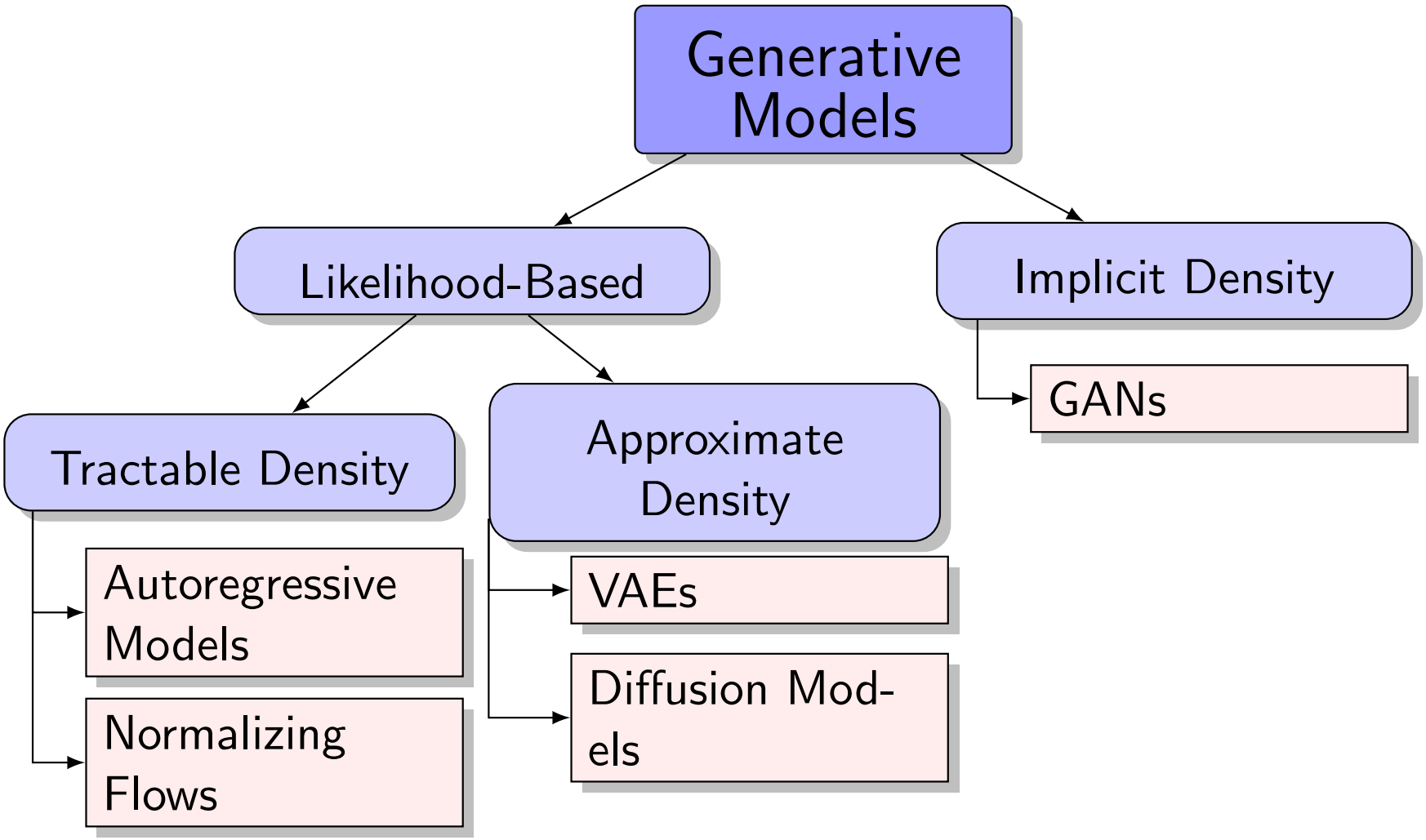
2025, Autumn

Generative Models Zoo



Outline

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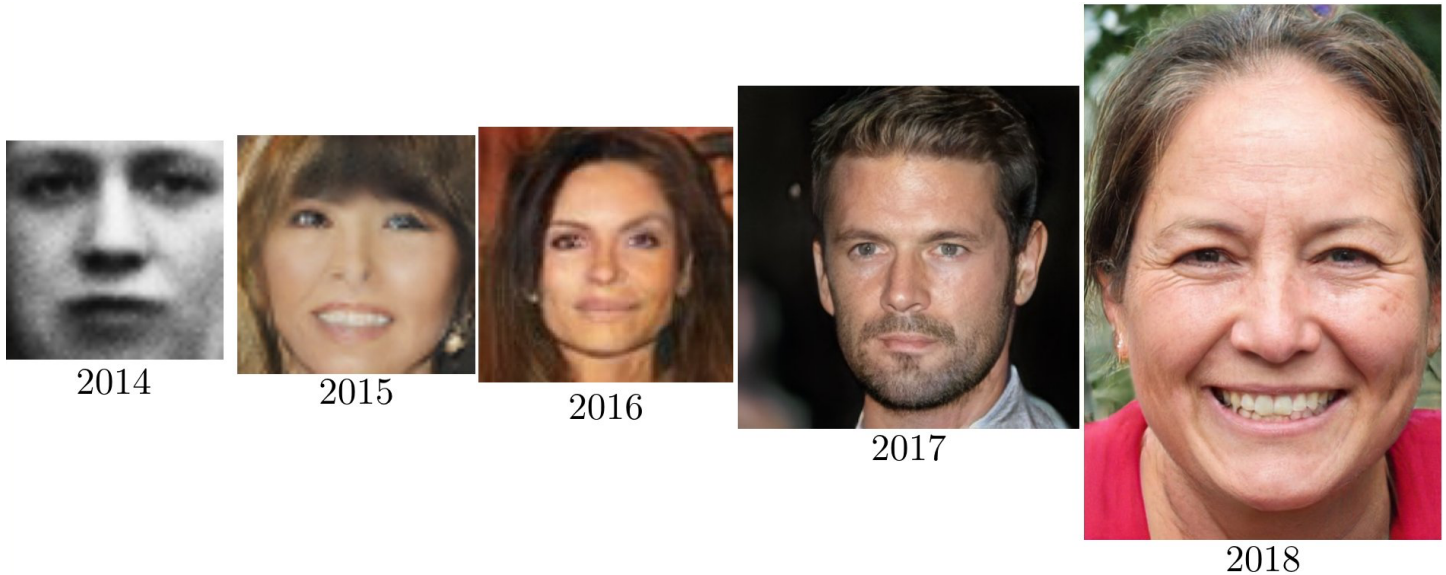
VAE – The First Scalable Approach for Image Generation

Kingma D.P., Welling M. Auto-Encoding Variational Bayes, 2013

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

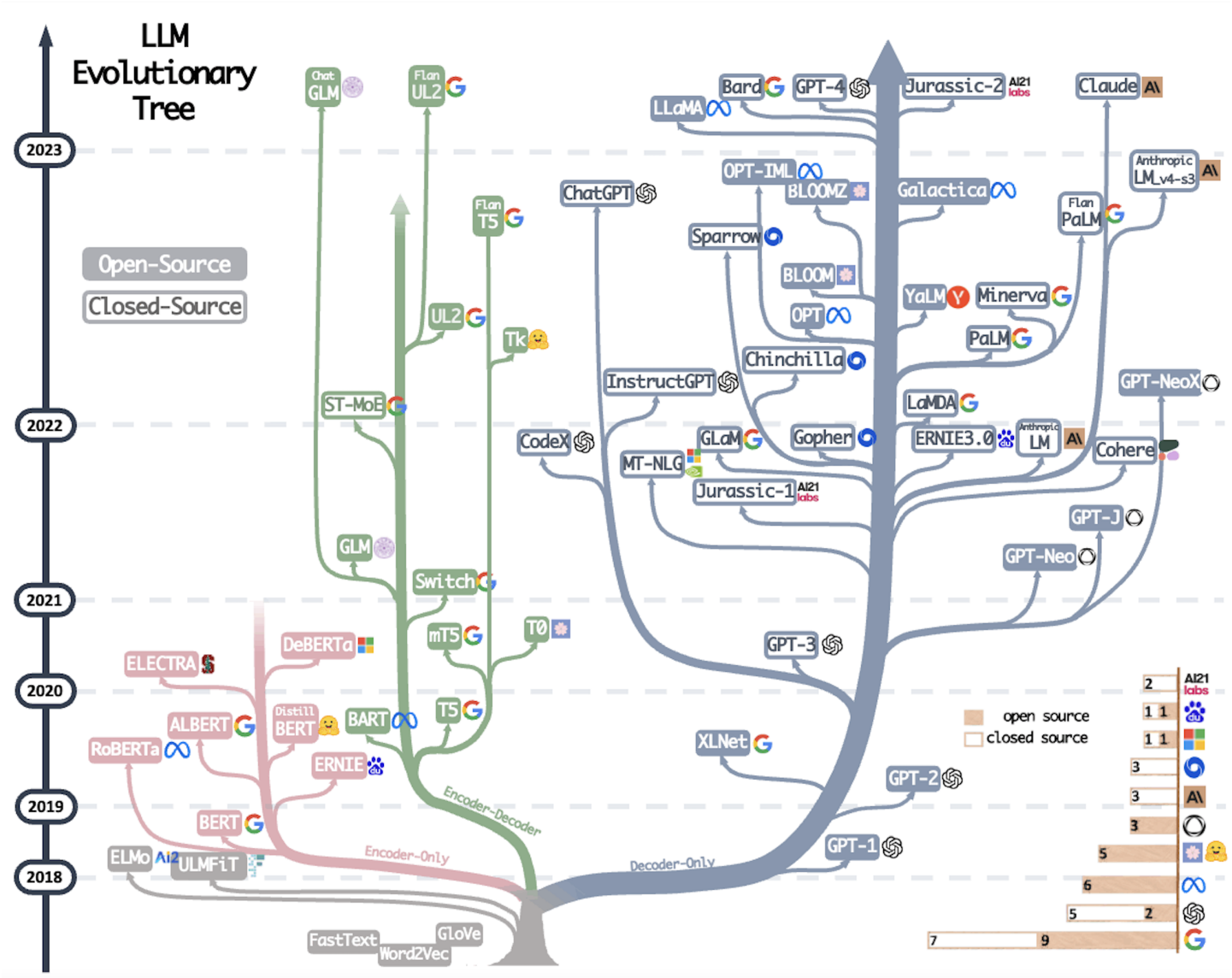


Image credit:
https://blog.biocomm.ai/2023/05/14/open-source-proliferation-llm-evolutionary-tree/

Denoising Diffusion Probabilistic Model

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Midjourney – Impressive Text-to-Image Results

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

Sora – Video Generation

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

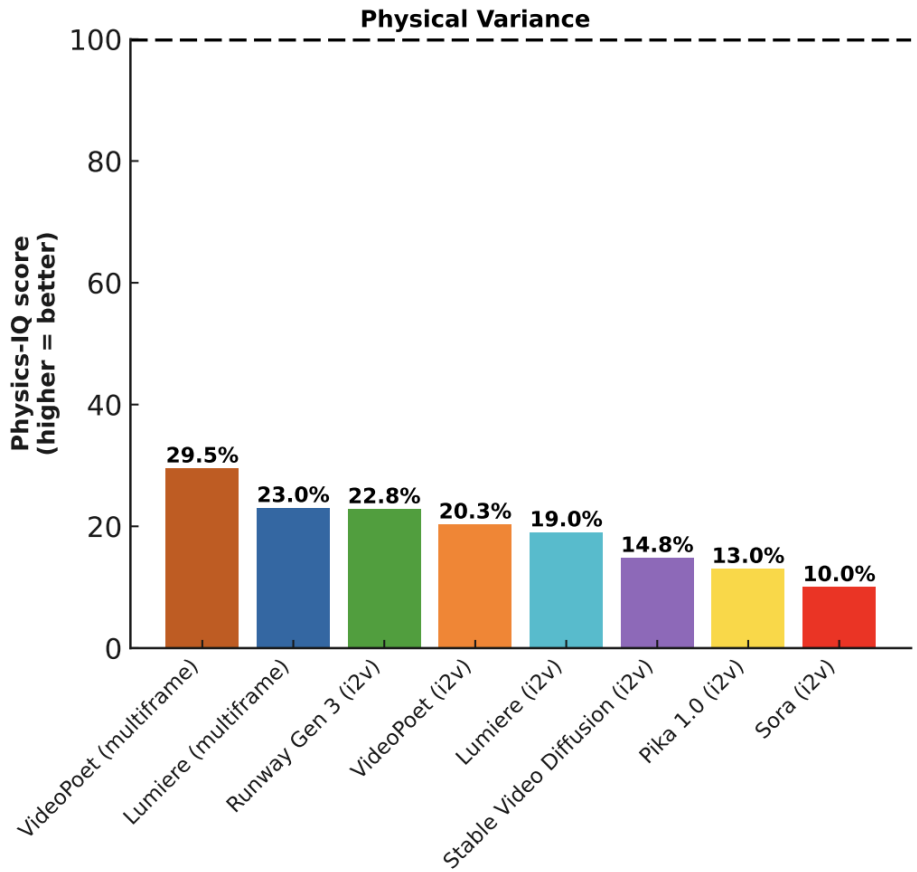
GPT4o Image Editing

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



Motamed S. et al. Do generative video models understand physical principles?, 2025

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Course Tricks I

Log-Derivative Trick

Given a differentiable function $p : \mathbb{R}^m \to \mathbb{R}$ (usually density function),

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

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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 $f : \mathbb{R}^m \to \mathbb{R}$ 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 $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^d$ 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)

Let $\mathbf{x} \in \mathbb{R}^m$ be a random vector with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ be a C^1-diffeomorphism ($\mathbf{f}$ and $\mathbf{f}^{-1}$ are continuously differentiable mappings). If $\mathbf{z} = \mathbf{f}(\mathbf{x})$, then

$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_\mathbf{f})| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right|$$

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

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 $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ 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 $p(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0)$.

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

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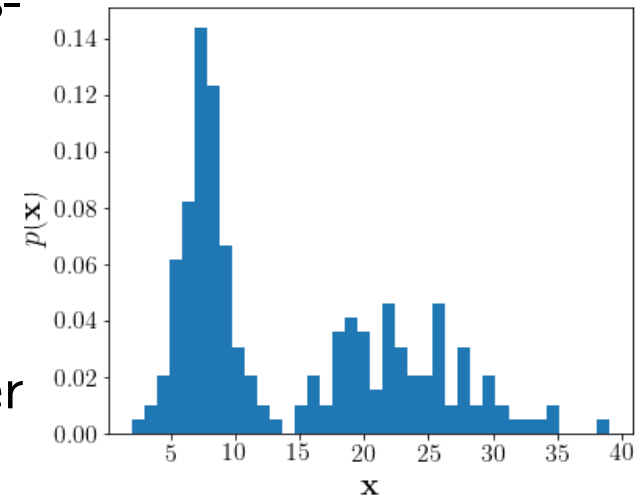
Note: here we use a strong assumption that our data is continuous (thus avoiding the domain of texts).

Histogram as a Generative Model

Assume $x \sim \text{Categorical}(\boldsymbol{\pi})$. 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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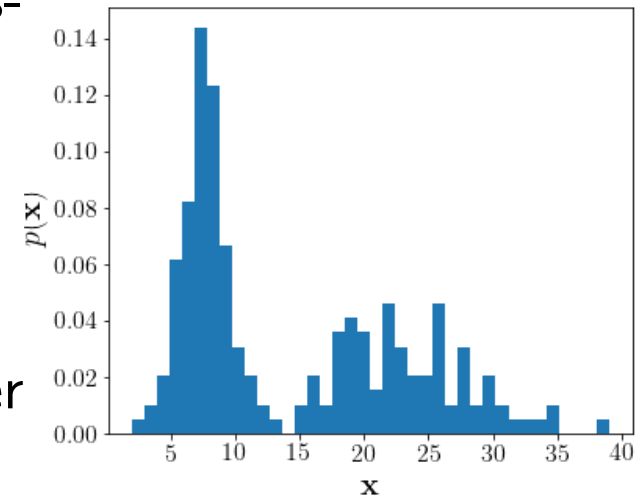

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MNIST example: 28×28 grayscale images, with each image $\mathbf{x} = (x_1, \ldots, x_{784})$, $x_i \in \{0, 1\}$:

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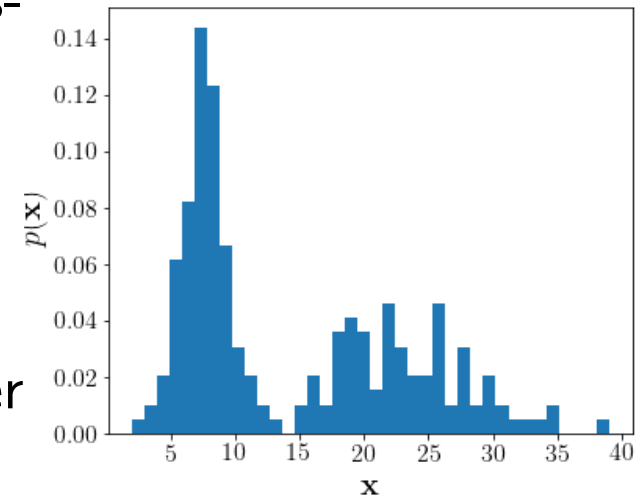

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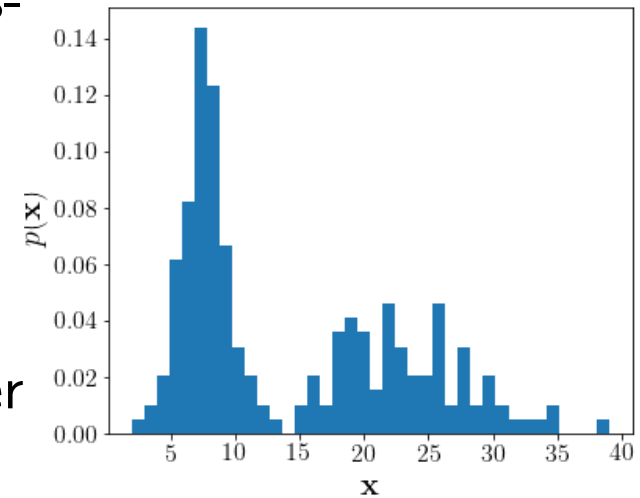

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Question: How many parameters are required in these cases?

$$p_{\text{data}}(\mathbf{x}) = p(x_1) \cdot p(x_2) \cdot \cdots \cdot p(x_m);$$
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Conditional Models

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- $\mathbf{y} = \emptyset$, $\mathbf{x}$ = image $\Rightarrow$ unconditional image model
- $\mathbf{y}$ = class label, $\mathbf{x}$ = image $\Rightarrow$ class-conditional image model
- $\mathbf{y}$ = text prompt, $\mathbf{x}$ = image $\Rightarrow$ text-to-image model
- $\mathbf{y}$ = image, $\mathbf{x}$ = image $\Rightarrow$ image-to-image model
- $\mathbf{y}$ = image, $\mathbf{x}$ = text $\Rightarrow$ image-to-text (image captioning) model
- $\mathbf{y}$ = English text, $\mathbf{x}$ = Russian text $\Rightarrow$ sequence-to-sequence model (machine translation) model
- $\mathbf{y}$ = sound, $\mathbf{x}$ = text $\Rightarrow$ speech-to-text (automatic speech recognition) model
- $\mathbf{y}$ = text, $\mathbf{x}$ = 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 $D : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ is called a **divergence** if

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Divergence Minimization Problem

$$\min_{\boldsymbol{\theta}} D(p_{\text{data}} \| p_{\boldsymbol{\theta}})$$

where $p_{\text{data}}(\mathbf{x})$ is the true data distribution and $p_{\boldsymbol{\theta}}(\mathbf{x})$ is the model distribution.

Forward KL vs Reverse KL (Kullback-Leibler Divergence)

Forward KL

$$\mathrm{KL}(p_{\text{data}} \| p_{\boldsymbol{\theta}}) = \int p_{\text{data}}(\mathbf{x}) \log \frac{p_{\text{data}}(\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{x})} d\mathbf{x} \to \min_{\boldsymbol{\theta}}$$

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Maximum Likelihood Estimation (MLE)

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

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

Forward KL vs Reverse KL: MLE as Forward KL

Forward KL

$$\mathrm{KL}(p_{\text{data}} \| p_\theta) = \int p_{\text{data}}(\mathbf{x}) \log \frac{p_{\text{data}}(\mathbf{x})}{p_\theta(\mathbf{x})} d\mathbf{x}$$

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&\approx -\frac{1}{n} \sum_{i=1}^{n} \log p_\theta(\mathbf{x}_i) + \text{const} \to \min_\theta .
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Maximum likelihood estimation is thus equivalent to minimizing a Monte Carlo estimate of the forward KL divergence.

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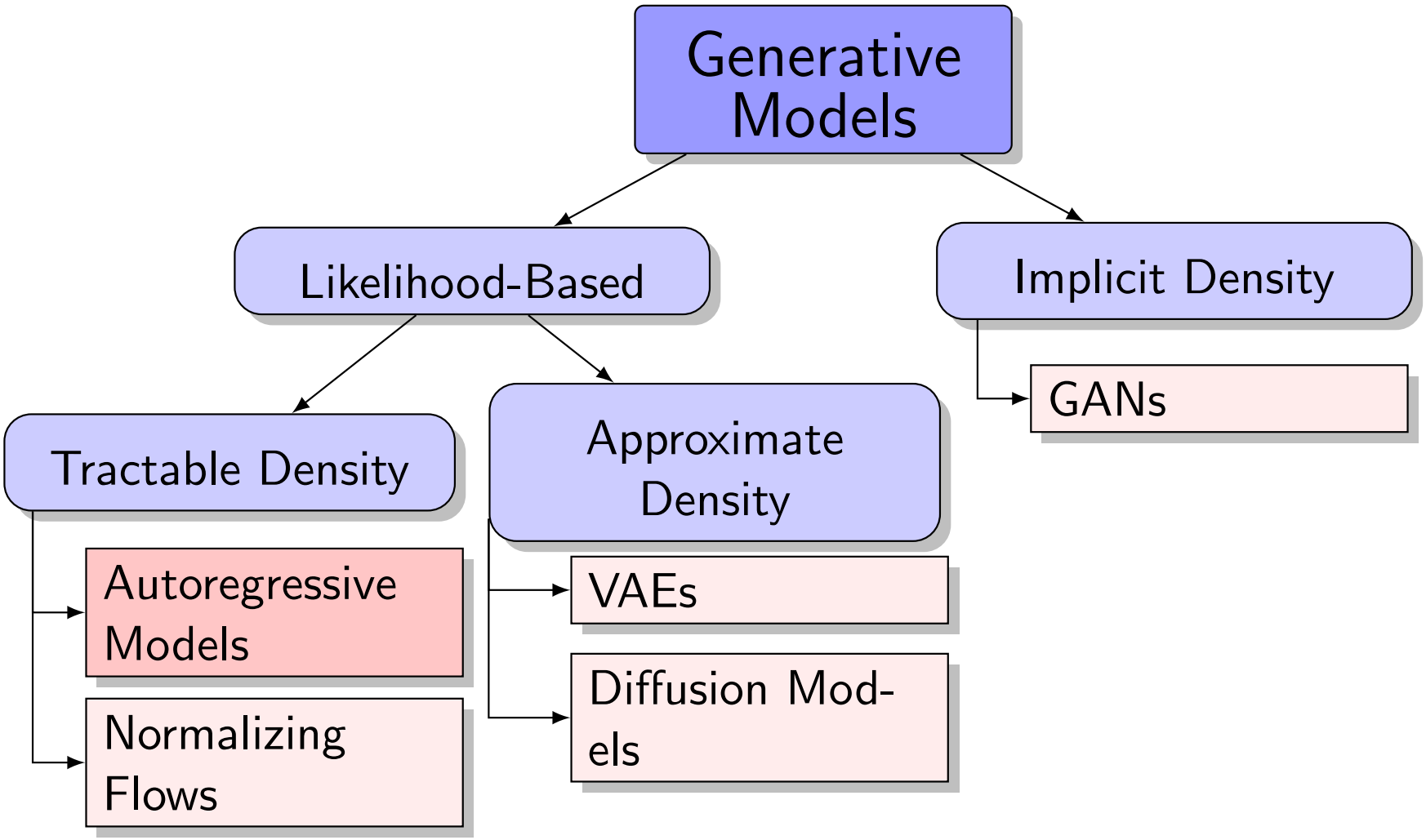
Outline

Generative Models Zoo



Autoregressive Modeling

MLE Problem

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

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

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Likelihood as a Product of Conditionals

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

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \prod_{j=1}^{m} p_{\boldsymbol{\theta}}(x_j | \mathbf{x}_{1:j-1}); \quad \log p_{\boldsymbol{\theta}}(\mathbf{x}) = \sum_{j=1}^{m} \log p_{\boldsymbol{\theta}}(x_j | \mathbf{x}_{1:j-1})$$

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Autoregressive Models

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

Autoregressive Models

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- Sampling is performed sequentially:
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  - ...
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- Each conditional $p_{\theta}(x_j | \mathbf{x}_{1:j-1})$ 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 $p_{\theta}(x_j|\mathbf{x}_{1:j-1})$ becomes intractable as the history $\mathbf{x}_{1:j-1}$ grows variable-length.

Image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

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Markov Assumption

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

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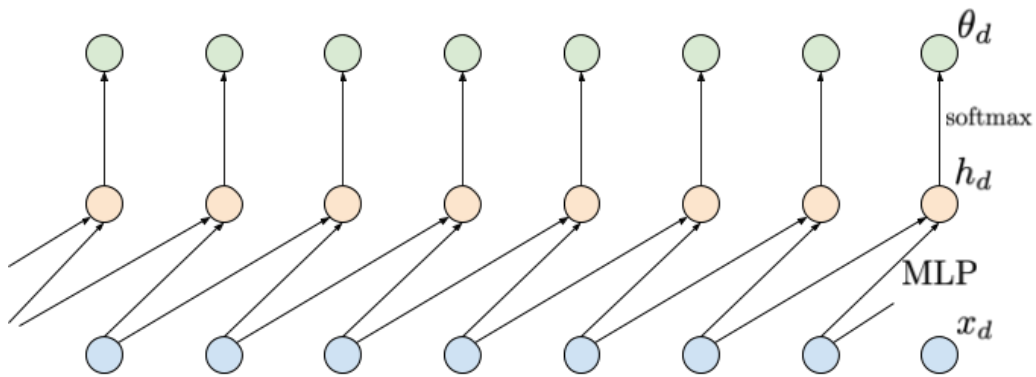
Example

- $d = 2$
- $x_j \in \{0, 255\}$
- $\mathbf{h}_j = \mathrm{MLP}_{\boldsymbol{\theta}}(x_{j-1}, x_{j-2})$
- $\boldsymbol{\pi}_j = \mathrm{softmax}(\mathbf{h}_j)$
- $p_{\boldsymbol{\theta}}(x_j|x_{j-1}, x_{j-2}) = \mathrm{Categorical}(\boldsymbol{\pi}_j)$



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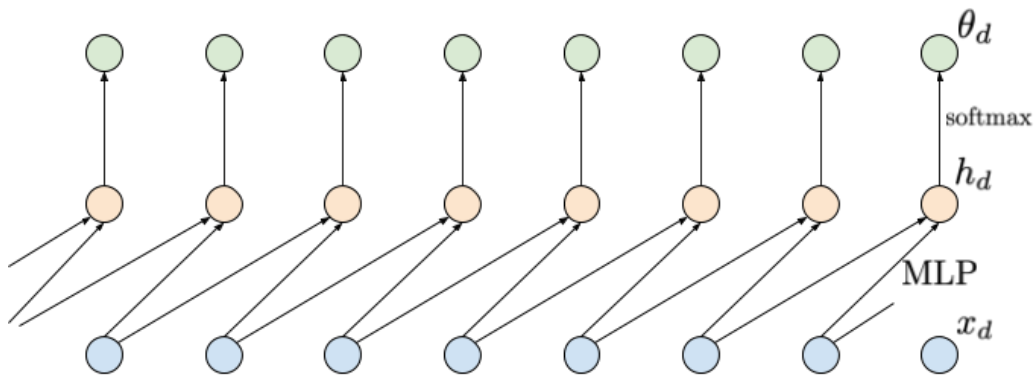

Can we also model continuous-valued data, not just the discrete case?

Image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Autoregressive Models: LLM

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

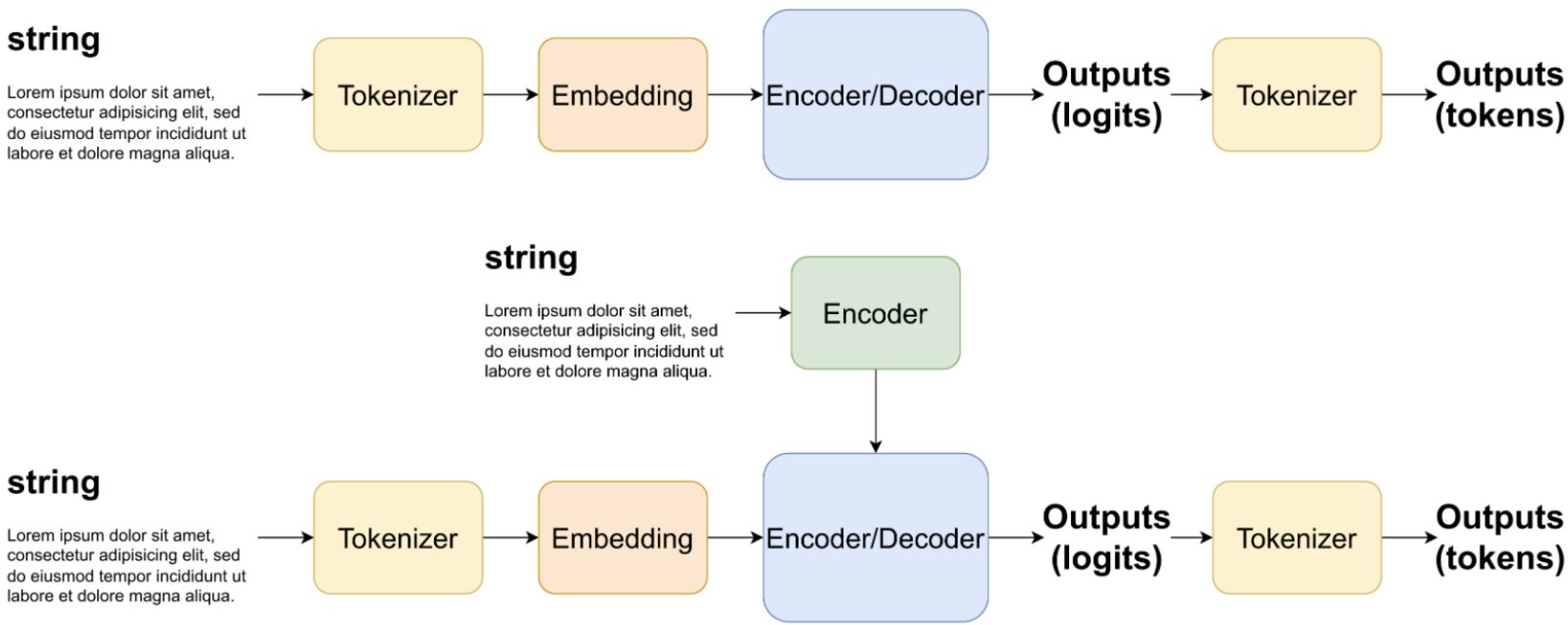

Image credit: https://jmtomczak.github.io/blog/20/20_llms.html

Autoregressive Models for Images

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

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

Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel Recurrent Neural Networks, 2016

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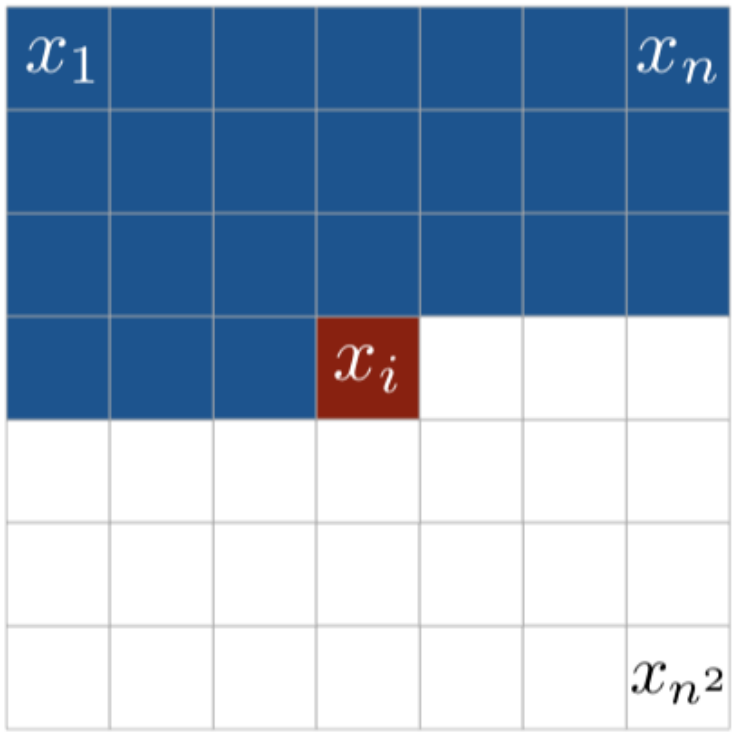
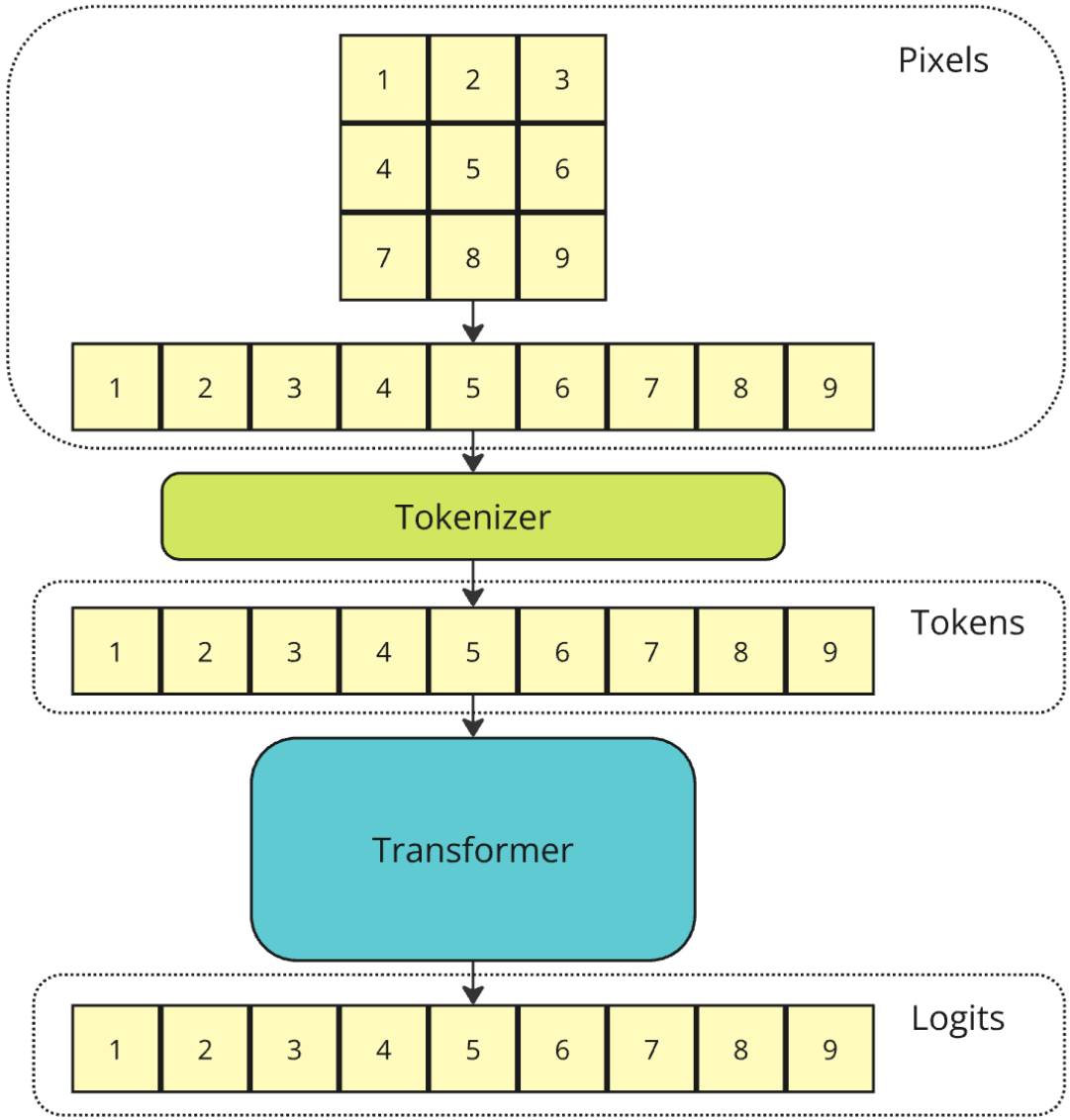
- A pixel ordering must be selected; the raster scan is a standard choice.
- RGB channel dependencies can be modeled explicitly as well.



Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel Recurrent Neural Networks, 2016

Autoregressive Models: ImageGPT



Chen M. et al. Generative Pretraining from Pixels, 2020

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 $p_{\theta}(x_j|\mathbf{x}_{1:j-1})$.
- ImageGPT applies a transformer architecture to sequences of raster-ordered image pixels.