Deep Generative Models

Lecture 1

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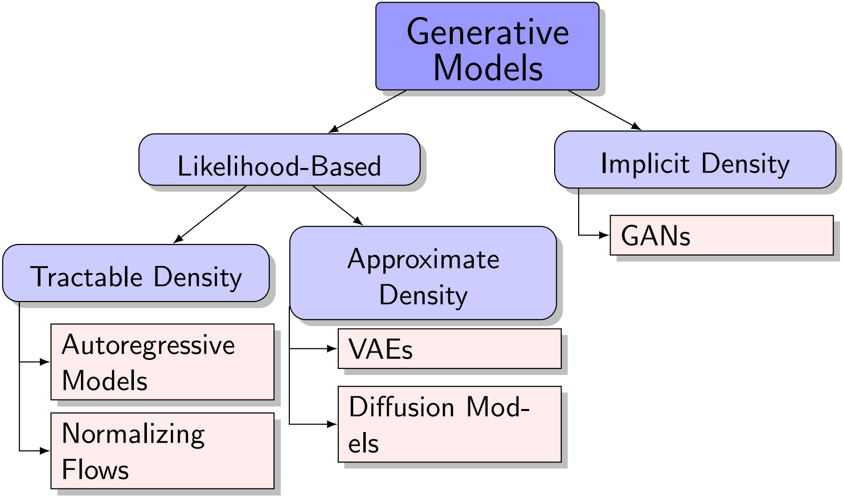
Generative Models Zoo



Outline

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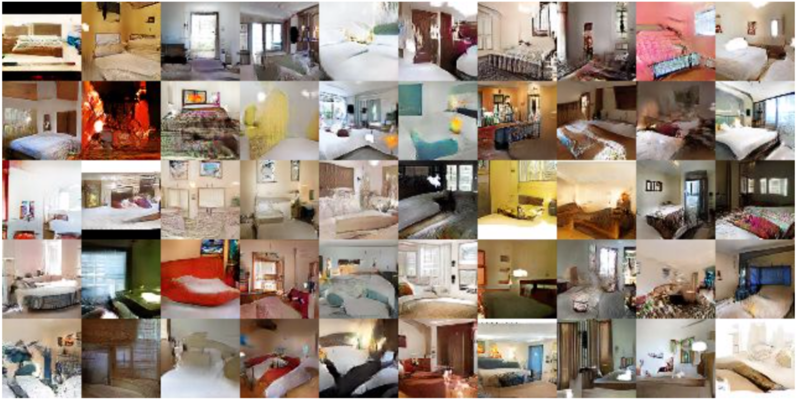
1. Generative Models Overview
2. Course Tricks
3. Problem Statement
4. Divergence Minimization Framework
5. Autoregressive Modeling

VAE – The First Scalable Approach for Image Generation

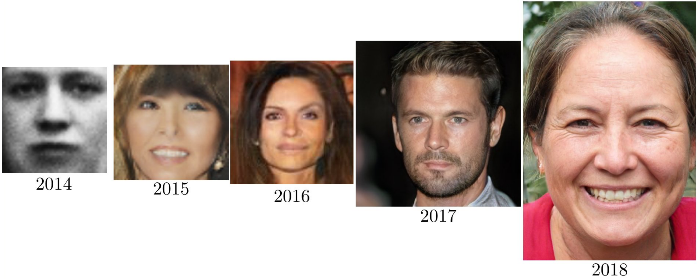
Kingma D.P., Welling M. Auto-Encoding Variational Bayes, 2013

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

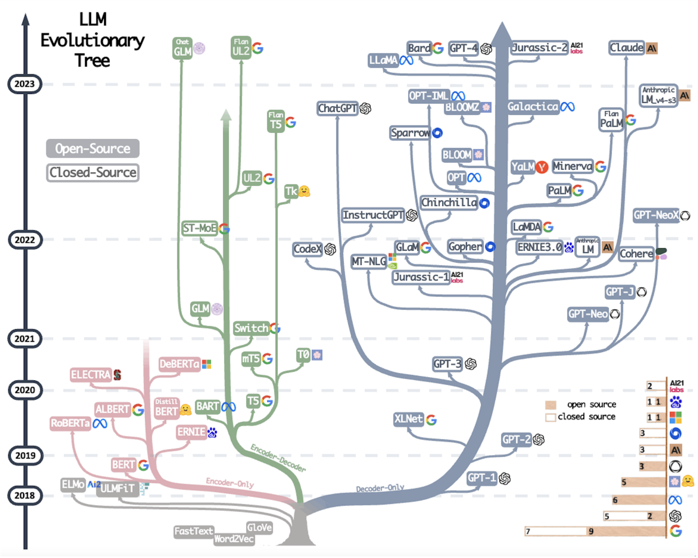


Image credit: https://blog.biocomm.ai/2023/05/14/open-source-proliferation-llm-evolutionary-tree/

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

Stable Diffusion 3 – Flow Matching


Image credit: https://stability.ai/news/stable-diffusion-3

Sora – Video Generation

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

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Course Tricks I

Log-Derivative Trick

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

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

Jensen's Inequality

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

Suppose $\mathbf{x}$ is a continuous random variable with density $p(\mathbf{x})$, and $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ 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.

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

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

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

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

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

Outline

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

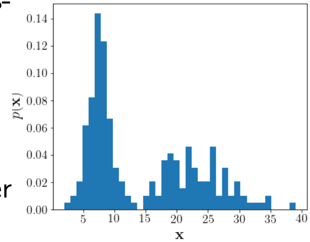
The data is high-dimensional and complex. For example, image datasets live in $\mathbb{R}^{\text{width}\times\text{height}\times\text{channels}}$. The curse of dimensionality makes accurately estimating $\pi(\mathbf{x})$ infeasible.

Histogram as a Generative Model

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



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

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

A complete histogram would require $2^{28\times28} - 1$ parameters for $\pi(\mathbf{x})$.

Question: How many parameters are required in these cases?

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

Problem Statement: Conditional Models

Conditional Models

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

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

Outline

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 $D : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ 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

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

Reverse KL

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

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.

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

Forward KL vs Reverse KL: MLE as Forward KL

Forward KL

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

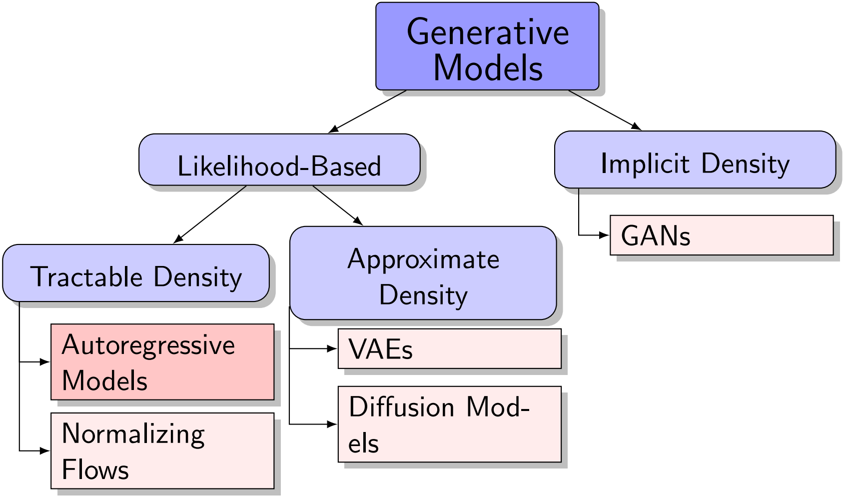
Maximum likelihood estimation is thus equivalent to minimizing a Monte Carlo estimate of the forward KL divergence.

Reverse KL

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

Outline

Generative Models Zoo



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 $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_m)$.
- 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

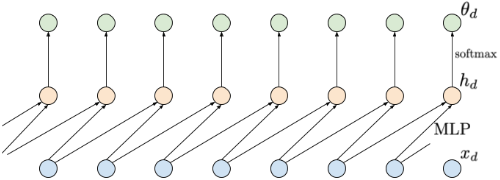
For large j, the conditional $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$ becomes intractable as the history $\mathbf{x}_{1:j-1}$ grows variable-length.

Markov Assumption

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

Example

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



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

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

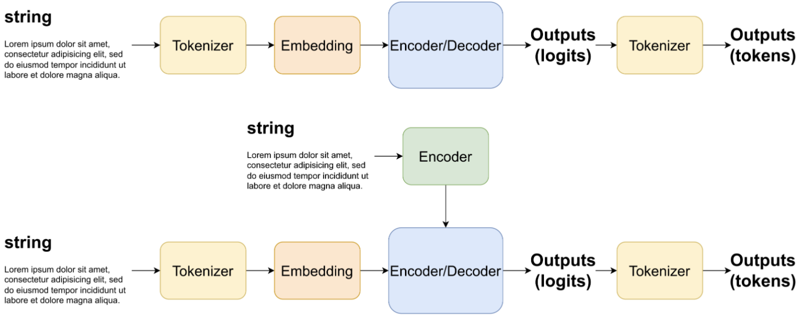


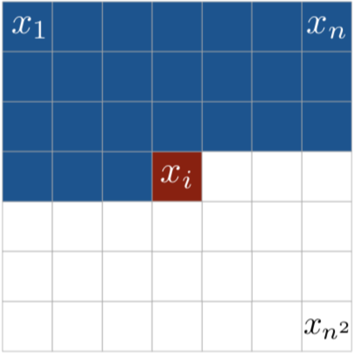
Image credit: https://jmtomczak.github.io/blog/20/20_llms.html

Autoregressive Models for Images

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

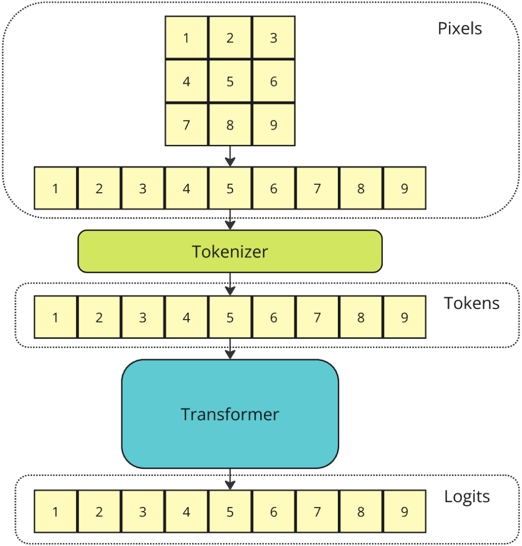
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{\text{width}\times\text{height}} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$$

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