

Deep Generative Models

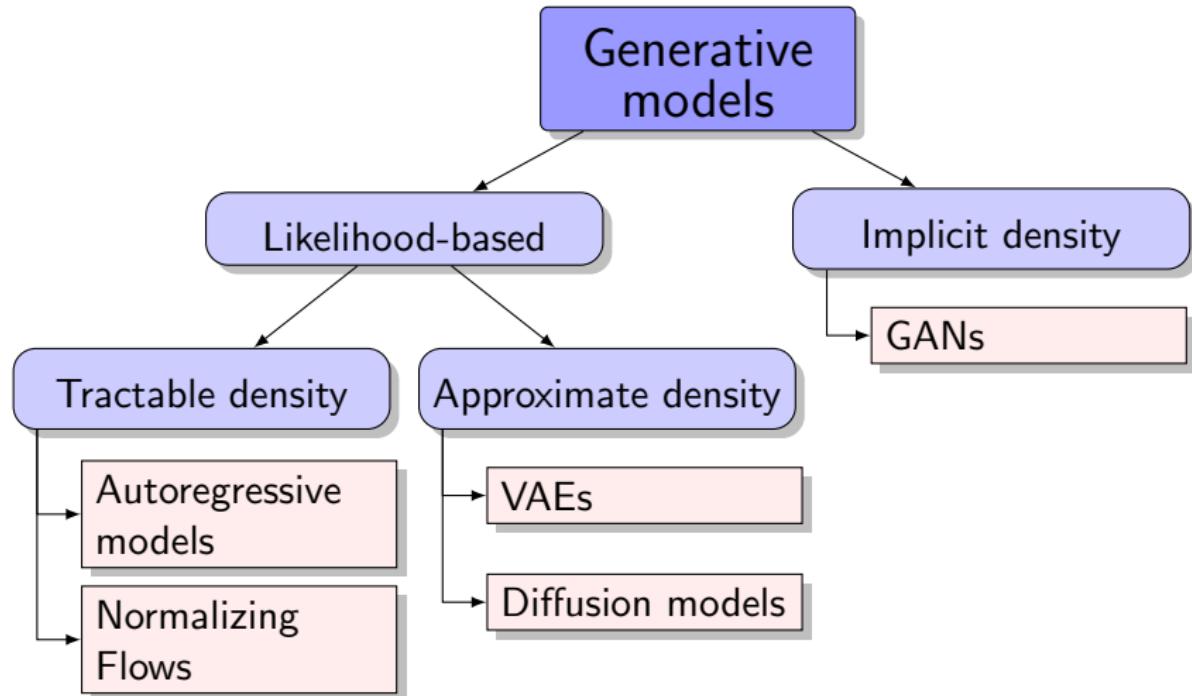
Lecture 1

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2024, Spring

Generative models zoo



Outline

1. Generative models overview
2. Problem statement
3. Divergence minimization framework
4. Autoregressive modelling

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VAE – first scalable approach for image generation



DCGAN – 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 generation of faces



Karras T., Laine S., Aila T. A style-based generator architecture for generative adversarial networks, 2018

VQ-VAE-2 – high quality generation without GANs



Razavi A., Oord A., Vinyals O. Generating Diverse High-Fidelity Images with VQ-VAE-2, 2019

Language modelling at scale

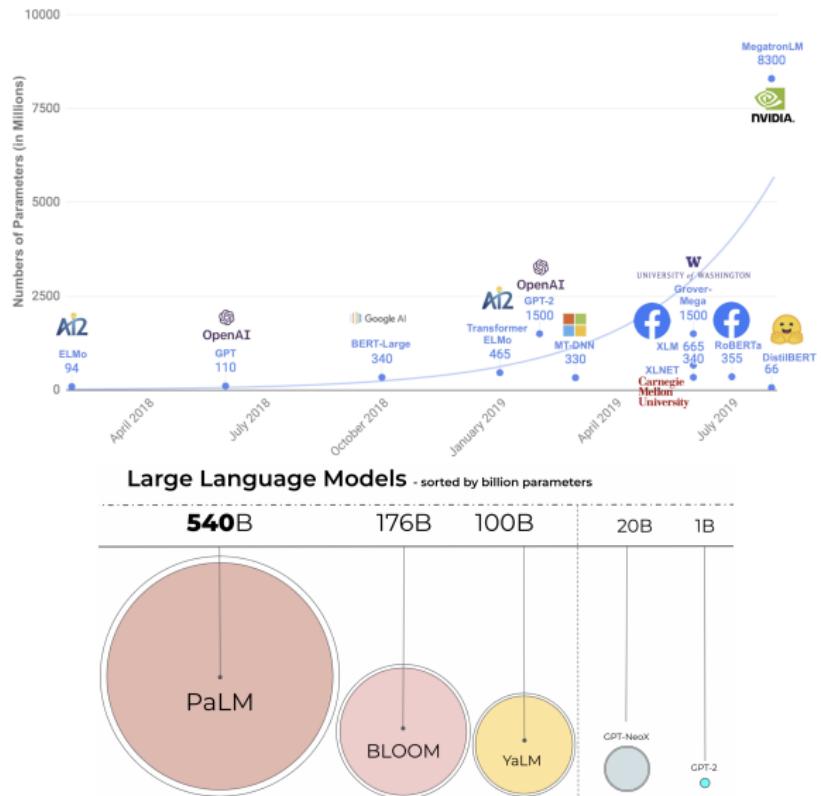


image credit: <http://jalammar.github.io/illustrated-gpt2>

image credit: <https://huggingface.co/blog/hf-bitsandbytes-integration>

DALL-E – cross-modal image-text model

TEXT PROMPT an armchair in the shape of an avocado. . .

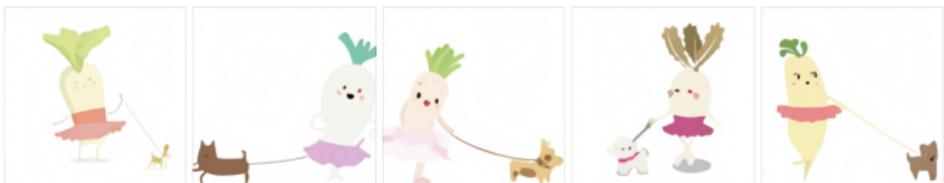
AI-GENERATED
IMAGES



Edit prompt or view more images↓

TEXT PROMPT an illustration of a baby daikon radish in a tutu walking a dog

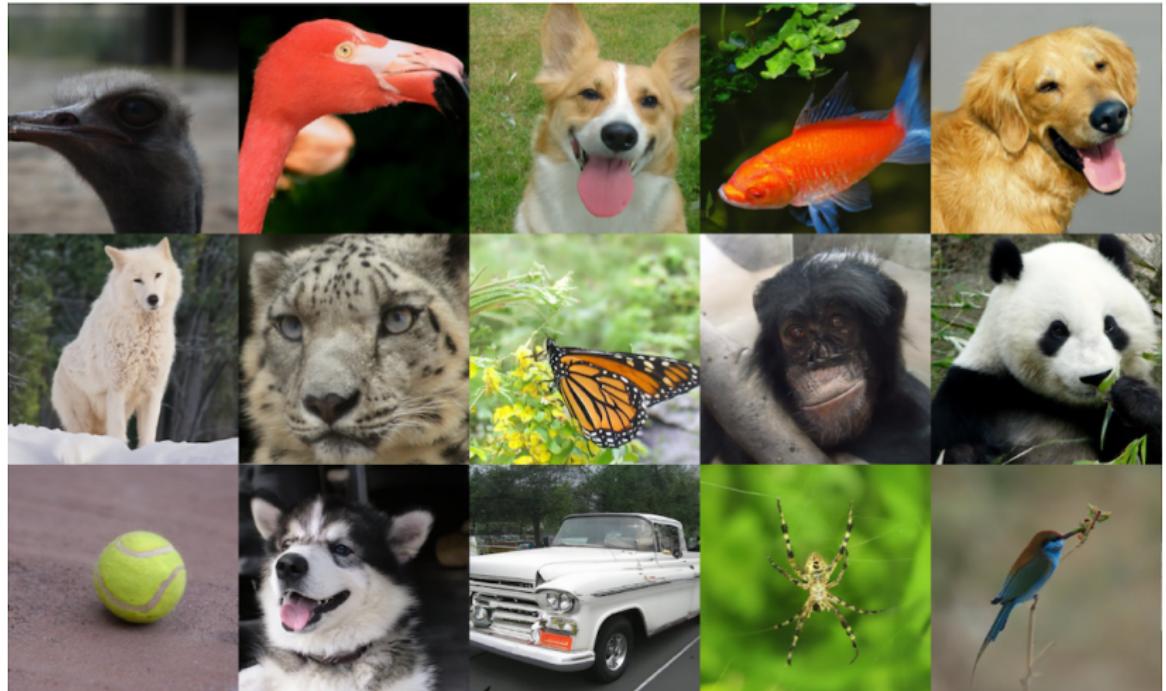
AI-GENERATED
IMAGES



Edit prompt or view more images↓

image credit: <https://openai.com/blog/dall-e/>
Ramesh A. et al. Zero-shot text-to-image generation, 2021

DDPM - diffusion model



Stable Diffusion - awesome text to image results



Rombach R., et al. *High-Resolution Image Synthesis with Latent Diffusion Models*,
2021

<https://github.com/CompVis/stable-diffusion>
LAION-5B dataset

Shedevrum - Yandex generative model



Кот ныряет в бассейн, как ребенок на обложке альбома Nevermind, реалистично



рука человека с пятью пальцами, ни четыремя, ни шестью, а с 5 (пять) пальцами

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Course tricks 1

Let $\mathbf{x} \in \mathbb{R}^m$ be a random variable with a density $p_x(\mathbf{x})$.

Law of the unconscious statistician (LOTUS)

Let $\mathbf{y} = f(\mathbf{x})$ with density $p_y(\mathbf{y})$. Then

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

Monte-Carlo estimation

Expected value could be estimated using only the samples:

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

Jensen's Inequality

Assume $f(\cdot)$ is a convex function. Then

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

Course tricks 2

Let $\mathbf{x} \in \mathbb{R}^m$ be a random variable with a density $p_{\mathbf{x}}(\mathbf{x})$.

Decomposition to conditionals

$$p(\mathbf{x}) = p(x_1) \cdot p(x_2|x_1) \cdot p(x_3|x_2, x_1) \cdots \cdots p(x_m|x_{m-1}, \dots, x_1).$$

Log-derivative trick

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

Dirac delta function

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

We could treat any deterministic variable \mathbf{x}_0 as a random variable with density $p(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_0)$.

Problem statement

We are given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \in \mathcal{X}$ (e.g. $\mathcal{X} = \mathbb{R}^m$) from unknown distribution $\pi(\mathbf{x})$.

Goal

We would like to learn a distribution $\pi(\mathbf{x})$ for

- ▶ evaluating $\pi(\mathbf{x})$ for new samples (how likely to get object \mathbf{x} ?);
- ▶ sampling from $\pi(\mathbf{x})$ (to get new objects $\mathbf{x} \sim \pi(\mathbf{x})$).

Challenge

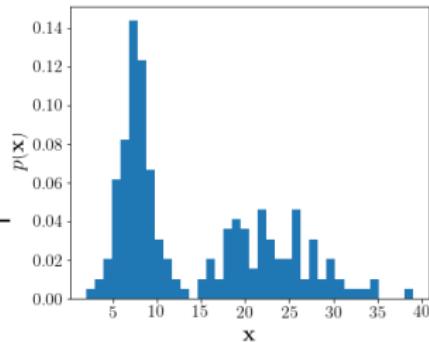
Data is complex and high-dimensional. E.g. the dataset of images lies in the space $\mathcal{X} \subset \mathbb{R}^{\text{width} \times \text{height} \times \text{channels}}$.

Histogram as a generative model

Let $x \sim \text{Categorical}(\pi)$. The histogram is totally defined by

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

Problem: curse of dimensionality (number of bins grows exponentially).



MNIST example: 28x28 gray-scaled images, each image is $\mathbf{x} = (x_1, \dots, x_{784})$, where $x_i \in \{0, 1\}$.

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

Hence, the histogram will have $2^{28 \times 28} - 1$ parameters to specify $\pi(\mathbf{x})$.

Question: How many parameters do we need in these cases?

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

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

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Divergences

Fix probabilistic model $p(\mathbf{x}|\theta)$ – the set of parameterized distributions.

Instead of searching true $\pi(\mathbf{x})$ over all probability distributions, learn function approximation $p(\mathbf{x}|\theta) \approx \pi(\mathbf{x})$.

What is a divergence?

Let \mathcal{S} be the set of all possible probability distributions. Then $D : \mathcal{S} \times \mathcal{S} \rightarrow \mathbb{R}$ is a divergence if

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

Divergence minimization task

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

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

f-divergence family

f-divergence

$$D_f(\pi || p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) = \int p(\mathbf{x}) f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) d\mathbf{x}.$$

Here $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

| Name | $D_f(P Q)$ | Generator $f(u)$ |
|-------------------|---|--|
| Kullback-Leibler | $\int p(x) \log \frac{p(x)}{q(x)} dx$ | $u \log u$ |
| Reverse KL | $\int q(x) \log \frac{q(x)}{p(x)} dx$ | $-\log u$ |
| Pearson χ^2 | $\int \frac{(q(x)-p(x))^2}{p(x)} dx$ | $(u-1)^2$ |
| Squared Hellinger | $\int \left(\sqrt{p(x)} - \sqrt{q(x)} \right)^2 dx$ | $(\sqrt{u}-1)^2$ |
| Jensen-Shannon | $\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx$ | $-(u+1) \log \frac{1+u}{2} + u \log u$ |
| GAN | $\int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx - \log(4)$ | $u \log u - (u+1) \log(u+1)$ |

Forward KL vs Reverse KL

Forward KL

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

Reverse KL

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

What is the difference between these two formulations?

Maximum likelihood estimation (MLE)

Let $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ be the set of the given i.i.d. samples.

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

Forward KL vs Reverse KL

Forward KL

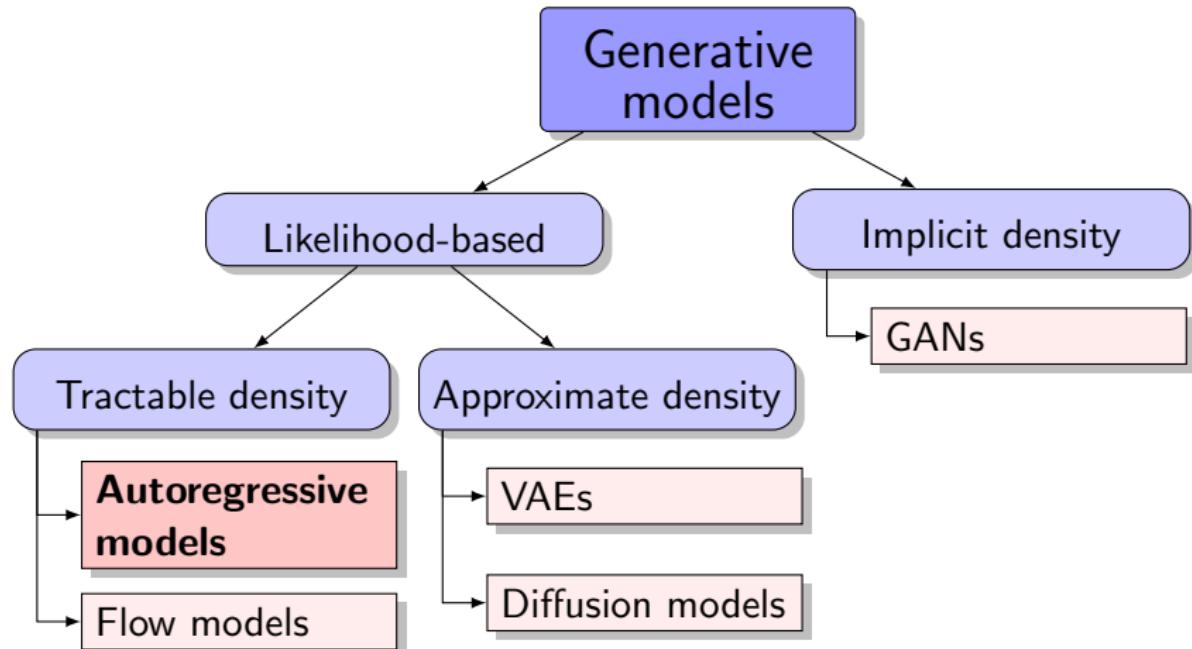
$$\begin{aligned} KL(\pi||p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\theta)} d\mathbf{x} \\ &= \int \pi(\mathbf{x}) \log \pi(\mathbf{x}) d\mathbf{x} - \int \pi(\mathbf{x}) \log p(\mathbf{x}|\theta) d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\theta) + \text{const}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

Maximum likelihood estimation is equivalent to minimization of the Monte-Carlo estimate of forward KL.

Reverse KL

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

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Autoregressive modelling

MLE problem

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

- ▶ We would like to solve the problem using gradient-based optimization.
- ▶ We have to efficiently compute $\log p(\mathbf{x}|\boldsymbol{\theta})$ and $\frac{\partial \log p(\mathbf{x}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}$.

Likelihood as product of conditionals

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

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

Example: $p(x_1, x_2, x_3) = p(x_2) \cdot p(x_1|x_2) \cdot p(x_3|x_1, x_2)$.

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 sequential:
 - ▶ sample $\hat{x}_1 \sim p(x_1|\boldsymbol{\theta})$;
 - ▶ sample $\hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta})$;
 - ▶ ...
 - ▶ sample $\hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$;
 - ▶ new generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.
- ▶ Each conditional $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$ could be modelled by neural network.
- ▶ Modelling all conditional distributions separately is infeasible and we would obtain separate models. To extend to high dimensions we could share parameters $\boldsymbol{\theta}$ across conditionals.

Autoregressive models: MLP

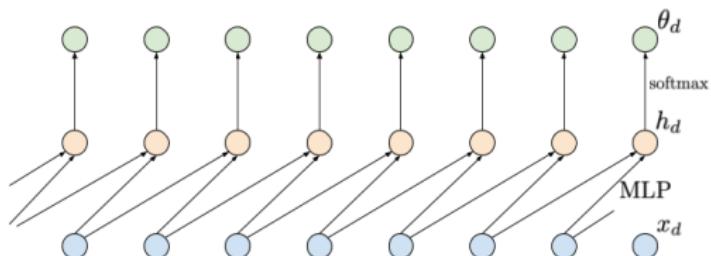
For large j the conditional distribution $p(x_j | \mathbf{x}_{1:j-1}, \theta)$ could be infeasible. Moreover, the history $\mathbf{x}_{1:j-1}$ has non-fixed length.

Markov assumption

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

Example

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



Is it possible to model continuous distributions instead of discrete one?

Autoregressive models: PixelCNN

Goal

Model a distribution $\pi(\mathbf{x})$ of natural images.

Solution

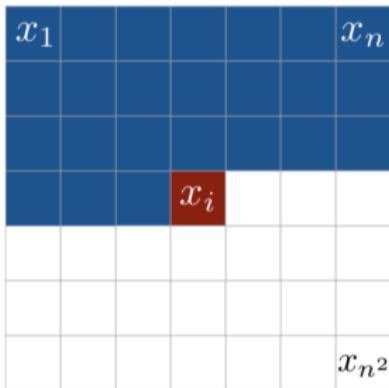
Autoregressive model on 2D pixels

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

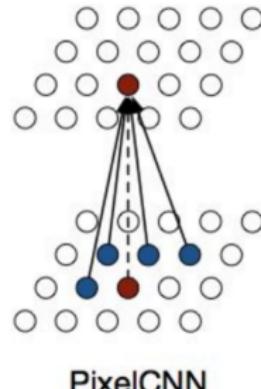
- ▶ We need to introduce the ordering of image pixels.
- ▶ The convolution should be **masked** to make them causal.
- ▶ The image has RGB channels, these dependencies could be addressed.

Autoregressive models: PixelCNN

Raster ordering



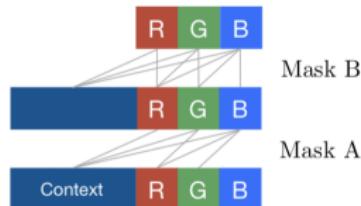
Dependencies between pixels



PixelCNN

Mask for the convolution kernel

| | | |
|---|---|---|
| 1 | 1 | 1 |
| 1 | 0 | 0 |
| 0 | 0 | 0 |



Summary

- ▶ We are trying to approximate the distribution of samples for density estimation and generation of new samples.
- ▶ To fit model distribution to the real data distribution one could use divergence minimization framework.
- ▶ Minimization of forward KL is equivalent to the MLE problem.
- ▶ Autoregressive models decompose the distribution to the sequence of the conditionals.
- ▶ Sampling from the autoregressive models is trivial, but sequential!
- ▶ To estimate density you need to multiply all conditionals $p(x_j | \mathbf{x}_{1:j-1}, \theta)$.
- ▶ PixelCNN model use masked causal convolutions (1D or 2D) to get autoregressive model.