

# Deep Generative Models

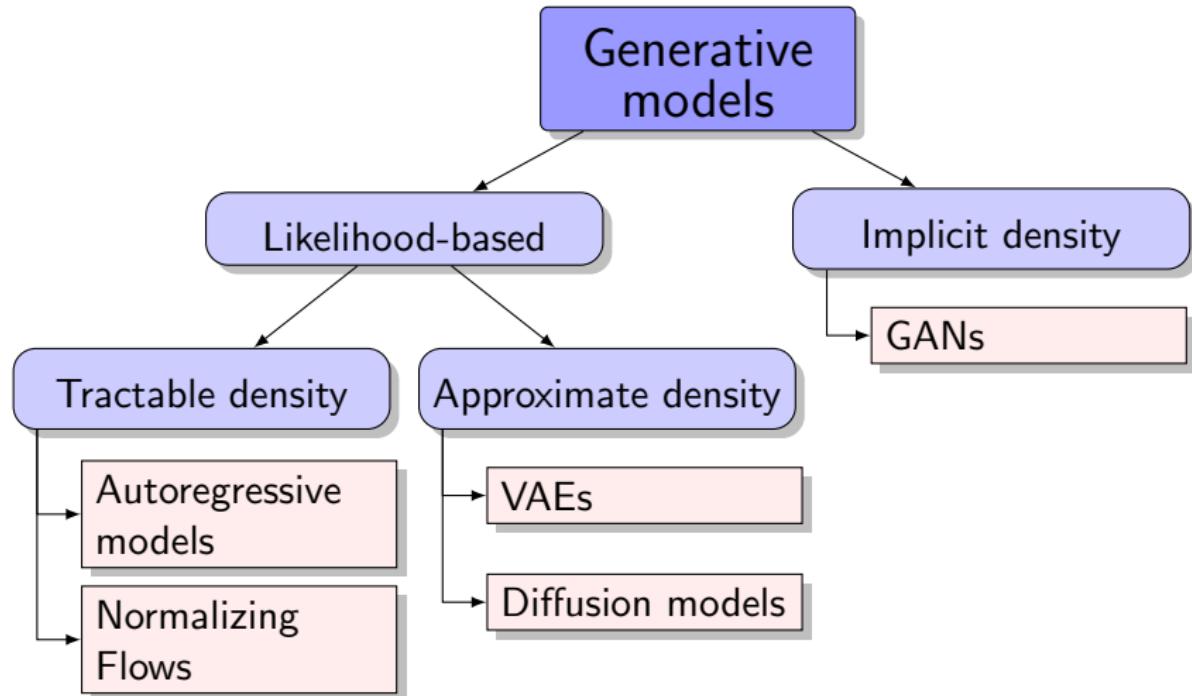
## Lecture 1

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# 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



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Radford A., Metz L., Chintala S. *Unsupervised representation learning with deep convolutional generative adversarial networks*, 2015

# StyleGAN – high quality generation of faces



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

## VQ-VAE-2 – high quality generation without GANs



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

# Language modelling at scale

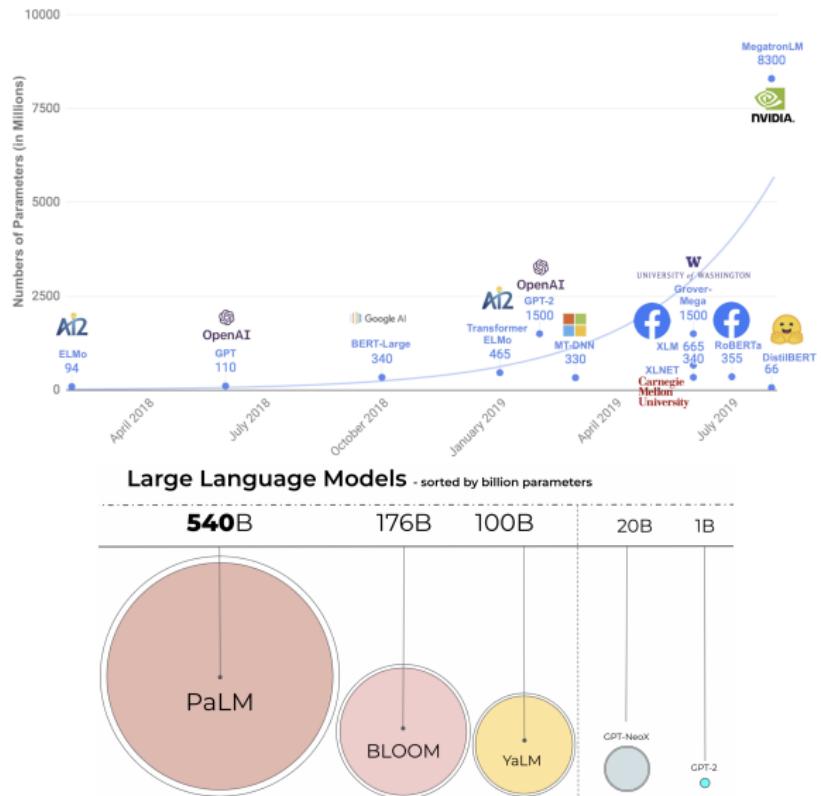


image credit: <http://jalammar.github.io/illustrated-gpt2>

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↓

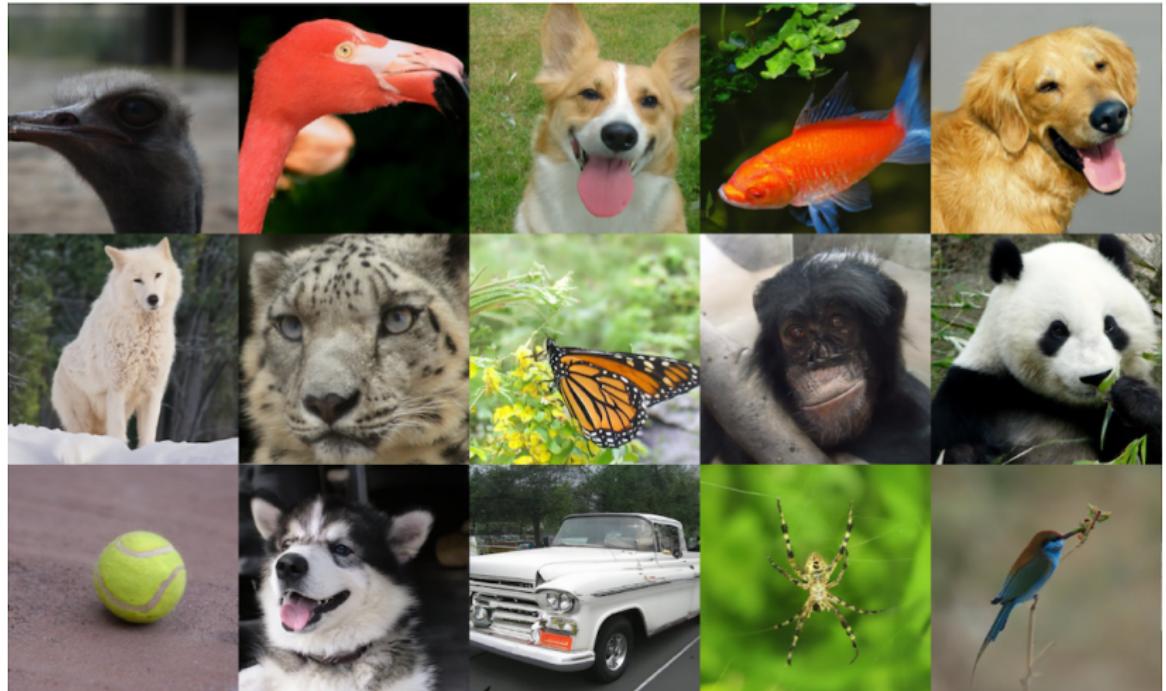
TEXT PROMPT    an illustration of a baby daikon radish in a tutu walking a dog

AI-GENERATED  
IMAGES



Edit prompt or view more images↓

# DDPM - diffusion model



# Stable Diffusion - awesome text to image results



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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

### Law of the unconscious statistician (LOTUS)

Let  $\mathbf{x}$  be a random variable with density  $p_x(\mathbf{x})$  and let  $\mathbf{y} = f(\mathbf{x})$  with density  $p_y(\mathbf{y})$ . Then

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

### Monte-Carlo estimation

Expected value could be estimated using only the samples:

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

## Course tricks 2

### Jensen's Inequality

Let  $\mathbf{x}$  be a random variable and  $f(\cdot)$  is a convex function. Then

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

### Decomposition to conditionals

Let  $\mathbf{x} = (x_1, x_2, \dots, x_m) \in \mathbb{R}^m$  be a random variable. Then

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

## 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

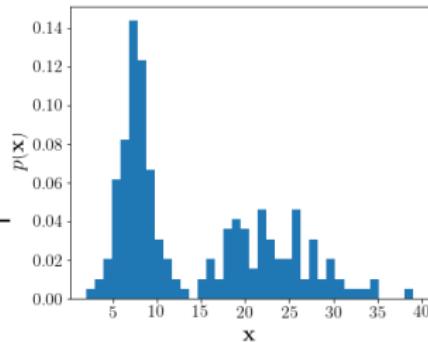
Data is complex and high-dimensional. E.g. the dataset of images lies in the space  $\mathcal{X} \subset \mathbb{R}^{\text{width} \times \text{height} \times \text{channels}}$ .

## 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 $\chi^2$	$\int \frac{(q(x)-p(x))^2}{p(x)} dx$	$(u-1)^2$
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

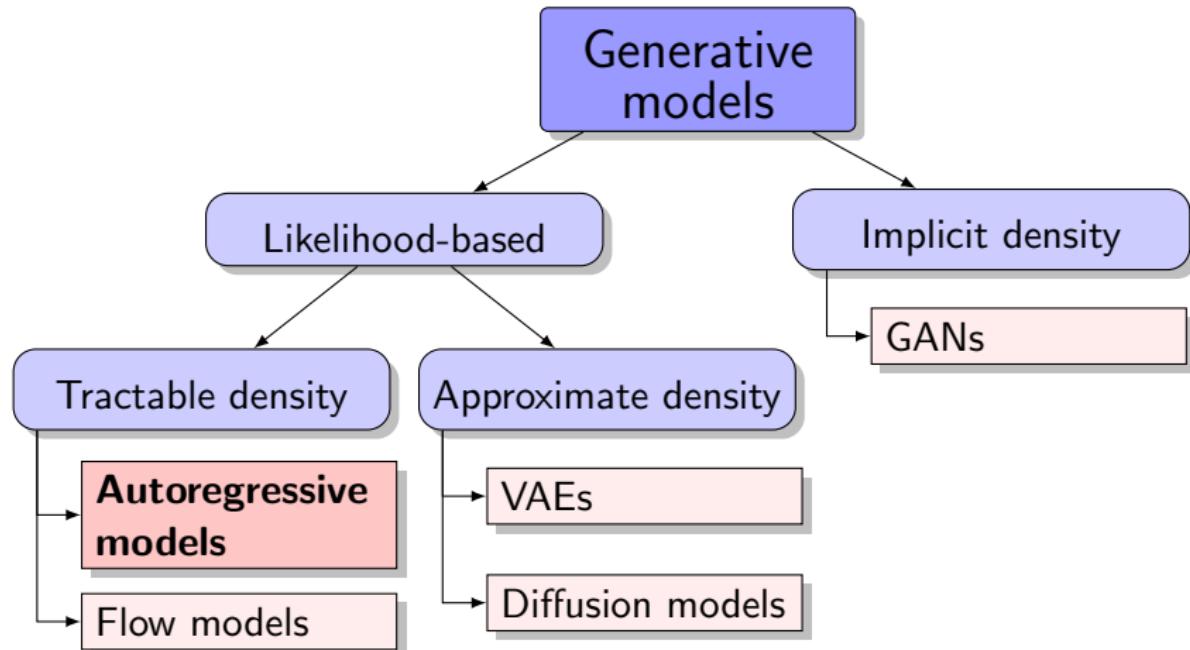
$$\begin{aligned} KL(\pi||p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\theta)} d\mathbf{x} \\ &= \int \pi(\mathbf{x}) \log \pi(\mathbf{x}) d\mathbf{x} - \int \pi(\mathbf{x}) \log p(\mathbf{x}|\theta) d\mathbf{x} \\ &= -\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\theta) + \text{const}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

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

### Reverse KL

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

# Generative models zoo



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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

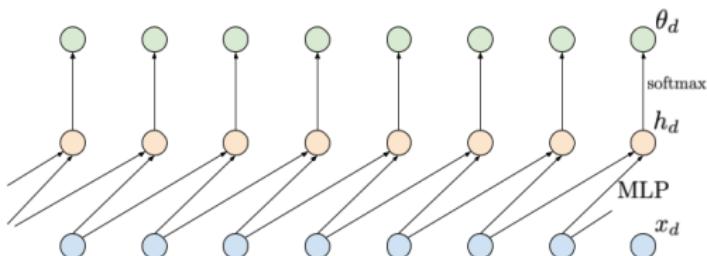
For large  $j$  the conditional distribution  $p(x_j | \mathbf{x}_{1:j-1}, \theta)$  could be infeasible. Moreover, the history  $\mathbf{x}_{1:j-1}$  has non-fixed length.

## 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

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

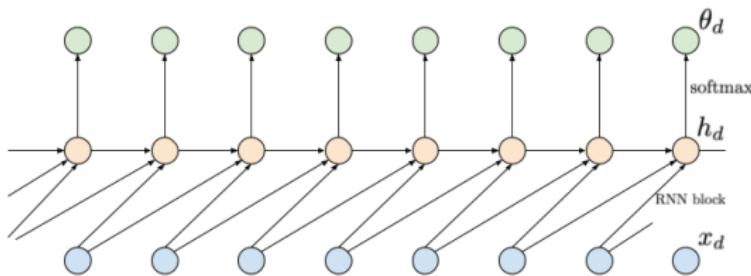


Is it possible to model continuous distributions instead of discrete one?

## Autoregressive models: RNN

- ▶ Previous model has **limited** memory  $d$ . It is insufficient for many modalities (e.g. for images and text).
- ▶ Recurrent NN fixes this problem and potentially could learn long-range dependencies:

$$p(x_j | \mathbf{x}_{1:j-1}, \theta) = p(x_j | \mathbf{h}_j, \theta), \quad \mathbf{h}_j = \text{RNN}(\mathbf{x}_{j-d:j-1}, \mathbf{h}_{j-1})$$



- ▶ Sequential computation of all conditionals  $p(x_j | \mathbf{x}_{1:j-1}, \theta)$ , hence, the training is slow.
- ▶ RNN suffers from vanishing and exploding gradients.

# Autoregressive models: PixelCNN

## Goal

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

## Solution

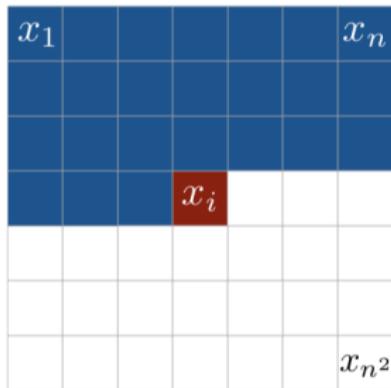
Autoregressive model on 2D pixels

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

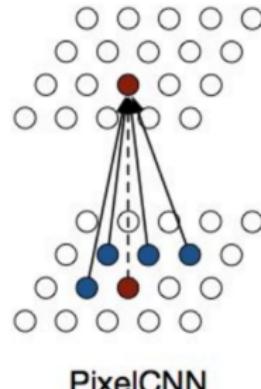
- ▶ We need to introduce the ordering of image pixels.
- ▶ The convolution should be **masked** to make them causal.
- ▶ The image has RGB channels, these dependencies could be addressed.

# Autoregressive models: PixelCNN

Raster ordering



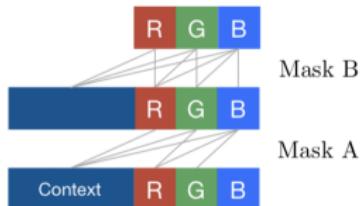
Dependencies between pixels



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  $p(x_j | \mathbf{x}_{1:j-1}, \theta)$ .
- ▶ Autoregressive models work on both continuous and discrete data.
- ▶ PixelCNN model use masked causal convolutions (1D or 2D) to get autoregressive model.