Deep Generative Models

Lecture 1

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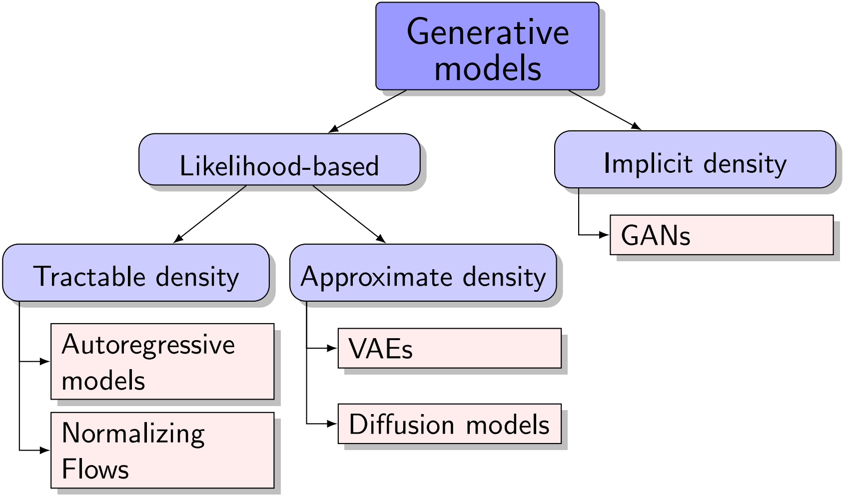
AI Masters

2024, Spring

Generative models zoo



Outline

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

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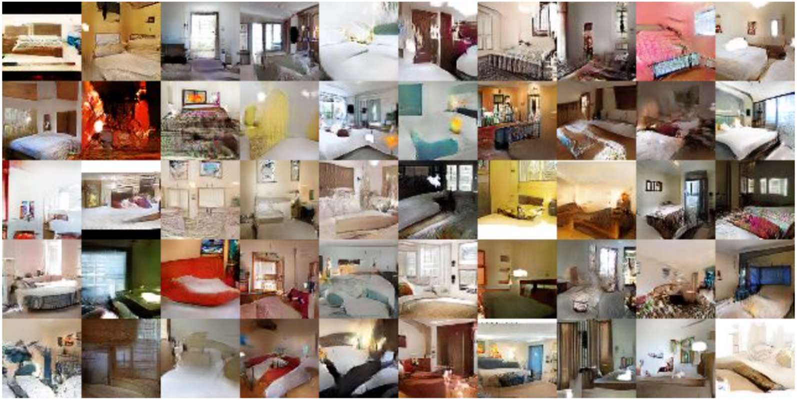
VAE – first scalable approach for image generation

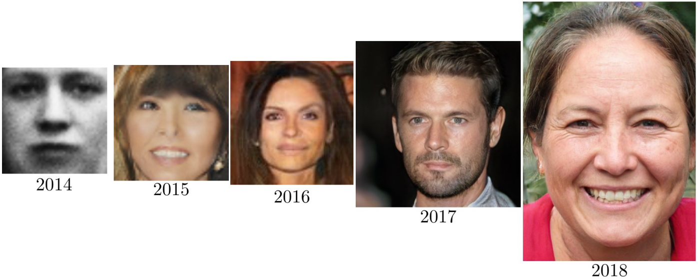
Kingma D. P., Welling M. *Auto-encoding variational bayes*, 2013

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

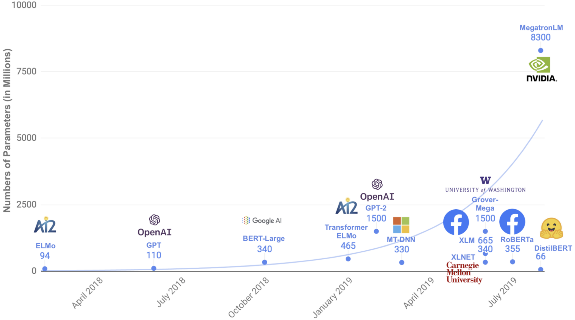


Karras T., Laine S., Aila T. A style-based generator architecture for generative adversarial networks, 2018

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



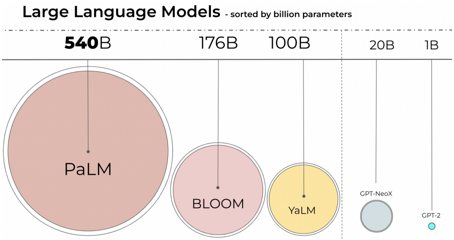


image credit: http://jalammar.github.io/illustrated-gpt2
image credit: https://huggingface.co/blog/hf-bitsandbytes-integration

Language modelling at scale

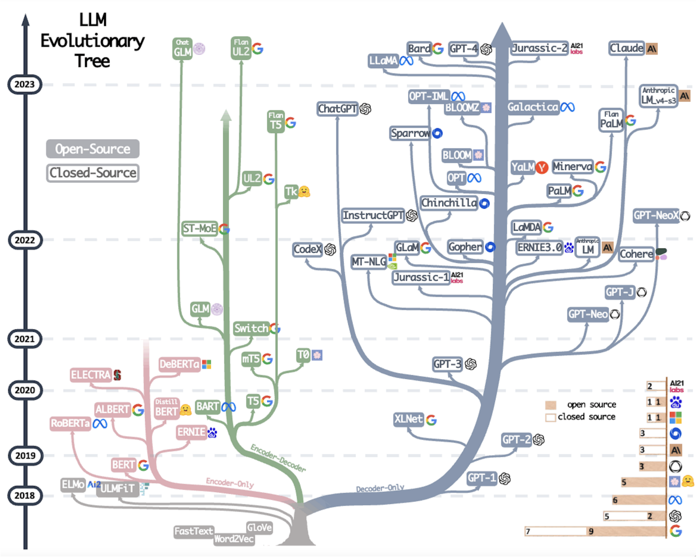


image credit:
https://blog.biocomm.ai/2023/05/14/open-source-proliferation-llm-evolutionary-tree/

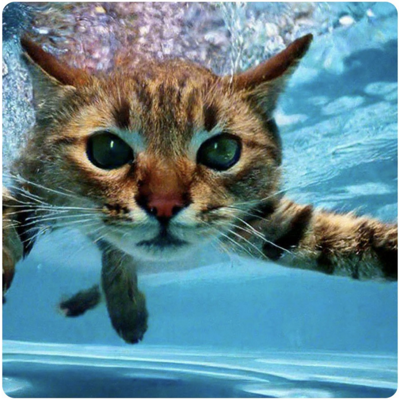
DDPM - diffusion model

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

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 $p_x(\mathbf{x})$.

Decomposition to conditionals

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

Log-derivative trick

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

Dirac delta function

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

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 $\mathbf{x}$?) – **density evaluation**;
- sampling from $\pi(\mathbf{x})$ (to get new objects $\mathbf{x} \sim \pi(\mathbf{x})$) – **generation**.

Challenge

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

Problem statement

Conditional model

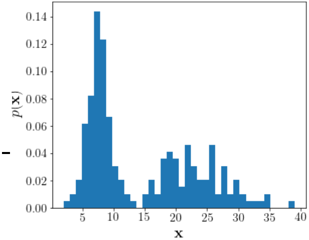
In practice the popular task is to create a conditional model $\pi(\mathbf{x}|\mathbf{y})$.

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

Histogram as a generative model

Let $x \sim \text{Categorical}(\boldsymbol{\pi})$. 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 $x_i = \{0, 1\}$.

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

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

What is a divergence?

Let $\mathcal{S}$ be the set of all possible probability distributions. Then $D : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ 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

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

where $\pi(\mathbf{x})$ is a true data distribution, $p(\mathbf{x}|\boldsymbol{\theta})$ 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 $f : \mathbb{R}_+ \to \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

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

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

Forward KL vs Reverse KL

Forward KL

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

Reverse KL

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

What 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.

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

Forward KL vs Reverse KL

Forward KL

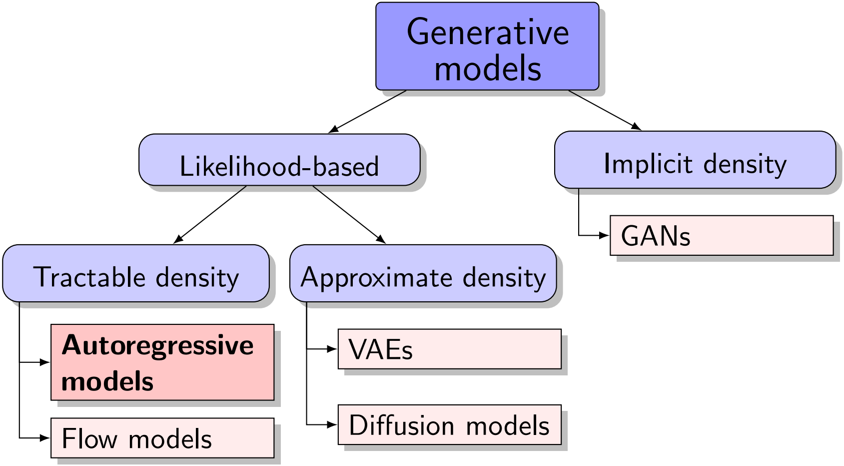
$$
\begin{aligned}
KL(\pi || p) &= \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \\
&= \int \pi(\mathbf{x}) \log \pi(\mathbf{x}) d\mathbf{x} - \int \pi(\mathbf{x}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{x} \\
&= -\mathbb{E}_{\pi(\mathbf{x})}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

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

Reverse KL

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

Generative models zoo



Outline

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

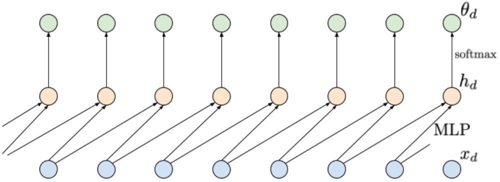
For large j the conditional distribution $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$ could be infeasible. Moreover, the history $\mathbf{x}_{1:j-1}$ has non-fixed length.

Markov assumption

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

Example

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



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

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

Autoregressive models: PixelCNN

Goal

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

Solution

Autoregressive model on 2D pixels

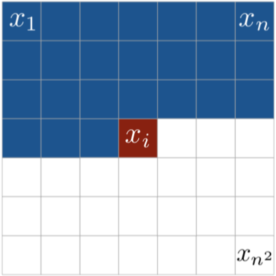
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{\text{width} \times \text{height}} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}).$$

- 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.

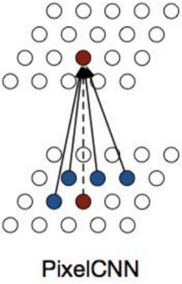
Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

Autoregressive models: PixelCNN

Raster ordering

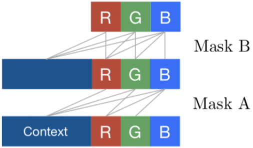


Dependencies between pixels



Mask for the convolution kernel

1	1	1
1	0	0
0	0	0



Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

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 $p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta})$.
- PixelCNN model use masked causal convolutions (1D or 2D) to get autoregressive model.