Deep Generative Models
Lecture 1

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Ozon Masters

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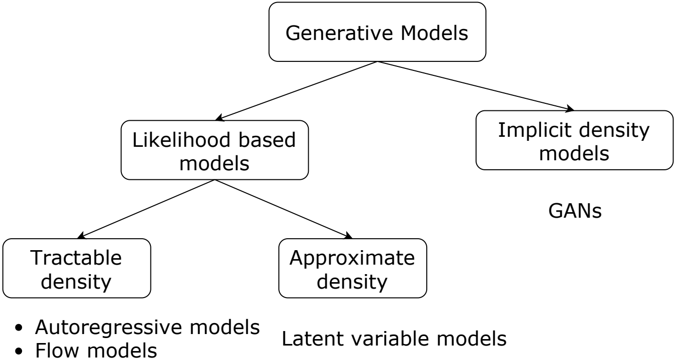
Logistics

- homeworks: 30 points
  - hw1: autoregressive models
  - hw2: latent variable models
  - hw3: flow models
  - hw4: adversarial models
- exam: 30 points
- final project: 40 points

Last year course page: link
Admission: link

Generative models zoo



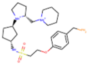
Applications

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .

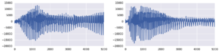
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Text analysis

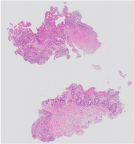
Image analysis



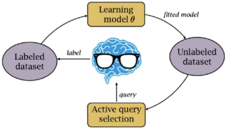
Graph analysis



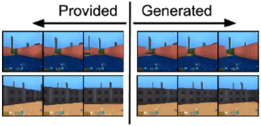
Audio analysis



Medical data



Active Learning



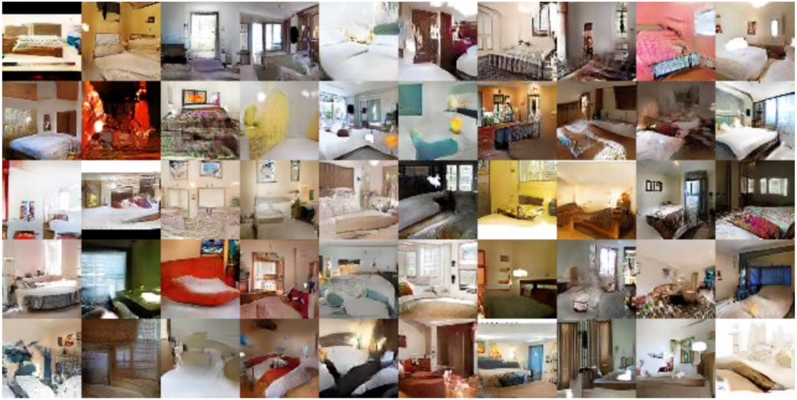
Reinforcement Learning

and more...

Applications: Image generation (VAE)

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

Applications: Image generation (DCGAN)

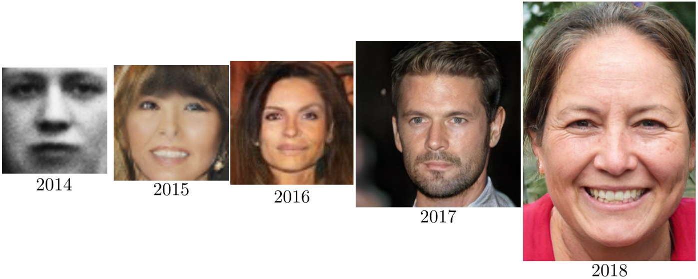


Radford A., Metz L., Chintala S. Unsupervised representation learning with deep convolutional generative adversarial networks, 2015

Applications: SuperResolution (SRGAN)

Ledig C. et al. Photo-realistic single image super-resolution using a generative adversarial network, 2016

Applications: Face generation (StyleGAN)

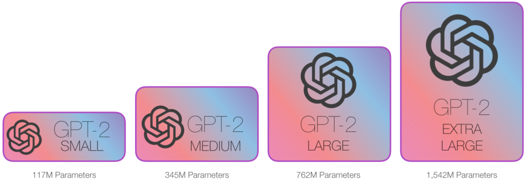


Karras T., Laine S., Aila T. A style-based generator architecture for generative adversarial networks, 2018

Applications: Face generation (VQ-VAE-2)

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

Applications: Language modelling



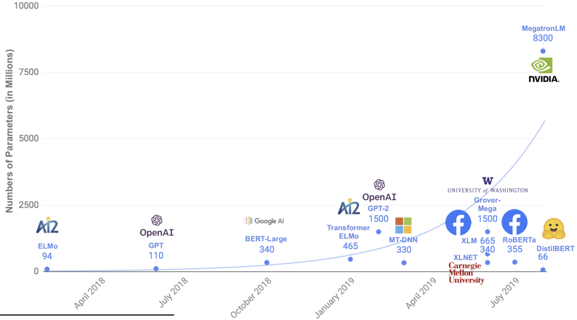
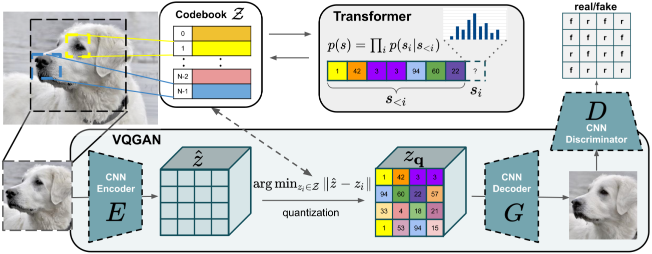


image credit: http://jalammar.github.io/illustrated-gpt2
Sanh V. et al. DistilBERT, a distilled version of BERT: smaller, faster, cheaper and lighter, 2019.

Applications: Image generation, new era



Esser P., Rombach R., Ommer B. Taming Transformers for High-Resolution Image Synthesis, 2020

Problem Statement

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

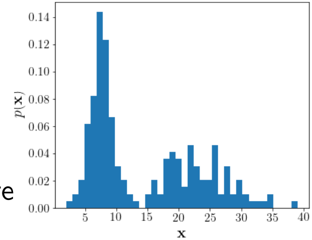
Challenge

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

Histogram as a generative model

Let $x \sim$ Categorical. The histogram is totally defined by

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



MNIST: 28x28 gray-scaled images each image is $\mathbf{x} = (x_1, \ldots, x_{784})$, where $x_i \sim \mathrm{Be}(p_i)$.
$2^{28\times 28} - 1$ parameters to specify $\pi(\mathbf{x})$

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

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

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

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

Maximum likelihood

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 $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

MLE problem

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

The problem is solved with SGD.

Requirements

- efficiently compute $\log p(\mathbf{x}|\boldsymbol{\theta})$;
- efficiently compute gradient of $\log p(\mathbf{x}|\boldsymbol{\theta})$.

Autoregressive model

MLE problem

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

Challenge

$p(\mathbf{x}|\boldsymbol{\theta})$ could be intractable.

Likelihood as product of conditionals

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

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

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

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{i=1}^{m} \log p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta})$$

- Sampling is sequential:
  - sample $\hat{x}_0 \sim p(x_1|\boldsymbol{\theta})$;
  - sample $\hat{x}_1 \sim p(x_2|x_1, \boldsymbol{\theta})$;
  - ...
  - sample $\hat{x}_n \sim p(x_n|\mathbf{x}_{1:n-1}, \boldsymbol{\theta})$;
  - new generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_n)$.
- Each conditional $p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta})$ 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

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

Markov assumption

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

Example

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

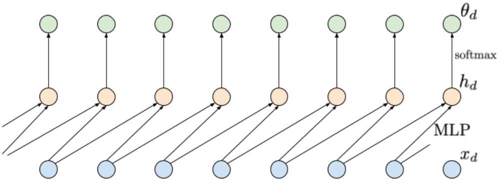
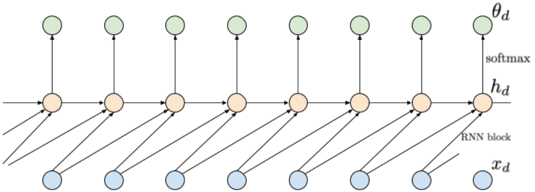


image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Autoregressive models

- 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:

$$p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta}) = p(x_i|\mathbf{h}_i, \boldsymbol{\theta}), \quad \mathbf{h}_i = \text{RNN}(\mathbf{x}_{i-1}, \mathbf{h}_{i-1})$$

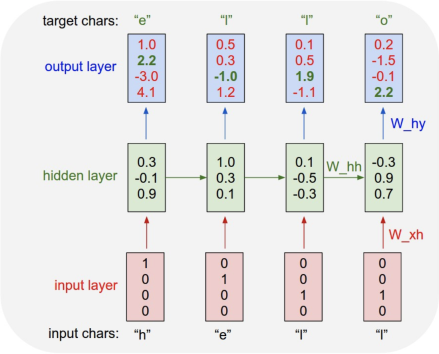


- Sequential computation of all conditionals $p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta})$, hence, the training is slow.
- RNN suffers from vanishing and exploding gradients.

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

Char RNN

Model tries to predict the next token (single letter) from previous context.

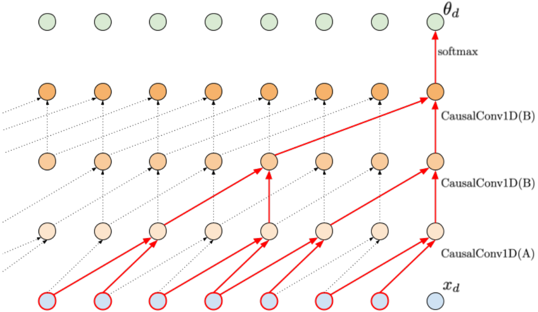



```
PANDARUS:
Alas, I think he shall be come approached and the day
When little srain would be attain'd into being never fed,
And who is but a chain and subjects of his death,
I should not sleep.

Second Senator:
They are away this miseries, produced upon my soul,
Breaking and strongly should be buried, when I perish
The earth and thoughts of many states.

DUKE VINCENTIO:
Well, your wit is in the care of side and that.

Second Lord:
They would be ruled after this chamber, and
my fair nues begun out of the fact, to be conveyed,
Whose noble souls I'll have the heart of the wars.

Clown:
Come, sir, I will make did behold your worship.

VIOLA:
I'll drink it.
```

image credit: http://karpathy.github.io/2015/05/21/rnn-effectiveness

Autoregressive models

- Convolutions could be used for autoregressive models, but they have to be **causal**.
- Try to find and understand the difference between Conv A/B.

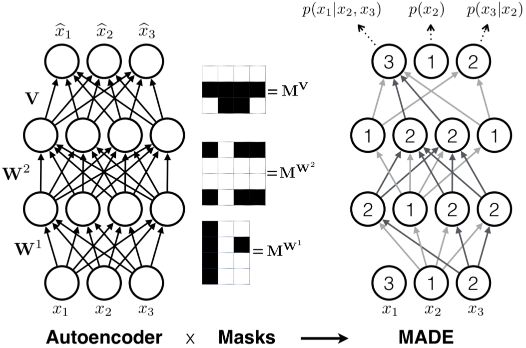


- Could learn long-range dependecies.
- Do not suffer from gradient issues.
- Easy to estimate probability for given input, but hard generation of new samples (the sequential process).

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

MADE

- Vanila autoencoder is not a generative model. Why?
- Let mask the weight matrices to make the model generative: $\mathbf{W}_M = \mathbf{W} \cdot \mathbf{M}$.



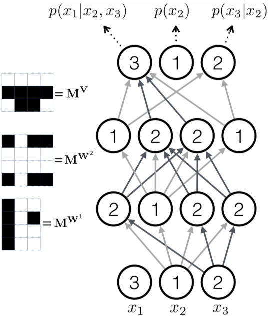
- The question is how to create matrices **M** which produce the autoregressive property?

Germain M. et al. Made: Masked autoencoder for distribution estimation, 2015

MADE

Masks generation

- Define the ordering of input elements from 1 to n.
- Assign the random number m from 1 to $n-1$ to each hidden unit. The number gives the maximum number of input units to which the unit can be connected.
- Connect each hidden unit with number m with the previous layer units which has the number is **less or equal** than m.
- Connect each output unit with number m with the previous layer units which has the number is **less** than m.



Germain M. et al. Made: Masked autoencoder for distribution estimation, 2015

WaveNet

Goal

Efficient generation of raw audio waveforms with natural sounds.

Solution

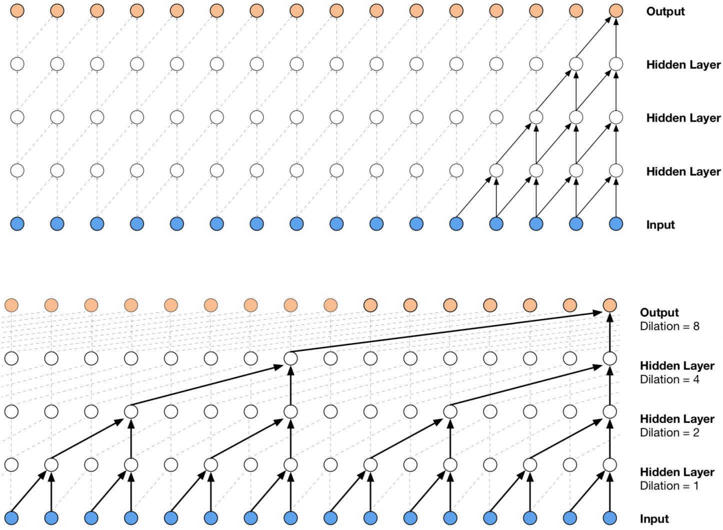
Autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{t=1}^{T} p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta}).$$

- Each conditional $p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta})$ models the distribution for the timestamp t.
- The model uses **causal** dilated convolutions.

Oord A. et al. Wavenet: A generative model for raw audio, 2016

WaveNet (2016)



Oord A. et al. Wavenet: A generative model for raw audio, 2016

PixelCNN

Goal

Model a distribution of natural images.

Solution

Autoregressive model

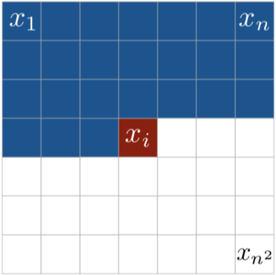
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{n^2} p(x_i|\mathbf{x}_{1:i-1}, \boldsymbol{\theta}).$$

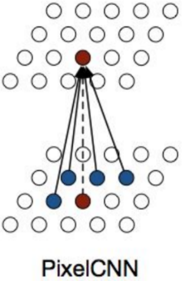
- **masked** convolutions;
- dependencies over RGB channels.

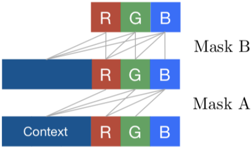
Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

PixelCNN (2016)

1	1	1
1	0	0
0	0	0







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

Summary

- Sampling from autoregressive models is trivial, but sequential
  - sample $x_0 \sim p(x_0)$;
  - sample $x_1 \sim p(x_1|x_0)$;
  - $\dots$.
- Estimating probability:

$$p(\mathbf{x}) = \prod_{i=1}^{m} p(x_i|\mathbf{x}_{1:i-1}).$$

- Work on both continuous and discrete data.
- There is no natural way to do unsupervised learning.