Deep Generative Models

Autoregressive Model

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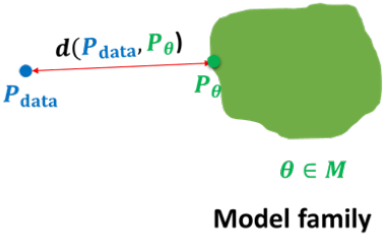
Introduction

1. **A Generative model** (GM) is a probability distribution $p(\mathbf{x})$.
   - A statistical GM is a trainable probabilistic model, $p_\theta(\mathbf{x})$.
   - A deep GM is a statistical generative model parametrized by a neural network.
2. A generative model needs
   - Data ($\mathbf{x}$): Complex, unstructured samples such as images, speech, molecules, text, etc.
   - Prior knowledge: parametric form (e.g., Gaussian, mixture, softmax), loss function (e.g., maximum likelihood, divergence), optimization algorithm, etc.

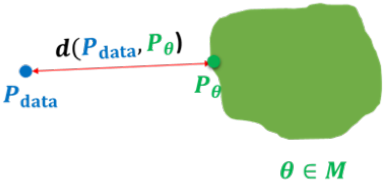
$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Credit: Aditya Grover

Introduction (Key Questions)

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$

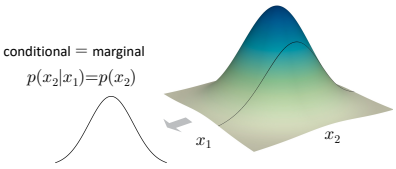


1. **A Representation:** how do we parameterize the joint distribution of many random variables?
2. **A Learning:** what is the right way to compare probability distributions?
3. **A Inference:** how do we invert (or encode) the generation process?

Credit: Aditya Grover

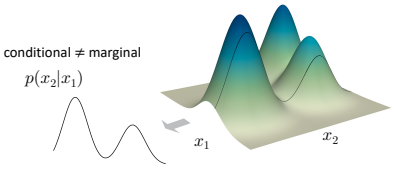
Independent random variables

$$p(x_1, x_2) = p(x_1)\, p(x_2)$$



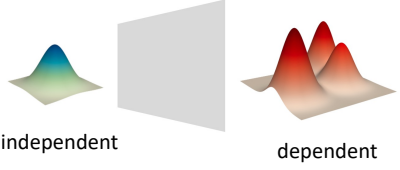
Dependent random variables

$$p(x_1, x_2) \neq p(x_1)\, p(x_2)$$



How to Model Joint Distributions?

1. **Solution 1:** Modeling by independent latents (e.g., VAE)
   - Mapping independent variables → dependent ones
   - Strict assumption for high-dim data.
   - Often with low-dim latents
   - A good building block, but often not sufficient

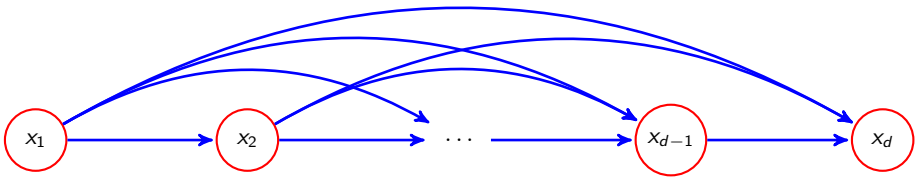


2. **Solution 2:** Modeling by conditional distributions

1. Suppose we have a dataset $S = \{x_1, x_2, \ldots, x_m\}$ of n-dimensional points $\mathbf{x}$.
2. For simplicity, we assume points are binary, i.e., $x \in \{0, 1\}^n$.
3. **Case 1:** Partitioning the input representation space $\mathcal{X}$
   - Using chain rule, we can factorize the joint distribution as

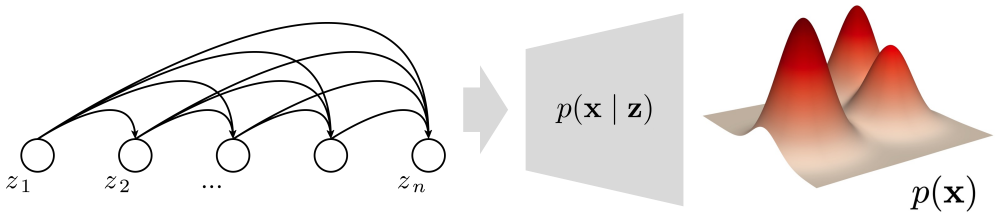
$$p(x) = p(x_1, x_2, \ldots, x_n) = \prod_{i=1}^{n} p(x_i | x_1, x_2, \ldots, x_{i-1}) = \prod_{i=1}^{n} p(x_i | \mathbf{x}_{<i})$$

     where $\mathbf{x}_{<i} = [x_1, x_2, \ldots, x_{i-1}]$ denotes vector of random variables with index less than i.
   - The chain rule factorization can be expressed graphically as a Bayesian network.



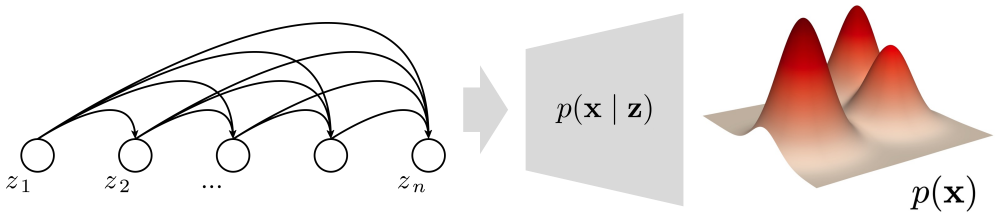
1. Suppose we have a dataset $S = \{x_1, x_2, \ldots, x_m\}$ of n-dimensional points $\mathbf{x}$.
2. For simplicity, we assume points are binary, i.e., $x \in \{0, 1\}^n$.
3. **Case 2:** Partitioning the latent representation space $\mathcal{Z}$ (Ex. VQ-VAE)

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x} \mid \mathbf{z})$$
$$\text{with} \quad p(\mathbf{z}) = p(z_1)p(z_2 \mid z_1)...p(z_n \mid z_1, z_2, ..., z_{n-1})$$

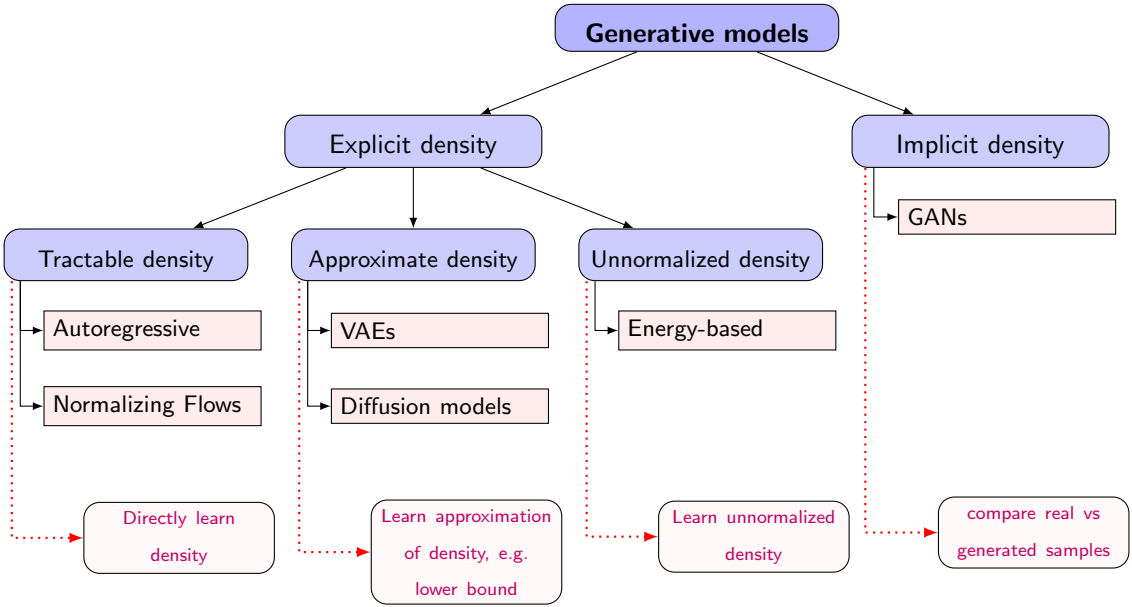


1. Suppose we have a dataset $S = \{x_1, x_2, \ldots, x_m\}$ of n-dimensional points $\mathbf{x}$.
2. For simplicity, we assume points are binary, i.e., $x \in \{0,1\}^n$.
3. **Case 3:** Partitioning the latent representation space $\mathcal{Z}$ (Ex. VQ-VAE)

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p(\mathbf{x} \mid \mathbf{z})$$
$$\text{with} \quad p(\mathbf{z}) = p(z_1)p(z_2 \mid z_1)...p(z_n \mid z_1, z_2, ..., z_{n-1})$$

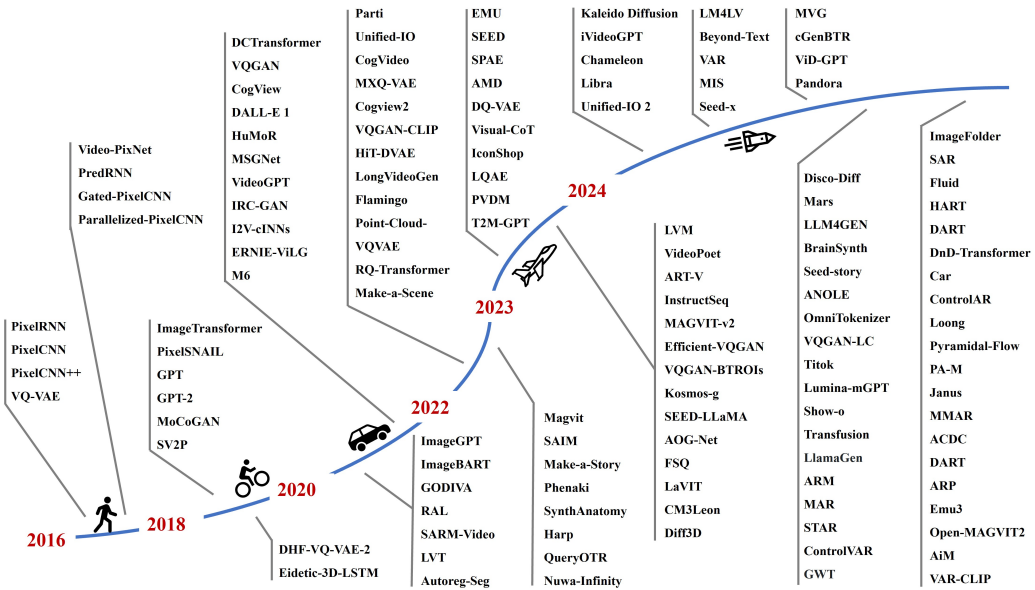


Generative models categories



Autoregressive models

A timeline of representative autoregressive models in vision



Autoregressive models

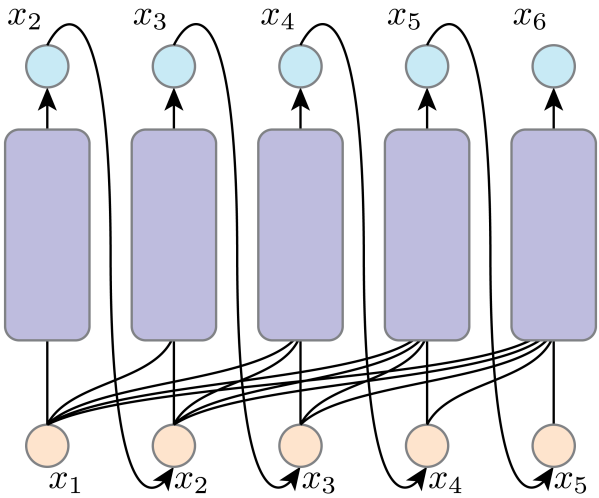
1. The autoregressive constraint is a way to model sequential data.
2. **Autoregressive** = **Auto** + **Regression**
   - **Auto:** Self

     using its own outputs as inputs for next perditions
   - **Regression:**

     estimating relationship between variables
3. Autoregressive implies an **inference-time** behavior
4. Training-time is not necessarily autoregressive

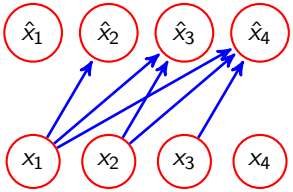
Autoregressive models inference

1. Factorization contains n factors and some factors contain many parameters: $O(2^n)$.
2. It is infeasible to learn such an exponential number of parameters.
3. AR models use (deep) neural network to parameterize these factors $p(x_i|x_{<i})$.



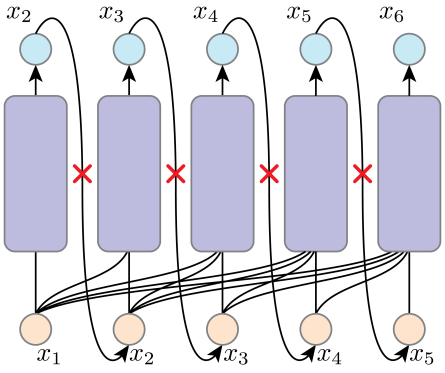
Autoregressive models

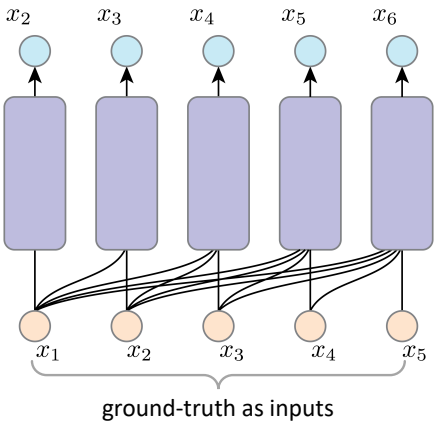
1. How to evaluate $p(x_1, \ldots, x_{900})$?
2. Multiply all the conditionals factors.
3. How to sample from $p(x_1, \ldots, x_{900})$?
   - Sample $\bar{x}_1 \sim p(x_1)$.
   - Sample $\bar{x}_2 \sim p(x_2|x_1 = \bar{x}_1)$.
   - Sample $\bar{x}_3 \sim p(x_3|x_1 = \bar{x}_1, x_2 = \bar{x}_2)$.
4. How many parameters? $1 + 2 + 3 + \ldots + n \approx \frac{n^2}{2}$



Autoregressive models training

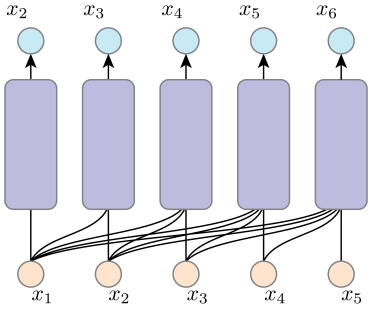
1. Usually **teacher-forcing** are used for training.
2. Inputs are not from previous outputs
3. Inputs are from ground-truth data



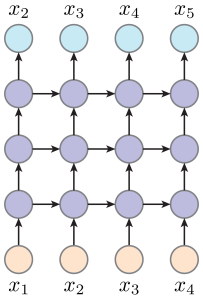


Autoregression is not architecture-specific.

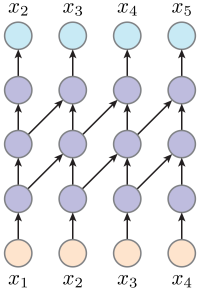
RNN



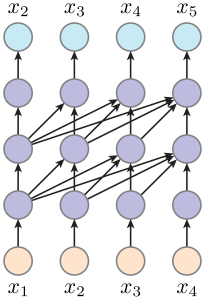
RNN



CNN



Attention



1. Suppose conditional distributions $p(x_i|x_{<i})$ correspond to Bernoulli random variables and learn a function mapping $x_1, x_2, \ldots, x_{i-1}$ to the mean of this distribution as

$$p_{\theta_i}(x_i|x_{<i}) = Bern(f_i(x_1, x_2, \ldots, x_{i-1}))$$

   θ_i denotes a set of parameters used to specify mean function $f_i : \{0,1\}^{i-1} \mapsto [0,1]$.

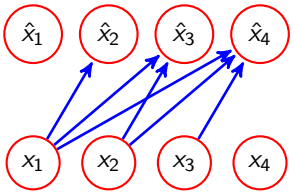
2. The number of parameters of an AR model equals to $\sum_{i=1}^{n} |\theta_i|$.
3. Tractable exact likelihood computations.
4. No complex integral over latent variables in likelihood
5. Slow sequential sampling process.
6. Cannot rely on latent variables.

1. In the simplest case, we can specify the function as a linear combination of the input elements followed by a sigmoid non-linearity (to restrict the output to lie between 0 and 1).
2. This gives us the formulation of a fully-visible sigmoid belief network (FVSBN).

$$f_i(x_1, x_2, \ldots, x_{i-1}) = \sigma\left(a_0^i + \sum_{j=1}^{i-1} a_j^i x_j\right)$$

where σ is sigmoid function and $\theta_i = \{a_0^i, \ldots, a_{i-1}^i\}$.

3. At the output layer we want to predict n conditional probability distributions while at the input layer we are given the n input variables.

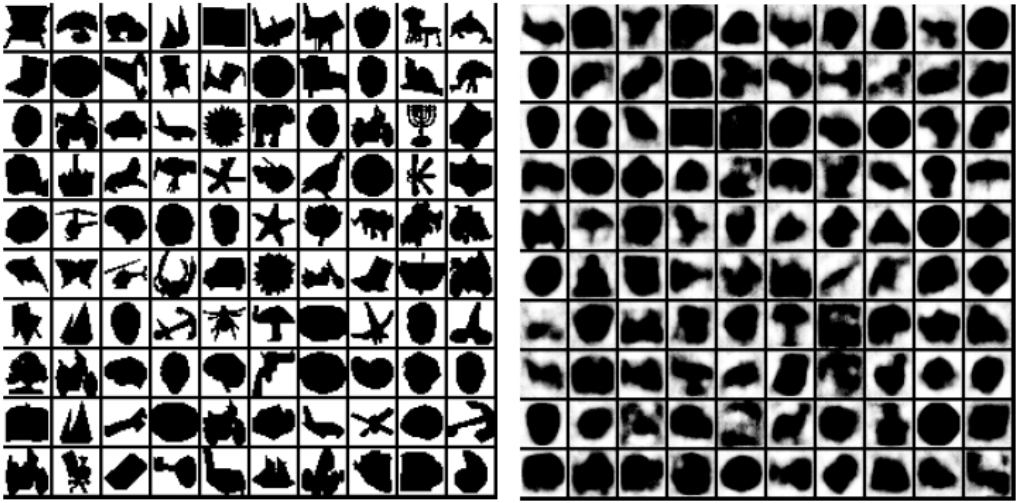


4. The conditional variables $x_i|x_1, \ldots, x_{i-1}$ are Bernoulli with parameters

$$\hat{x}_i = p(x_i = 1|x_1, \ldots, x_{i-1}; \theta_i) = \sigma\left(a_0^i + \sum_{j=1}^{i-1} a_j^i x_j\right)$$

FVSBN results (Gan et al. 2015)

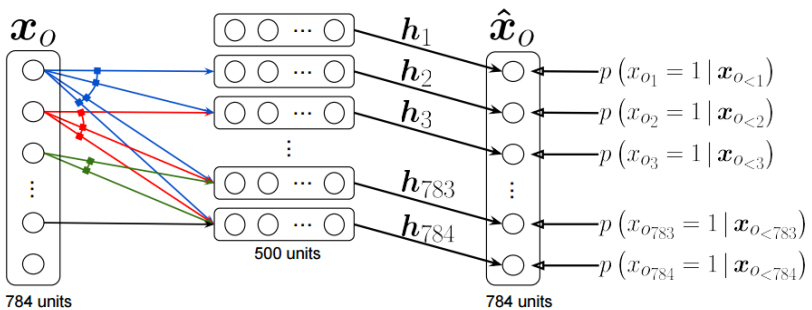
1. Left: Training (Caltech 101 Silhouettes) Right: Samples from the model



1. To increase the expressiveness of an autoregressive generative model, we can use more flexible parameterizations for the mean function such as MLP instead of logistic regression.
2. For example, consider the case of a neural network with one hidden layer.
3. The mean function for variable i can be expressed as

$$\mathbf{h}_i = \sigma(A_i \mathbf{x}_{<i} + \mathbf{c}_i)$$
$$f_i(x_1, x_2, \ldots, x_{i-1}) = \sigma\left(\mathbf{a}^i \mathbf{h}_i + b_i\right)$$

   where $\mathbf{h}_i \in \mathbb{R}^d$ is hidden layer activations of MLP.
4. Hence, we have the following architecture



5. Total number of parameters is dominated by matrices A_i and given by $O(nd + n)$.

1. The Neural Autoregressive Density Estimator (NADE) provides an alternate MLP-based parameterization that is more statistically and computationally efficient than the given approach (Larochelle and Murray 2011).
2. In NADE, parameters are shared across the functions used for evaluating the conditionals.
3. The hidden layer activations are specified as

$$\mathbf{h}_i = \sigma(W_{.,<i}\mathbf{x}_{<\mathbf{i}} + \mathbf{c})$$
$$\hat{x}_i = p(x_i = 1|x_1, \ldots, x_{i-1}; \boldsymbol{\theta}^i) = \sigma(\boldsymbol{\alpha}^{(i)}\mathbf{h}_i + b_i)$$

4. $\theta = \{W \in \mathbb{R}^{d\times n}, \mathbf{c} \in \mathbb{R}^d, \{\boldsymbol{\alpha}^{(i)} \in \mathbb{R}^d\}_{i=1}^n, \{b_i \in \mathbb{R}\}_{i=1}^n\}$ is the full set of parameters.
5. The weight matrix W and the bias vector c are shared across the conditionals.

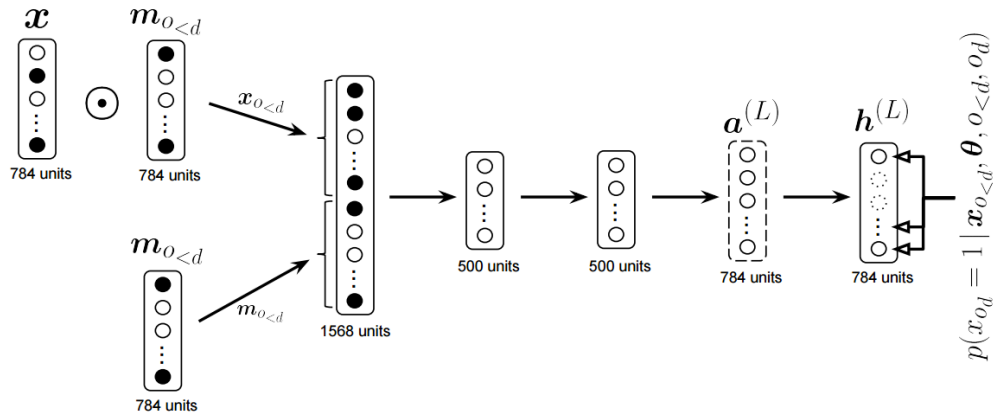
1. Sharing parameters has two benefits:
   - The total number of parameters gets reduced from $O(n^2 d)$ to $O(nd)$.
   - Hidden unit activations can be evaluated in $O(nd)$ time via

$$\mathbf{h}_i = \sigma(\mathbf{a}_i)$$
$$\mathbf{a}_{i+1} = \mathbf{a}_i + W[., i]x_i$$

   with the base case given by $\mathbf{a}_1 = \mathbf{c}$.

2. Training of NADE is done by minimizing $-\frac{1}{T}\sum_{i=1}^{T} \log p(x_i)$
3. Samples from NADE trained on a binary version of MNIST.

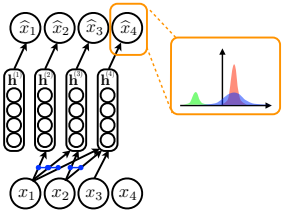
1. The input to the network (DeepNADE) is the concatenation of the masked data and the mask itself (Uria, Côté, et al. 2016).
2. This allows the network to identify cases when input data is truly zero from cases when input data is zero because of the mask.
3. NADE also explored other autoencoder architectures such as convolutional neural networks
4. DeepNade with two hidden layers



1. The RNADE algorithm extends NADE to learn generative models over real-valued data (Uria, Murray, and Larochelle 2013).
2. The conditionals are modeled via a continuous distribution such as mixture of K Gaussian.

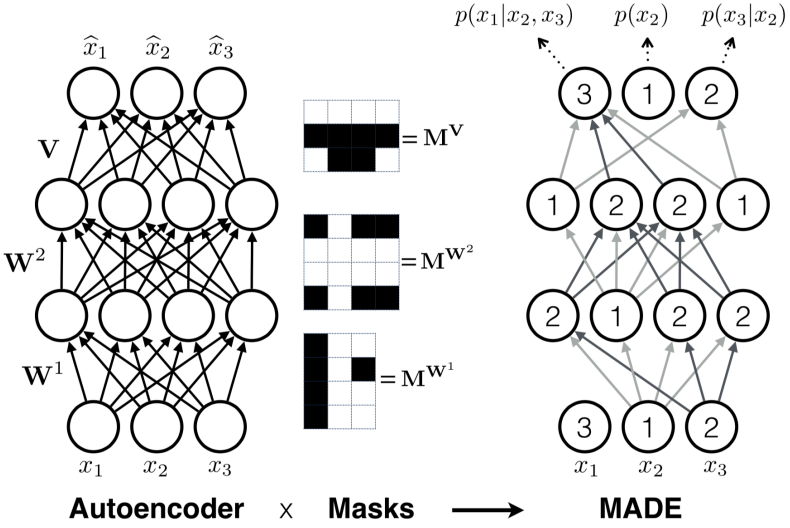
$$p(x_i|x_{<i}) = \sum_{j=1}^{K} \pi_{ij} \mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$$

- Output of the network are parameters of a mixture model for $p(x_k|x_{<k})$
- Means are $\mu_{i,k} = b_{i,k}^{\mu_i} + \boldsymbol{\alpha}_{i,k}^{\mu_i} h_i$
- Standard deviations are $\sigma_{i,k} = \exp\left(b_{i,k}^{\sigma_i} + \boldsymbol{\alpha}_{i,k}^{\sigma_i} h_i\right)$
- Mixing weights are $\pi_{i,k} = softmax\left(b_{i,k}^{\pi_i} + \boldsymbol{\alpha}_{i,k}^{\pi_i} h_i\right)$



3. Please study DocNADE.

1. MADE is an autoencoder that preserves autoregressive property (Germain et al. 2015).



Masked Autoencoder for Distribution Estimation (MADE)

1. MADE is a specially designed architecture to enforce the autoregressive property in the autoencoder efficiently.
2. MADE removes the contribution of certain hidden units by using mask matrices so that each input dimension is reconstructed only from previous dimensions in a given ordering in a single pass.
3. In a multilayer fully-connected neural network, say, we have L hidden layers with weight matrices $\mathbf{W}^1, \ldots, \mathbf{W}^L$ and an output layer with weight matrix V. The output $\hat{x}$ has dimensions $\hat{x}_i = p(x_i | x_{1:i-1})$
4. Without any mask, we have

$$\begin{aligned}
\mathbf{h}^0 &= \mathbf{x} \\
\mathbf{h}^l &= \text{activation}^l(\mathbf{W}^l \mathbf{h}^{l-1} + \mathbf{b}^l) \\
\hat{\mathbf{x}} &= \sigma(\mathbf{V}\mathbf{h}^L + \mathbf{c})
\end{aligned}$$

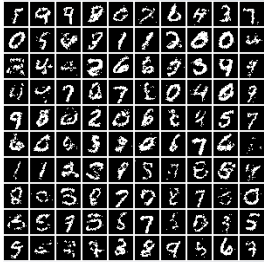
1. Without any mask, we have

$$\mathbf{h}^0 = \mathbf{x}$$
$$\mathbf{h}^l = \text{activation}^l(\mathbf{W}^l\mathbf{h}^{l-1} + \mathbf{b}^l)$$
$$\hat{\mathbf{x}} = \sigma(\mathbf{V}\mathbf{h}^L + \mathbf{c})$$

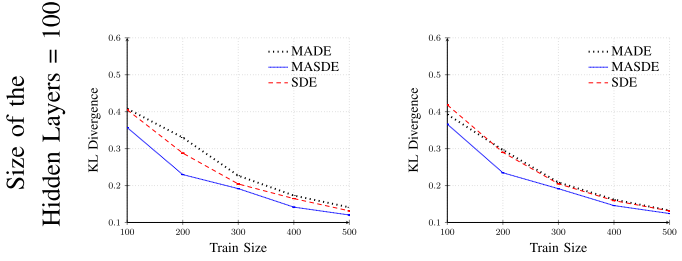
2. To zero out some connections between layers, we can simply element-wise multiply every weight matrix by a binary mask matrix.

$$\mathbf{h}^l = \text{activation}^l((\mathbf{W}^l \odot \mathbf{M}^{\mathbf{W}^l})\mathbf{h}^{l-1} + \mathbf{b}^l)$$
$$\hat{\mathbf{x}} = \sigma((\mathbf{V} \odot \mathbf{M}^{\mathbf{V}})\mathbf{h}^L + \mathbf{c})$$

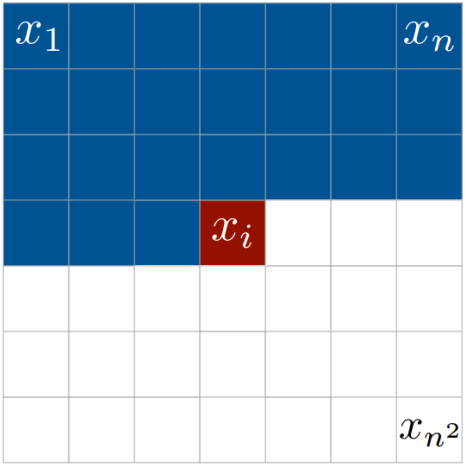
3. Mask matrix is constructed by a labeling process.



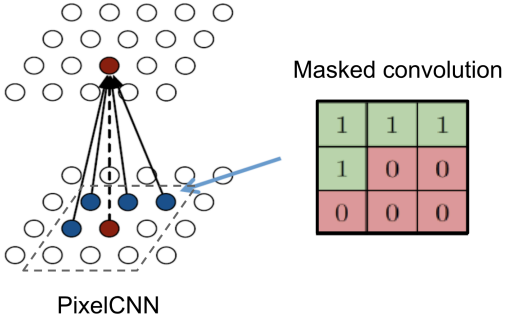
1. This method is used when the structure (Markov random field) of the data is known (Khajenezhad, Madani, and Beigy 2021).
2. In structured distributions, the graph structure of the variables declares their conditional dependencies.
3. Therefore, having a graph structure, each of the chain rule conditional terms might be presentable by a conditional probability on a smaller set of variables.
4. For each i, we assume there is a subset $B_i \subseteq \{1, \ldots, i-1\}$ such that $p(x_i|x_{<i}) = p(x_i|x_{B_i})$.
5. Use an auoencoder that has the above autoregressive property and mask matrix is constructed by a labeling process.
6. MASDE needs a smaller training set in comparison with its counterparts.



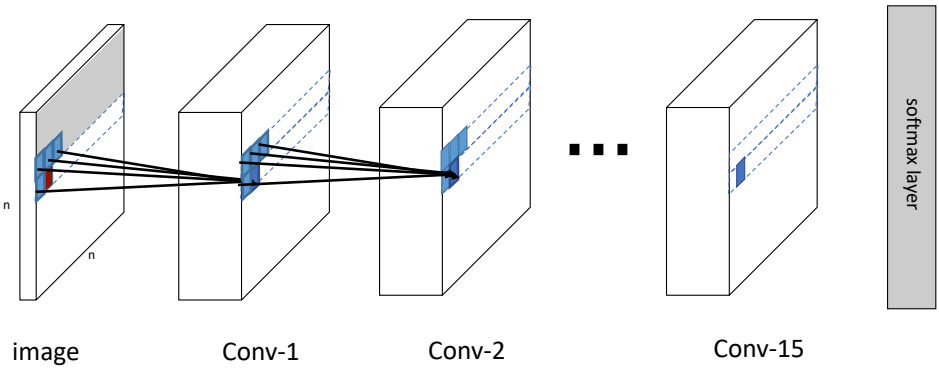
1. PixelRNN is a deep generative model for images (Oord, Kalchbrenner, and Kavukcuoglu 2016).
2. Dependency on previous pixels modeled using an RNN (LSTM).



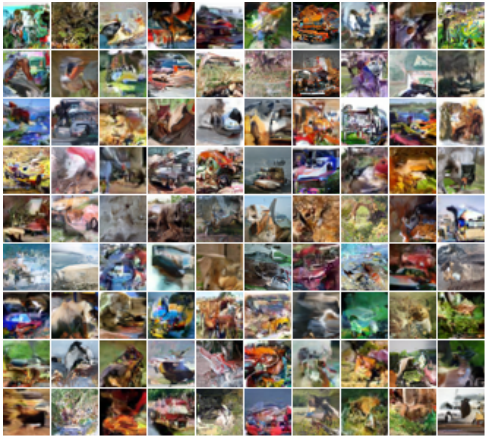
1. The main drawback of PixelRNN is that training is very slow.
2. PixelCNN uses standard convolutional layers to capture a bounded receptive field and compute features for all pixel positions at once (Oord, Kalchbrenner, Espeholt, et al. 2016).
3. In PixelCNN, pooling layers are not used.
4. Masks are adopted in the convolutions to restrict the model from violating the conditional dependence.



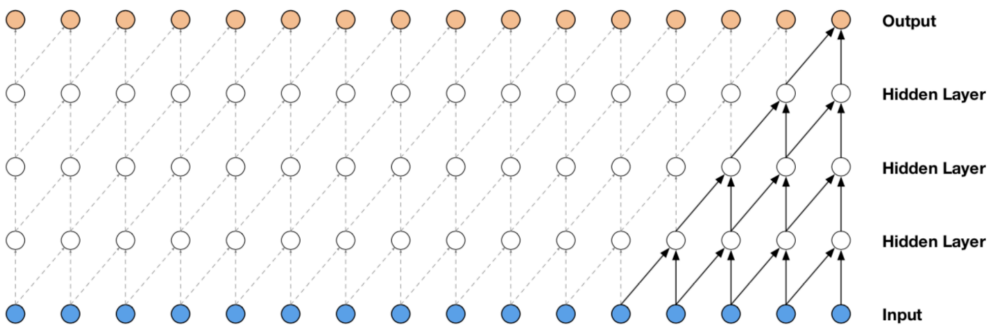
5. Please also PixelCNN++ (Salimans et al. 2017).


n
n
softmax layer
image
Conv-1
Conv-2
Conv-15

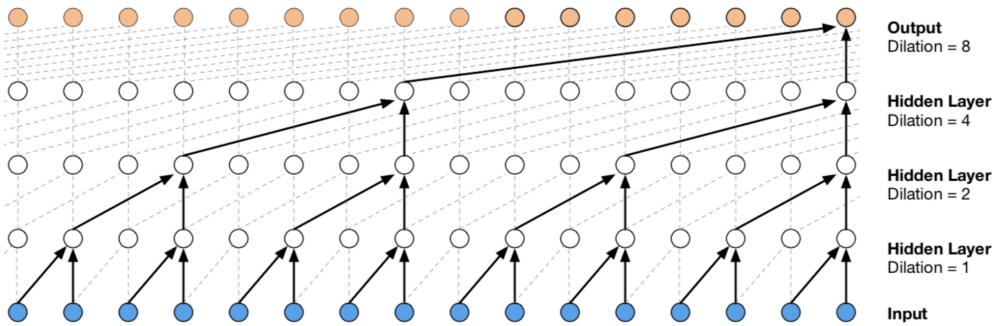
1. The training set (CIFAR-10 (left)) and the samples generated by the PixelCNN (right).



1. WaveNet is very similar to PixelCNN but applied to 1-D audio signals (Oord, Dieleman, et al. 2016).
2. WaveNet consists of a stack of causal convolution which is a convolution operation designed to respect the ordering.
3. Causal convolutions used for temporal data which ensures the model cannot violate the ordering in which we model the data: the prediction $p(x_{t+1}|x_1, \ldots, x_t)$.
4. The causal convolution in WaveNet is simply to shift the output by a number of timestamps to the future so that the output is aligned with the last input element.



1. One big drawback of convolution layer is a very limited size of receptive field.
2. WaveNet therefore adopts dilated convolution, where the kernel is applied to an evenly-distributed subset of samples in a much larger receptive field of the input.



1. The attention make it possible to do sequence to sequence modeling without recurrent network units (Vaswani et al. 2017).
2. The transformer model is entirely built on the self-attention mechanisms without using sequence-aligned recurrent architecture.

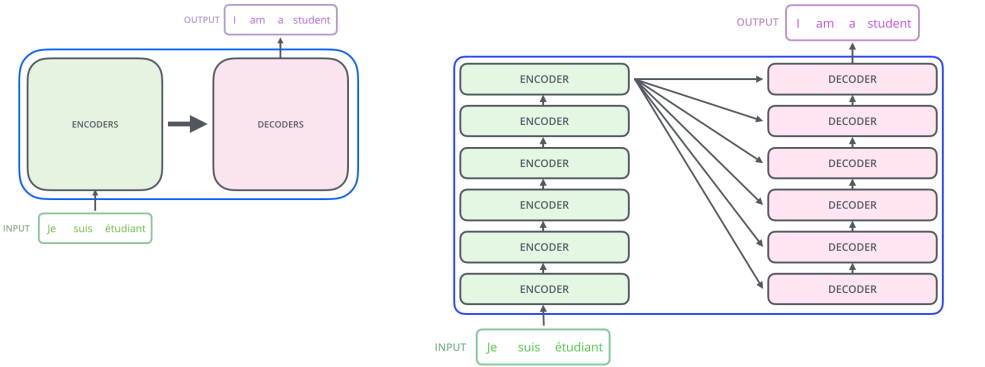


Figure: Jay Alammar

3. The encoding component is a stack of six encoders.
4. The decoding component is a stack of decoders of the same number.

References

Reading

1. Chapter 22 of Probabilistic Machine Learning: Advanced Topics (Murphy 2023).
2. Chapter 2 of Deep Generative Modeling (Tomczak 2024).
3. Papee A Survey on Vision Autoregressive Model (Jiang and Huang 2024).

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Questions?