Statistical Models & Computing Methods

Lecture 17: Autoregressive Models

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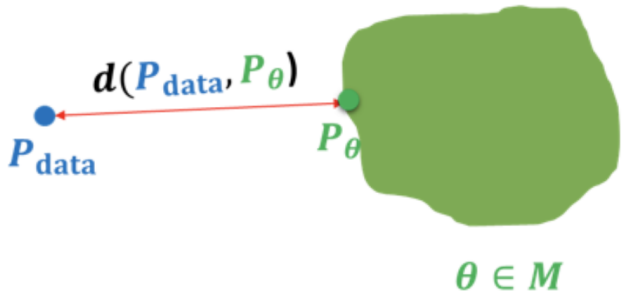
Introduction

- Statistical models and inference methods allow us to learn and explain the generative process of the observed data.
- However, real data distributions are often too complicated to be handled by standard statistical models in a satisfactory manner.
- In this lecture, we will introduce some recent techniques that combine deep neural networks and statistical inference methods for expressive generative models.
- The materials for deep generative models are mainly adapted from Ermon and Grover, 2019.

We are given a training set of examples, e.g., images of dogs

$x_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Goal: learn a probability distribution $p(x)$ over x such that

- Generation: If we sample $x_{\text{new}} \sim p(x)$, x_{new} should look like a real image.
- Density estimation: $p(x)$ should be high if x looks like a real image, and low otherwise (anomaly detection).
- Unsupervised representation learning: We should be able to learn high level features of these images, e.g., ears, tail, etc.

Two key questions: (1) How to construct $p(x)$? (2) How to learn $p(x)$?

Chain Rule in Probability

We can decompose the joint probability using Chain Rule

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$

Fully general (exponential size, no free lunch)

- Bayes Net: assumes conditional independencies; tabular representations via conditional probability tables (CPT)

$$p(x_1, x_2, x_3, x_4) \approx p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)$$

- Neural Models: assume specific functional form for the conditionals. A sufficiently deep neural net can approximate any function.

$$p(x_1, x_2, x_3, x_4) \approx p(x_1)p(x_2|x_1)p_{\text{Neural}}(x_3|x_1, x_2) \\ p_{\text{Neural}}(x_4|x_1, x_2, x_3)$$

- Input features $X \in \{0,1\}^n$, response variable $Y \in \{0,1\}$.
- For classification, we care about $p(Y|x)$, and assume that

$$p(Y = 1|x; \alpha) = f(x, \alpha)$$

- Logistic regression: let $z(\alpha, x) = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i$

$$p_{\text{logit}}(Y = 1|x; \alpha) = \sigma(z(\alpha, x)), \quad \sigma(z) = \frac{1}{1 + \exp(-z)}$$

- Neural Nets: let $h(x; A, b)$ be a non-linear transformation of the input features.

$$p_{\text{Neural}}(Y = 1|x; \alpha, A, b) = \sigma(z(\alpha, h))$$

More parameters $\Rightarrow$ more flexibility. Can repeat multiple times to get a multilayer perceptron.

Example: MNIST

Consider a dataset $\mathcal{D}$ of handwritten digits (binarized MNIST)

- Each image has $n = 28 \times 28 = 784$ pixels. Each pixel can either be black (0) or white (1).
- **Goal:** Learn a probability distribution $p(x) = p(x_1, \ldots, x_{784})$ over $x \in \{0, 1\}^{784}$ such that $x \sim p(x)$ looks like a handwritten digit.
- Two step process as mentioned before:
  - Parameterize a family of flexible models $\{p_\theta(x), \theta \in \Theta\}$
  - Search for model parameters θ based on training data $\mathcal{D}$

We start with the first step.

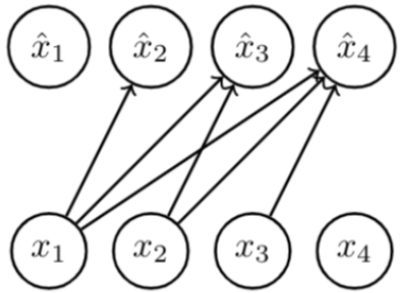
- Pick an order of all random variables, i.e., raster scan order of pixels from top-left (x_1) to bottom-right ($x_{n=784}$)
- Without loss of generality, we can use chain rule for factorization

$$p(x_1, \ldots, x_n) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2) \cdots p(x_n|x_1, \ldots, x_{n-1})$$

- However, the above parameterization is too heavy to be practical. We can use neural models to simplify it

$$p(x_1, \ldots, x_{784}) = p(x_1; \alpha^1)p_{\text{logit}}(x_2|x_1; \alpha^2) \cdots p_{\text{logit}}(x_n|x_1, \ldots, x_{n-1}; \alpha^n)$$

Remark: This is a modeling assumption. We are using parameterized functions to predict next pixel given all the previous ones (autoregressive models).



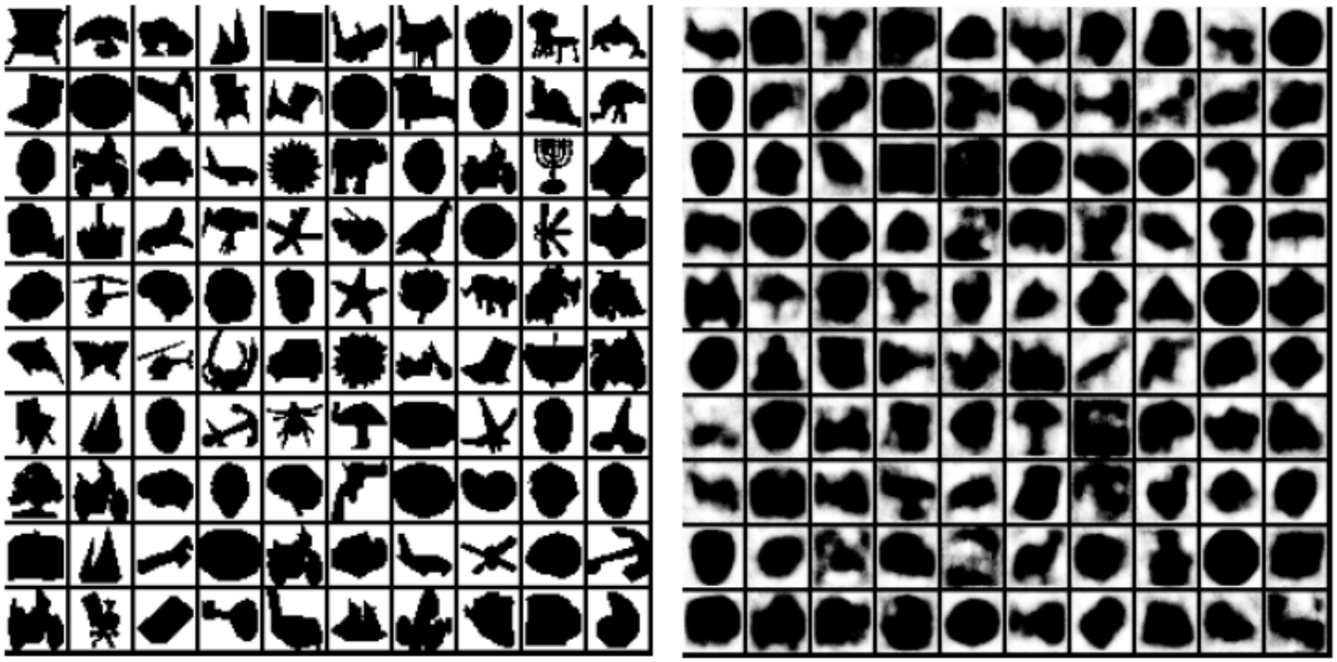
FVSBN

- The conditional distributions $X_i|X_{<i}$ are Bernoulli with parameters

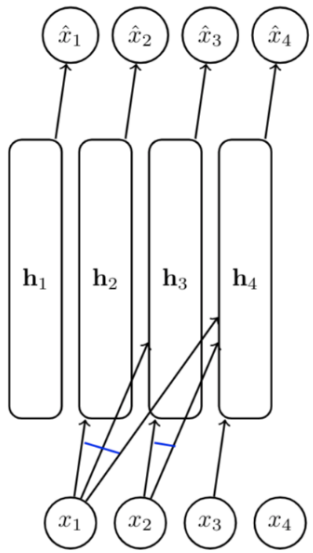
$$p(x_i = 1|x_{<i}; \alpha^i) = \sigma(\alpha_0^i + \sum_{j=1}^{i-1} \alpha_j^i x_j)$$

- We can evaluate $p(x)$ as a product of all the conditionals.
- How to sample from $p(x)$? Sequential sampling!
  - Sample $\bar{x}_1 \sim p(x_1)$
  - Sample $\bar{x}_i \sim p(x_i|x_{<i}), \quad i = 2, \ldots, n$
- How many parameters do we have? $\sum_{i=1}^{n} i = O(n^2)$

Training data on the left (*Caltech 101 Silhouettes*). Samples from the model on the right.



Adapted from Gan et al., 2015

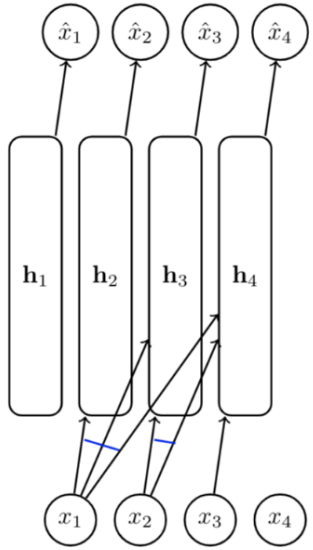


NADE

- Use one layer neural network instead of logistic regression

$$p(x_i = 1|x_{<i}; A_i, c_i, \alpha_i, b_i) = \sigma(\alpha_i^T h_i + b_i), \quad h_i = \sigma(A_i x_{<i} + c_i)$$

- For example: $h_2 = \sigma\left(A_2 x_1 + c_2\right)$, $h_2 = \sigma\left(A_3 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + c_3\right)$



NADE

- Tie weights to reduce the number of parameters

  $$p(x_i = 1|x_{<i}; A_i, c_i, \alpha_i, b_i) = \sigma(\alpha_i^T h_i + b_i), \quad h_i = \sigma(W_{.,<i} x_{<i} + c)$$

- For example: $h_2 = \sigma\left([w_1] x_1 + c\right)$, $h_3 = \sigma\left([w_1\ w_2]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + c\right)$

- If $h_i \in \mathbb{R}^d$, weights $W \in \mathbb{R}^{d \times n}$, biases $c \in \mathbb{R}^d$, and n logistic regression coefficient $\alpha_i, b_i \in \mathbb{R}^{d+1}$. Probability is evaluated in $O(nd)$.

NADE Results

Samples on the left. Conditional probabilities on the right.

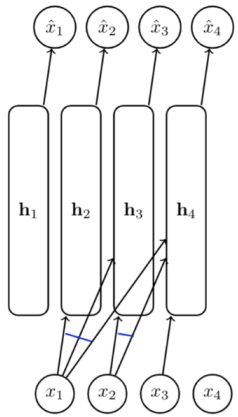
Adapted from Larochelle and Murray, 2011

- What about multi-class discrete random variables $X_i \in \{1, \ldots, K\}$? E.g., pixel intensities varying from 0 to 255
- One solution: use categorical distribution instead of a binary one

$$x_i | x_{<i} \sim \text{Cat}(\pi_i), \quad \pi_i = \text{softmax}(\alpha_i^T h_i + b_i)$$

- Softmax generalizes the sigmoid/logistic function $\sigma(\cdot)$ and transforms a vector of K numbers into a vector of K probabilities

$$\text{softmax}(a) = \left(\frac{\exp(a_1)}{\sum_i \exp(a_i)}, \cdots, \frac{\exp(a_K)}{\sum_i \exp(a_i)} \right)$$



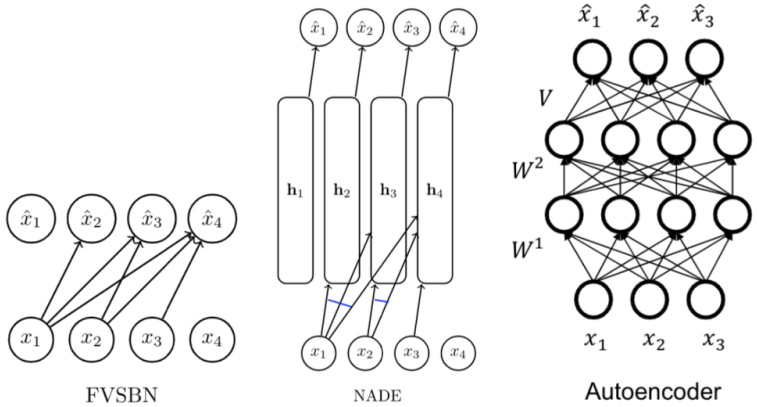
NADE

- How to model continuous random variables $X_i \in \mathbb{R}$? E.g., speech signals.
- Solution: Use a continuous distribution instead! For example, a mixture of K Gaussians

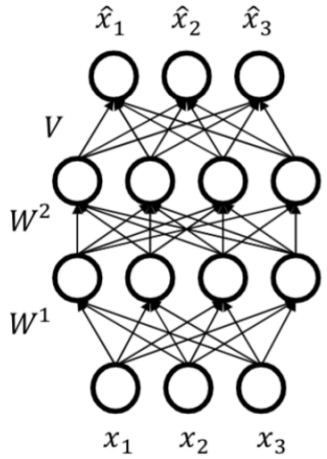
$$p(x_i|x_{<i}) = \frac{1}{K}\sum_{j=1}^{K}\mathcal{N}\left(\mu_i^j, (\sigma_i^j)^2\right)$$

where μ_i^j, σ_i^j can be functions of h_i, e.g., neural networks. Can use exponential function to ensure $\sigma_i^j > 0$.

Autoregressive Models vs Autoencoders

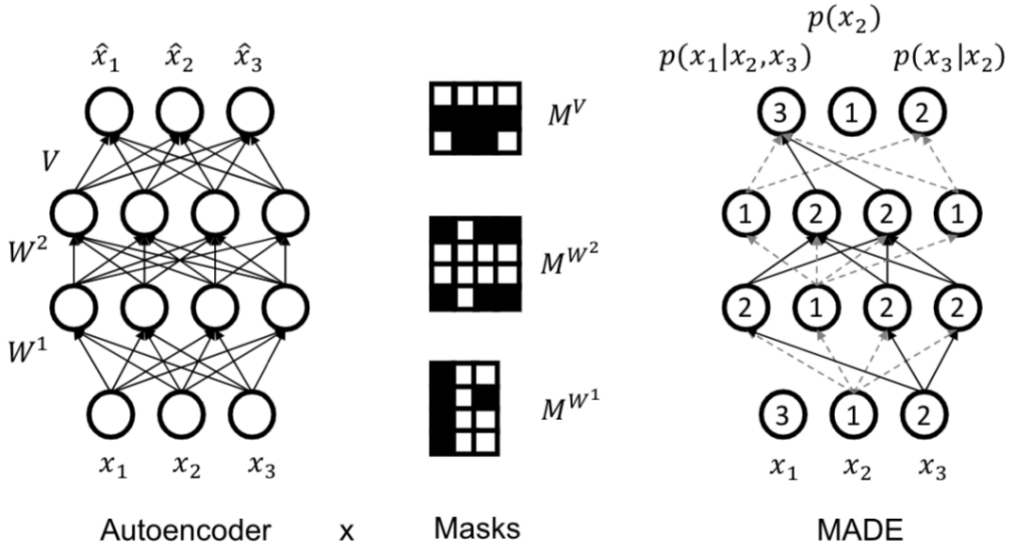


- FVSBN and NADE look similar to an autoencoder.
- Encoder $e(\cdot)$. E.g., $e(x) = \sigma(W^2(W^1 x + b^1) + b^2)$.
- Decoder such that $d(e(x)) \approx x$. E.g., $d(h) = \sigma(Vh + c)$.
- Autoencoder can be trained by minimizing some loss function, e.g., cross-entropy/mean square error.
- In practice, e and d are often constrained so that we don't learn identity mappings. Hopefully, $e(x)$ would be a meaningful, compressed representation of x.
- Note that a vanilla autoencoder is not a generative model



Autoencoder

- Can we get a generative model from an autoencoder?
- We need to make sure it corresponds to an autoregressive architecture, which requires a pre-specified order, say $x_1, x_2, \ldots, x_n$, then $\hat{x}_i$ can only depend on $x_{<i}$, $\forall i$.
- Benefit: we can use a single neural network to produce all the parameters, In contrast, NADE requires n passes. Much more efficient on modern hardware.



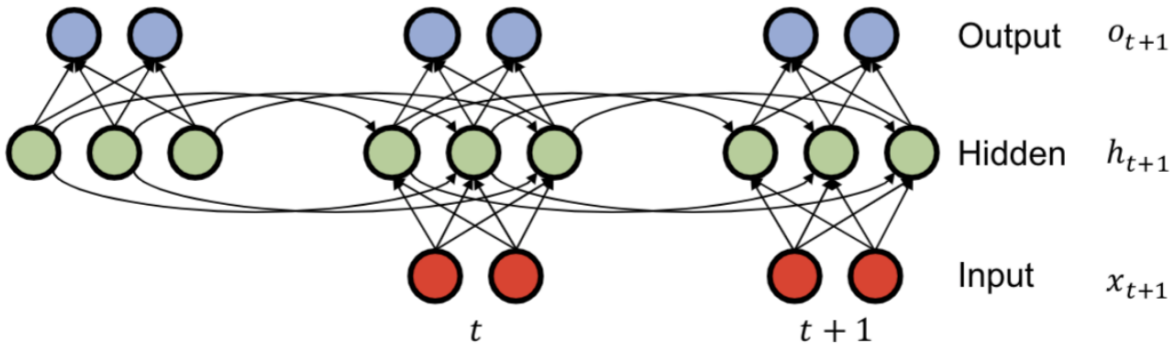
- Challenge: An autoencoder that is autoregressive.
- Solution: use mask to disallow certain paths (Germain et al., 2015).

$$h^\ell(x) = \sigma((W^\ell \odot M^{W^\ell})h^{\ell-1}(x) + b^\ell), \quad \ell = 1, \ldots, L$$

where the masks satisfies

$$M^{W^\ell}_{k',k} = \mathbf{1}_{m^\ell(k') \geq m^{\ell-1}(k)}, \; 1 \leq \ell \leq L, \quad M^V_{d,k} = \mathbf{1}_{d > m^L(k)}.$$

- Challenge: In autoregressive models, the history $x_{1:t-1}$ in conditional distributions $p(x_t|x_{<t};\alpha^t)$ keeps getting longer.
- Idea: keep a summary and recursively update it

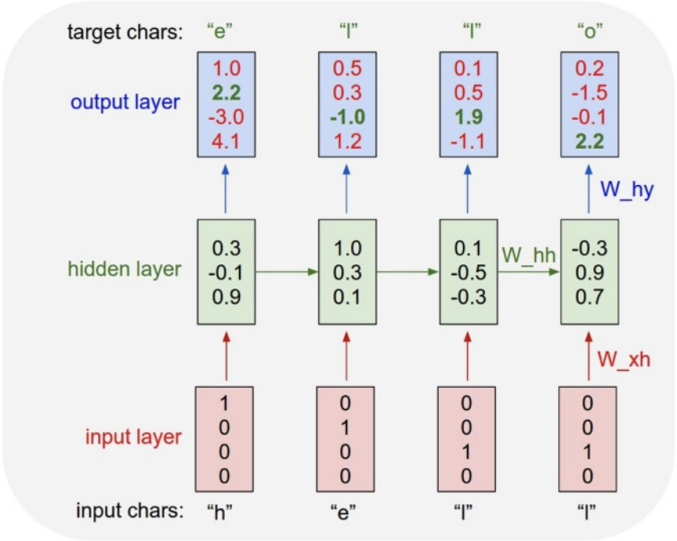


$$\text{update rule: } h_{t+1} = \tanh(W_{hh}h_t + W_{xh}x_{t+1})$$

$$\text{output: } o_{t+1} = W_{hy}h_{t+1}$$

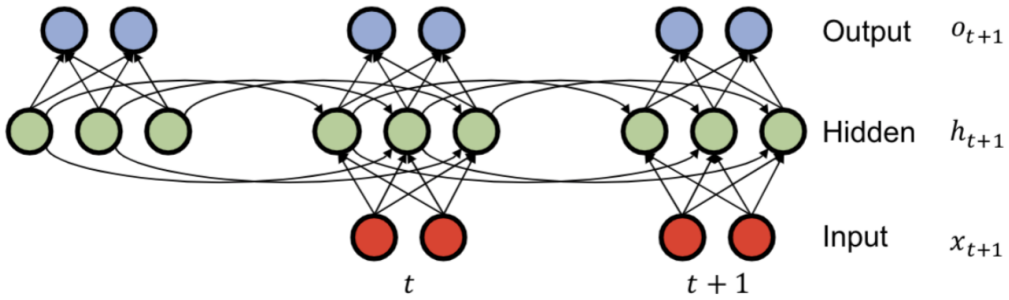
$$\text{initialization: } h_0 = b_0$$

- h_t is a summary of the inputs seen till time t
- o_{t-1} specifies parameters for conditional $p(x_t|x_{<t})$
- Parameterized by b_0, and matrices W_{hh}, W_{xh}, W_{hy}. Constant number of parameters w.r.t. n.



- Suppose $x_i \in \{h, e, l, o\}$. Use one-hot encoding (e.g., h encoded as $[1, 0, 0, 0]$, e encoded as $[0, 1, 0, 0]$.
- Autoregressive modeling: $p(x = hello) = p(x_1 = h)p(x_2 = e|x_1 = h) \cdots p(x_5 = o|x_1 = h, x_2 = e, x_3 = l, x_4 = l)$
- For example:

$$p(x_2 = e|x_1 = h) = \text{softmax}(o_1) = \frac{\exp(2.2)}{\exp(1.0) + \cdots + \exp(4.0)}$$



Pros:

- Can be applied to sequences of arbitrary length.
- Very general: for every computable function, there exists a finite RNN that can compute it.

Cons:

- Still requires an ordering
- Sequential likelihood evaluation (very slow for training)
- Sequential generation (unavoidable in an autoregressive model)
- Can be difficult to train (vanishing/exploding gradients)

Examples: Character RNN

Train 3-layer RNN with 512 hidden nodes on all the works of Shakespeare. Then sample from the model:

> KING LEAR: O, if you were a feeble sight, the courtesy of your law,
> Your sight and several breath, will wear the gods
> With his heads, and my hands are wonder'd at the deeds,
> So drop upon your lordship's head, and your opinion
> Shall be against your honour.

Remark: generation happens character by character. Needs to learn valid words, grammar, punctuation, etc.

Train on Wikipedia. Then sample from the model:

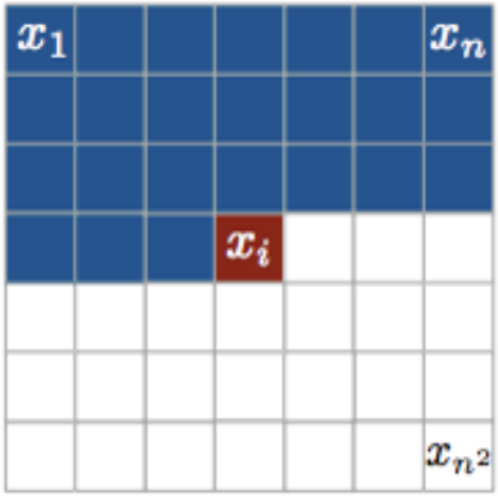
> Naturalism and decision for the majority of Arab countries' capitalide was grounded by the Irish language by [[John Clair]], [[An Imperial Japanese Revolt]], associated with Guangzham's sovereignty. His generals were the powerful ruler of the Portugal in the [[Protestant Immineners]], which could be said to be directly in Cantonese Communication, which followed a ceremony and set inspired prison, training. The emperor travelled back to [[Antioch, Perth, October 25—21]] to note, the Kingdom of Costa Rica, unsuccessful fashioned the [[Thrales]], [[Cynth's Dajoard]], known in western [[Scotland]], near Italy to the conquest of India with the conflict.

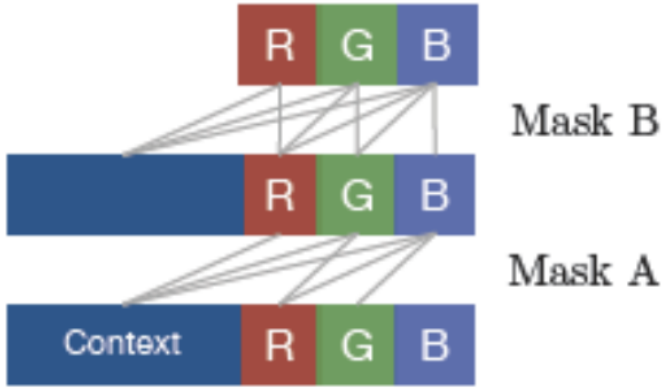
Remark: correct Markdown syntax. Opening and closing of brackets [[·]]

Examples: Character RNN

Train on data set of baby names. Then sample from the model:

Rudi Levette Berice Lussa Hany Mareanne Chrestina Carissy Marylen Hammine Janye Marlise Jacacrie Hendred Romand Charienna Nenotto Ette Dorane Wallen Marly Darine Salina Elvyn Ersia Maralena Minoria Ellia Charmin Antley Nerille Chelon Walmor Evena Jeryly Stachon Charisa Allisa Anatha Cathanie Geetra Alexie Jerin Cassen Herbett Cossie Velen Daurenge Robester Shermond Terisa Licia Roselen Ferine Jayn Lusine Charyanne Sales Sanny Resa Wallon Martine Merus Jelen Candica Wallin Tel Rachene Tarine Ozila Ketia Shanne Arnande Karella Roselina Alessia Chasty Deland Berther Geamar Jackein Mellisand Sagdy Nenc Lessie Rasemy Guen Gavi Milea Anneda Margoris Janin Rodelin Zeanna Elyne Janah Ferzina Susta Pey Castina



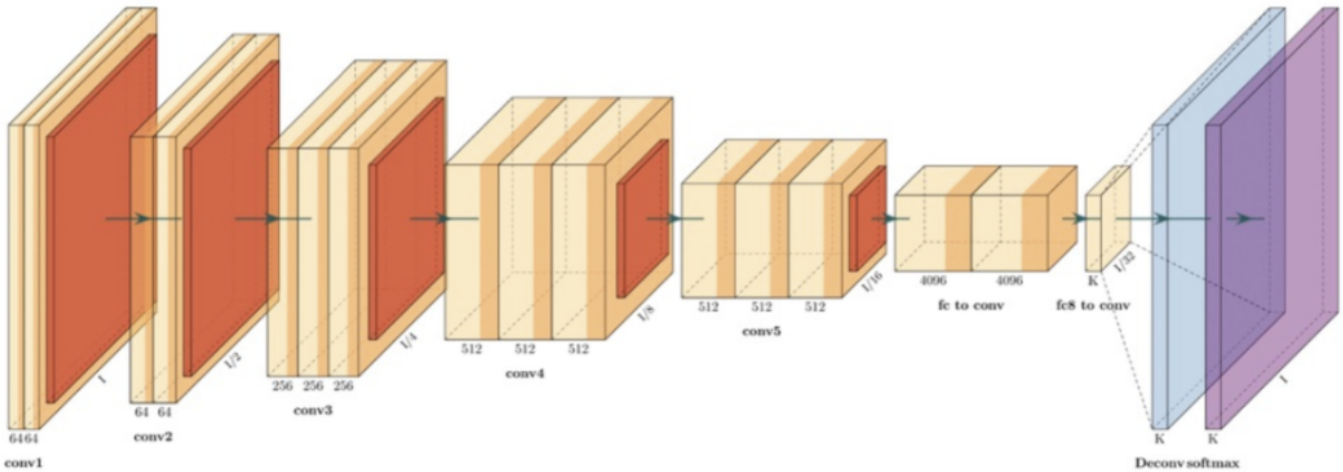


- Model images pixel by pixel using raster scan order
- Each pixel conditional $p(x_t|x_{1:t-1})$ needs to specify 3 colors

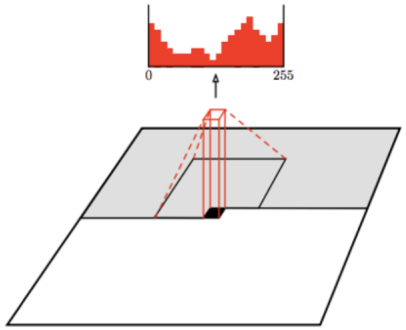
$$p(x_t|x_{1:t-1}) = p(x_t^{\text{red}}|x_{1:t-1})p(x_t^{\text{green}}|x_{1:t-1}, x_t^{\text{red}})p(x_t^{\text{blue}}|x_{1:t-1}, x_t^{\text{red}}, x_t^{\text{green}})$$

- Conditionals modeled using RNN variants. LSTM + Masking (like MADE)

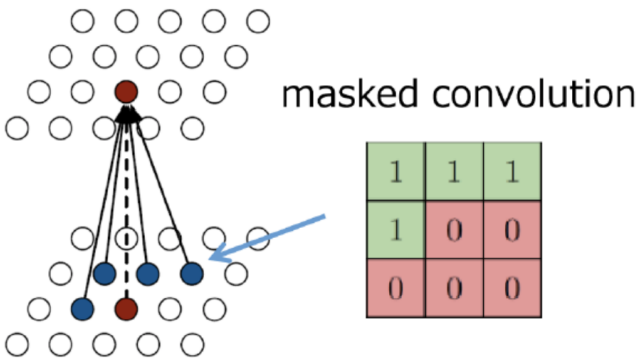
Results on downsampled ImageNet. Very slow: sequential likelihood evaluation.

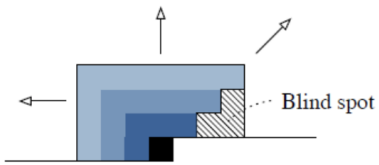


Convolutions are natural for image data and easy to parallelize on modern hardware.

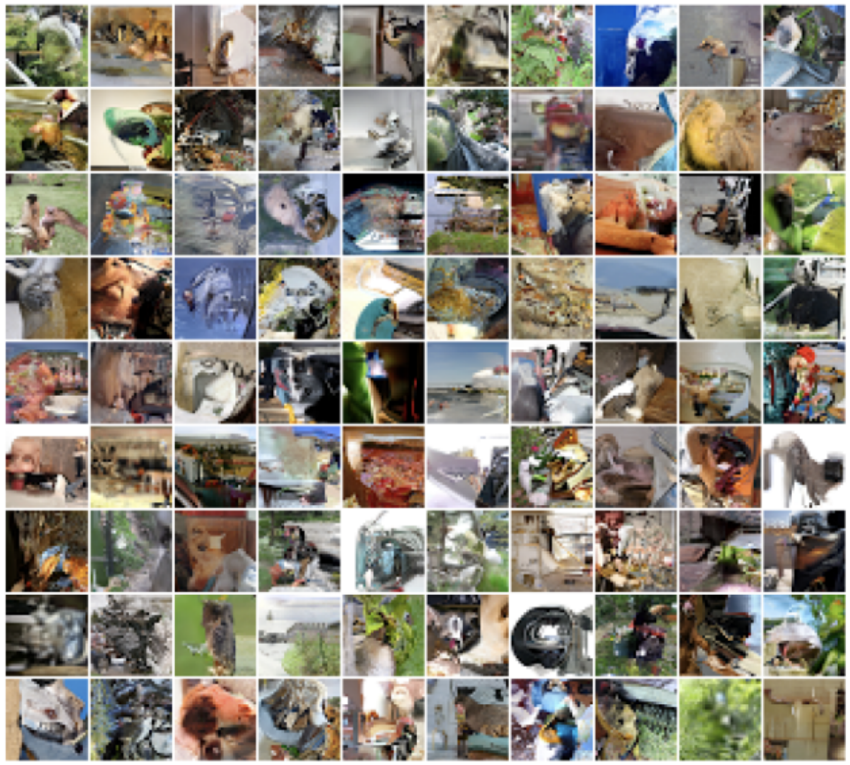


Idea: use convolutional architecture to predict next pixel given context (a neighborhood of pixels)
Challenge: Has to be autoregressive. Masked convolutions preserve raster scan order. Additional masking for colors order.



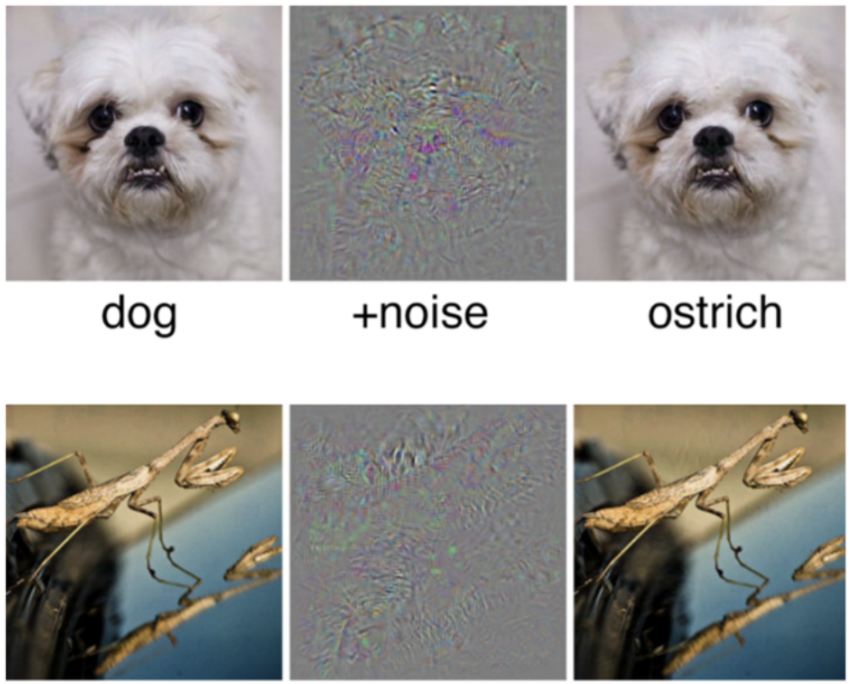


Examples: Pixel CNN

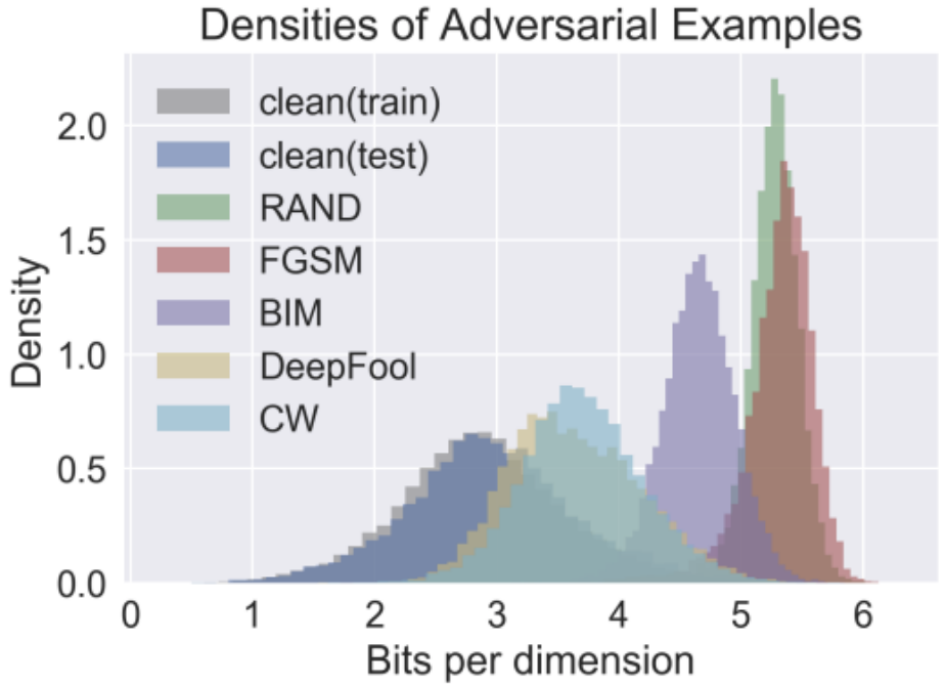


Samples from the PixelCNN model trained on Imagenet (32×32 pixels). Similar performance to PixelRNN, but much faster.

Machine learning methods are vulnerable to adversarial examples

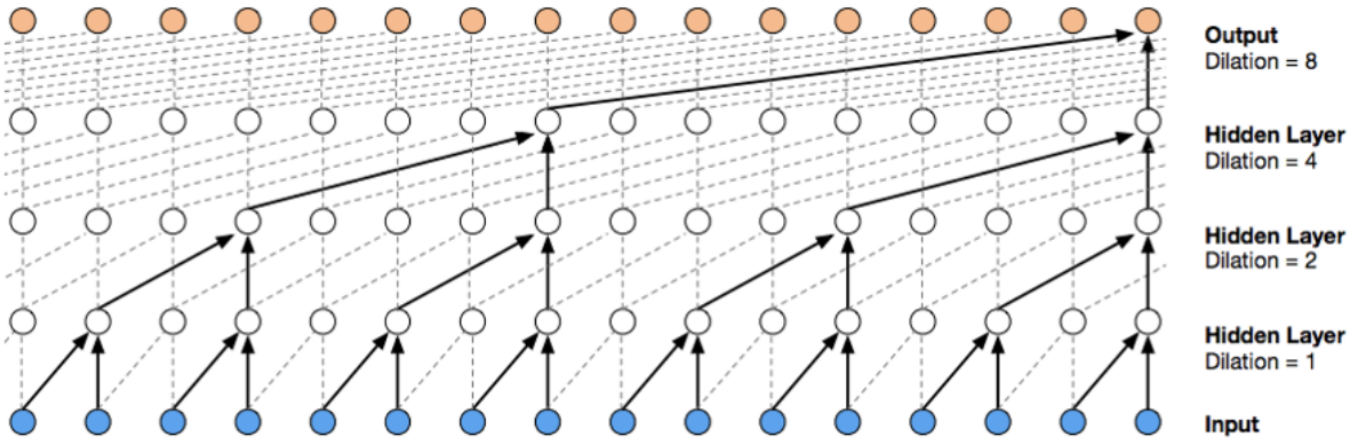


Can we detect them?



- Train a generative model $p(x)$ on clean inputs (PixelCNN)
- Given a new input $\bar{x}$, evaluate $p(\bar{x})$
- Adversarial examples are significantly less likely under $p(x)$

State of the art model for speech:



Dilated convolutions increases the receptive field: kernel only touches the signal at every 2^d entries.

Summary of Autoregressive Models

- Easy to sample from via sequential sampling

$$x_0 \sim p(x_0),\ x_1 \sim p(x_1|x_0),\ \ldots,\ x_n \sim p(x_n|x_{<n})$$

- Easy to compute probability $p(x)$

$$p(x) = p(x_0)p(x_1|x_0)\cdots p(x_n|x_{<n})$$

  Ideally, these conditional distributions can be computed in parallel for fast training

- Easy to extend to continuous variables. For example, $p(x_t|x_{<t}) = \mathcal{N}(\mu_\theta(x_{<t}), \Sigma_\theta(x_{<t})))$ or mixture of logistics
- No natural way to get features, cluster points, do unsupervised learning
- Next, we will discuss learning methods for autoregressive models

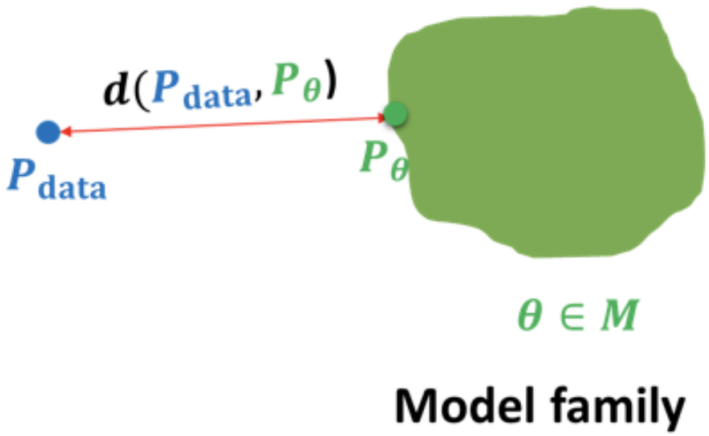
- Assume that the domain is governed by some underlying distribution p_{data}.
- We are given a dataset $\mathcal{D}$ of m samples from p_{data}. Each sample is an assignment of values to the variables, e.g., $X_{\text{bank}} = 1, X_{\text{dollar}} = 0, \ldots, Y = 1$ or pixel intensities.
- The standard assumption is that the data instances are independent and identically distributed (IID)
- We are also given a family of models $\mathcal{M}$, and our task is to learn some "good" model $\hat{\mathcal{M}} \in \mathcal{M}$ that defines a distribution $p_{\hat{\mathcal{M}}}$. For example
  - All Bayes nets with a given graph structure, for all possible choices of the CPD tables
  - A FVSBN for all possible choice of the logistic regression parameters. $\mathcal{M} = \{p_\theta; \theta \in \Theta\}$, where θ is the concatenation of all logistic regression coefficients.

Goal of Learning

- The goal of learning is to return a model $\hat{\mathcal{M}}$ that precisely captures the distribution p_{data} from which our data was sampled
- This is in general not achievable because of
  - limited data only provides a rough approximation of the true underlying distribution
  - can not handle too complicated models due to computational reasons
- Binary MNIST Example: The number of possible states is $2^{784} \approx 10^{236}$. Even 10^7 training examples provide extremely sparse coverage!
- We want to select $\hat{\mathcal{M}}$ to provide the "best" approximation to the underlying distribution p_{data}
- So, what is the "best"?

- If our goal is to learn the full distribution so that later we can answer any probabilistic inference query, we can view the learning problem as density estimation.
- Therefore, we want to construct p_θ as "close" as possible to p_{data} (where we assume the dataset $\mathcal{D}$ come from)

$x_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



- How do we measure "closeness"?

- One possibility is to use KL-divergence

$$\begin{aligned}\mathrm{KL}(p_{\text{data}}\|p_\theta) &= \mathbb{E}_{x\sim p_{\text{data}}}\left(\log\frac{p_{\text{data}}(x)}{p_\theta(x)}\right)\\ &= \sum_x p_{\text{data}}(x)\log\frac{p_{\text{data}}(x)}{p_\theta(x)}\end{aligned}$$

- Minimizing KL divergence is equivalent to maximizing the expected log-likelihood

$$\arg\min_{p_\theta}\mathrm{KL}(p_{\text{data}}\|p_\theta) = \arg\max_{p_\theta}\mathbb{E}_{x\sim p_{\text{data}}}\log p_\theta(x)$$

  - Ask that p_θ assign high probability to instances sampled from p_{data} so as to reflect the true distribution
  - Heavily penalize samples x where $p_\theta(x)\approx 0$

- Remark: we do not know how close we are to the data distribution since we do not know p_{data}

- Log-likelihood of an autoregressive model

$$\ell(\theta) = \log p(\theta, \mathcal{D}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \text{pa}(x_i)^{(j)}; \theta_i)$$

- This is an empirical version of $\mathbb{E}_{x \sim p_{\text{data}}} \log p_\theta(x)$. Its negative value can be taken as an Empirical Risk
- Can be trained via gradient ascent

$$\theta^{t+1} = \theta^{(t)} + \alpha_t \nabla_\theta \ell(\theta^t)$$

- When the data size m is large, we can use stochastic gradient ascent

$$\nabla_\theta \ell(\theta) \approx m \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \text{pa}(x_i)^{(j)}; \theta_i), \quad x^{(j)} \sim \mathcal{D}$$

- Empirical risk minimization can easily overfit the data. One extreme case is that the model just memorizes all the training data.
- In practice, people usually care more about generalization: how the model performs on samples that have not yet been seen.
- Thus, we typically restrict the hypothesis space of distributions that we search over, which involves a Bias-Variance trade off
  - Limited hypothesis space might not be able to represent p_{data}, leading to large bias
  - Highly expressive hypothesis space learns too much from the dataset $\mathcal{D}$ (together with random noises), and small perturbations on $\mathcal{D}$ can result in very different estimates, i.e., large variance

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