Autoregressive Models

Volodymyr Kuleshov

Cornell Tech

Lecture 3

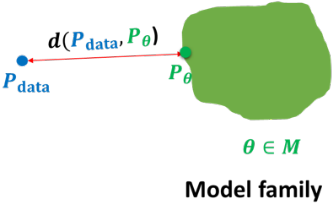
Announcements

- Assignment 1 will be released tonight on Gradescope
- It will be due in two weeks.
- Slides have been posted to Canvas (under Files).

The Task of Generative Modeling

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

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



Our Goal: define a probability distribution $p(x)$ over images x such that

- **Generation:** If we sample $x_{new} \sim p(x)$, x_{new} should look like a dog.
- **Representation Learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc.
- **Density Estimation:** $p(x)$ should be high if x looks like a dog, and low otherwise (*anomaly detection*)

Step 1: How to represent $p(x)$ (today). Step 2: how to learn it (next lecture).

Recap: Bayesian Networks vs Neural Models

Last class, we say three ways of defining a model $p(x)$:

- Using the Chain Rule

$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2)p(x_4 \mid x_1, x_2, x_3)$$

  Pros: no modeling assumptions on p. Cons: # parameters exponential in n.

- As a Bayes Net:

$$p(x_1, x_2, x_3, x_4) \approx p_{\mathrm{CPT}}(x_1)p_{\mathrm{CPT}}(x_2 \mid x_1)p_{\mathrm{CPT}}(x_3 \mid \cancel{x_1}, x_2)p_{\mathrm{CPT}}(x_4 \mid x_1, \cancel{x_2, x_3})$$

  Makes conditional independence assumptions. Uses tabular representations via conditional probability tables (CPT) to define each factor. Compact.

- Via Parametric Neural Models

$$p(x_1, x_2, x_3, x_4) \approx p(x_1)p(x_2 \mid x_1)p_{\mathrm{Neural}}(x_3 \mid x_1, x_2)p_{\mathrm{Neural}}(x_4 \mid x_1, x_2, x_3)$$

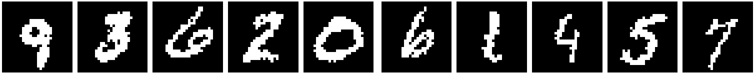
  Assumes specific parametric form for the conditionals (like in logistic regression). A sufficiently deep neural net can approximate any function.

Lecture Outline

1. **Basic Autoregressive Models**
    - Sigmoid Belief Networks: Models Based on Logistic Regression
    - NADE: From Logistic Regression to Multi-Layer Perceptrons
    - Autoregressive Models Are Masked Autoencoders
2. Recurrent Neural Networks as Autoregressive Models
3. Modern Autoregressive Models
    - PixelRNN and PixelCNN
    - WaveNet

Running Example: A Generative Model for MNIST

Suppose we are given 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).
- **Our Goal:** Learn a probability distribution $p(x) = p(x_1, \cdots, x_{784})$ over $x \in \{0, 1\}^{784}$ such that when $x \sim p(x)$, x looks like a digit
- Two step process:
  1. Parameterize a model family $\{p_\theta(x), \theta \in \Theta\}$ [This lecture]
  2. Search for model parameters θ based on training data $\mathcal{D}$ [Next lecture]

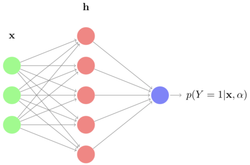
Recall: Neural Models for Classification

Consider binary classification of $Y \in \{0, 1\}$ from input features $X \in \{0, 1\}^n$.

- Discriminative models parameterize $p(Y \mid \mathbf{x})$, and assume that

$$p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = f(\mathbf{x}, \boldsymbol{\alpha})$$

- **Logistic regression**: let $z(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i$.
  $p_{\mathrm{logit}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = \sigma(z(\boldsymbol{\alpha}, \mathbf{x}))$, where $\sigma(z) = 1/(1 + e^{-z})$
- **Multi-Layer Perceptron**: Let $\mathbf{h}(A, \mathbf{b}, \mathbf{x})$ be a non-linear transformation of the input features. $p_{\mathrm{MLP}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}, A, \mathbf{b}) = \sigma(\alpha_0 + \sum_{i=1}^{h} \alpha_i \mathbf{h}_i)$
  - Increased flexibility
  - Increased # of parameters: $A, \mathbf{b}, \boldsymbol{\alpha}$



An Autoregressive Model From Logistic Regression

Let's define our first model. First, pick an ordering of the variables, e.g., a raster scan ordering of pixels from top-left (X_1) to bottom-right ($X_{n=784}$)

- Without loss of generality, we can use chain rule for factorization

$$p(x_1, \cdots, x_{784}) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2) \cdots p(x_n \mid x_1, \cdots, x_{n-1})$$

- Some conditionals are too complex to be stored in tabular form. Instead, we parameterize the conditionals using **logistic regression**:

$$p(x_1, \cdots, x_{784}) = p_{\mathrm{CPT}}(x_1; \alpha^1) p_{\mathrm{logit}}(x_2 \mid x_1; \boldsymbol{\alpha}^2) p_{\mathrm{logit}}(x_3 \mid x_1, x_2; \boldsymbol{\alpha}^3) \cdots \\ p_{\mathrm{logit}}(x_n \mid x_1, \cdots, x_{n-1}; \boldsymbol{\alpha}^n)$$

- More explicitly:
  - $p_{\mathrm{CPT}}(X_1 = 1; \alpha^1) = \alpha^1$, $p(X_1 = 0) = 1 - \alpha^1$
  - $p_{\mathrm{logit}}(X_2 = 1 \mid x_1; \boldsymbol{\alpha}^2) = \sigma(\boldsymbol{\alpha}_0^2 + \boldsymbol{\alpha}_1^2 x_1)$
  - $p_{\mathrm{logit}}(X_3 = 1 \mid x_1, x_2; \boldsymbol{\alpha}^3) = \sigma(\boldsymbol{\alpha}_0^3 + \boldsymbol{\alpha}_1^3 x_1 + \boldsymbol{\alpha}_2^3 x_2)$
- We have made a **modeling assumption**. We are using parameterized functions (e.g., logistic regression above) to predict next pixel given all the previous ones. Example of **autoregressive** model.

An Autoregressive Model From Logistic Regression

- Note that in our model

  $$p(x_1, \cdots, x_{784}) = p_{\mathrm{CPT}}(x_1; \alpha^1) p_{\mathrm{logit}}(x_2 \mid x_1); \boldsymbol{\alpha} \cdots p_{\mathrm{logit}}(x_n \mid x_1, \cdots, x_{n-1}; \boldsymbol{\alpha}^n)$$

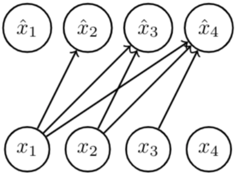
  each term $p_{\mathrm{logit}}(x_i \mid x_1, \cdots, x_{i-1}; \boldsymbol{\alpha}^i)$ is a conditional Bernoulli.
- We use $\hat{x}$ to denote the parameter of the Bernoulli:

  $$\hat{x}_i = p(X_i = 1 | x_1, \cdots, x_{i-1}; \boldsymbol{\alpha}^i) = p(X_i = 1 | x_{<i}; \boldsymbol{\alpha}^i) = \sigma(\alpha_0^i + \sum_{j=1}^{i-1} \alpha_j^i x_j)$$

- We may think of $\hat{x}_i$ as:
  - The probability that pixel i is on.
  - A prediction of the next pixel x_i given the previous pixels $x_{<i}$.
  - A reconstruction of x_i from partial input $x_{<i}$ (more on this later)

Fully Visible Sigmoid Belief Network (FVSBN)

The model we defined is called a Fully Visible Sigmoid Belief Network (FVSBN). Here is its computational graph:



FVSBN

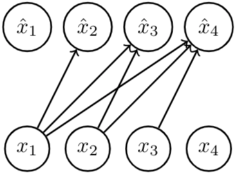
How do we use this model for the generative modeling tasks we defined earlier?

- How to evaluate $p(x_1, \cdots, x_{784})$? Multiply all the conditionals (factors)
  - First, we compute the parameters $\hat{x}_i$ of each Bernoulli distribution
  - Then we evaluate $p(x_1, \cdots, x_{784})$. In the above example:

$$p(X_1 = 0, X_2 = 1, X_3 = 1, X_4 = 0) = (1 - \hat{x}_1) \times \hat{x}_2 \times \hat{x}_3 \times (1 - \hat{x}_4)$$
$$= (1 - \hat{x}_1) \times \hat{x}_2(X_1 = 0) \times \hat{x}_3(X_1 = 0, X_2 = 1) \times (1 - \hat{x}_4(X_1 = 0, X_2 = 1, X_3 = 1))$$

Fully Visible Sigmoid Belief Network (FVSBN)

The model we defined is called a Fully Visible Sigmoid Belief Network (FVSBN). Here is its computational graph:

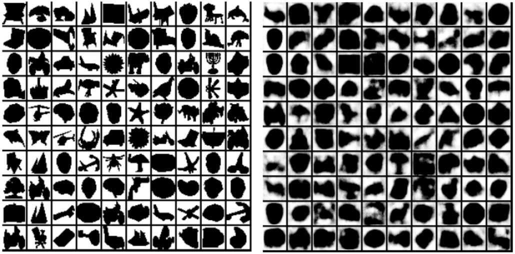


FVSBN

How do we use this model for the generative modeling tasks we defined earlier?

- How to sample from $p(x_1, \cdots, x_{784})$?
  1. Sample $\overline{x}_1 \sim p(x_1)$ (`np.random.choice([1,0],p=[`$\hat{x}_1, 1 - \hat{x}_1$`])`)
  2. Sample $\overline{x}_2 \sim p(x_2 \mid x_1 = \overline{x}_1) = \text{Ber}(\hat{x}_2)$
  3. Sample $\overline{x}_3 \sim p(x_3 \mid x_1 = \overline{x}_1, x_2 = \overline{x}_2) = \text{Ber}(\hat{x}_2) \cdots$
- How many parameters? $1 + 2 + 3 + \cdots + n \approx n^2/2$

FVSBN Results

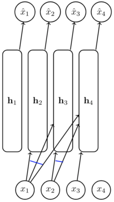


Training data on the left (*Caltech 101 Silhouettes*). Samples from the model on the right.

Figure from *Learning Deep Sigmoid Belief Networks with Data Augmentation, Gan et al. 2015*.

From Logistic Regression to Multi-Layer Perceptrons

We may improve our model by replacing logistic regression with a neural network with one hidden layer $\mathbf{h}_i$:



NADE

- We now compute $\hat{x}_i$ using a neural network:

$$\mathbf{h}_i = \sigma(A_i \mathbf{x}_{<i} + \mathbf{c}_i)$$

$$\hat{x}_i = p(x_i | x_1, \cdots, x_{i-1}; \underbrace{A_i, \mathbf{c}_i, \boldsymbol{\alpha}_i, b_i}_{\text{parameters}}) = \sigma(\boldsymbol{\alpha}_i \mathbf{h}_i + b_i)$$

- For example $\mathbf{h}_2 = \sigma\left(\underbrace{\begin{pmatrix} \vdots \end{pmatrix}}_{A_2} x_1 + \underbrace{\begin{pmatrix} \vdots \end{pmatrix}}_{c_2} \right)$ $\mathbf{h}_3 = \sigma\left(\underbrace{\begin{pmatrix} \vdots & \vdots \end{pmatrix}}_{A_3} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \underbrace{\begin{pmatrix} \vdots \end{pmatrix}}_{c_3} \right)$

From Logistic Regression to Multi-Layer Perceptrons

- We also want to tie weights to *reduce the number of parameters* and *speed up computation* (see blue dots in the figure):

$$\mathbf{h}_i = \sigma(W_{\cdot,<i}\mathbf{x}_{<i} + \mathbf{c})$$

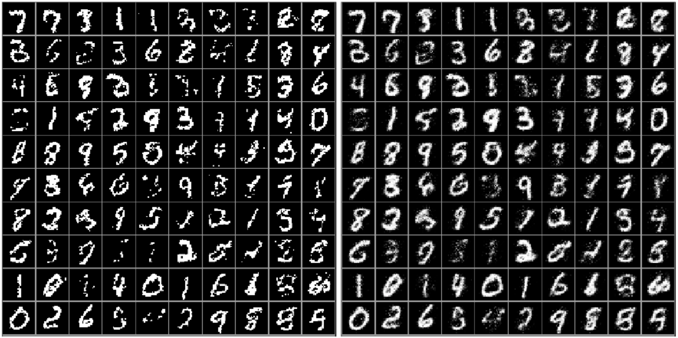
$$\hat{x}_i = p(x_i|x_1, \cdots, x_{i-1}) = \sigma(\boldsymbol{\alpha}_i\mathbf{h}_i + b_i)$$

- For example $\mathbf{h}_2 = \sigma\left(\underbrace{\begin{pmatrix} \vdots \\ w_1 \\ \vdots \end{pmatrix}}_{A_2} x_1\right)$ $\mathbf{h}_3 = \sigma\left(\underbrace{\begin{pmatrix} \vdots & \vdots \\ w_1 & w_2 \\ \vdots & \vdots \end{pmatrix}}_{A_3} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right)$ $\mathbf{h}_4 = \sigma\left(\underbrace{\begin{pmatrix} \vdots & \vdots & \vdots \\ w_1 & w_2 & w_3 \\ \vdots & \vdots & \vdots \end{pmatrix}}_{A_3} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}\right)$

- If $\mathbf{h}_i \in \mathbb{R}^d$, how many total parameters? Linear in n: weights $W \in \mathbb{R}^{d\times n}$, biases $c \in \mathbb{R}^d$, and n logistic regression coefficient vectors $\boldsymbol{\alpha}_i, b_i \in \mathbb{R}^{d+1}$. Probability is evaluated in $O(nd)$.

NADE: Neural Autoregressive Density Estimation

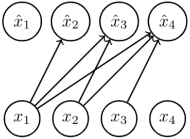
This yields a model called Neural Autoregressive Density Estimation (NADE).



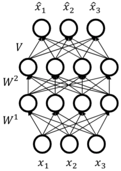
Samples on the left. Conditional probabilities $\hat{x}_i$ on the right.
Figure from *The Neural Autoregressive Distribution Estimator, 2011*.

Autoregressive Models vs. Autoencoders

On the surface, FVSBN and NADE look similar to an **autoencoder**:



FVSBN



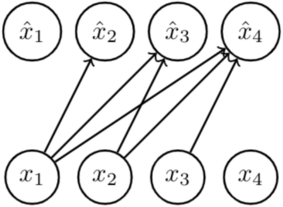
Autoencoder

An autoencoder consists of the following components:

- an **encoder** $e(\cdot)$. E.g., $e(x) = \sigma(W^2(W^1x + b^1) + b^2)$
- a **decoder** such that $d(e(x)) \approx x$. E.g., $d(h) = \sigma(Vh + c)$.
- Loss function, for example:
$$\min_{W^1,W^2,b^1,b^2,V,c} \sum_{x \in \mathcal{D}} \sum_i (x_i - \hat{x}_i)^2$$
- e and d are constrained so that we don't learn identity mappings. Hope that $e(x)$ is a meaningful, compressed representation of x (feature learning)
- A vanilla autoencoder is *not* a generative model: it does not define a distribution over x we can sample from to generate new data points.

Autoregressive Models vs. Autoencoders

An autoregressive model looks like an auto-encoder that predicts a shifted input.

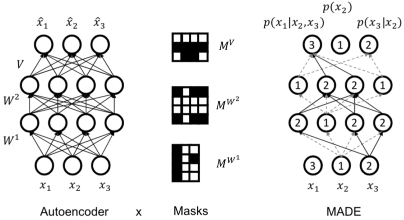


FVSBN

- In this figure, $\hat{x}_i$ is the prediction for x_i (the parameters of $p(x_i|x_{<i})$).
- Since $\hat{x}_i$ should only depend on its ancestors, it only gets edges from $x_{<i}$.
- As a result, the product of the $p(x_i|x_{<i})$ is a valid probability distribution.
- In practice, we can construct this computational graph by taking an auto-encoder and setting ("masking") some of its weights to zero (this deletes their edges in the graph).

MADE: Masked Autoencoder for Distribution Estimation

MADE is an algorithm for masking edges in an autoencoder.



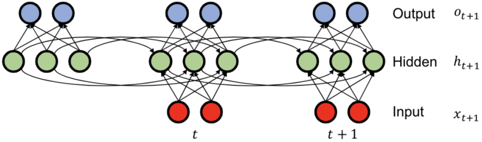
1. **Challenge**: An autoencoder that is autoregressive (DAG structure)
2. **Solution**: use masks to disallow certain paths (Germain et al., 2015). Suppose ordering is x_1, x_2, x_3.
    1. The unit producing the parameters for $p(x_1)$ is not allowed to depend on any input. Unit for $p(x_2|x_1)$ only on x_1. And so on...
    2. For each unit in a hidden layer, pick an integer i in $[1, n-1]$. That unit is allowed to depend only on the first i inputs. We mask or **zero-out the weights** to make this happen.
    3. Add mask to preserve this invariant: connect to all units in previous layer with smaller or equal assigned number (strictly $<$ in final layer)

Lecture Outline

1. Basic Autoregressive Models
   - Sigmoid Belief Networks: Models Based on Logistic Regression
   - NADE: From Logistic Regression to Multi-Layer Perceptrons
   - Autoregressive Models Are Masked Autoencoders
2. **Recurrent Neural Networks as Autoregressive Models**
3. Modern Autoregressive Models
   - PixelRNN and PixelCNN
   - WaveNet

RNN: Recurrent Neural Nets

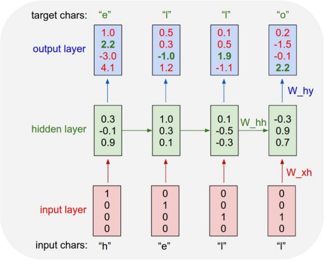
Challenge: model $p(x_t | x_{1:t-1}; \boldsymbol{\alpha}^t)$. "History" $x_{1:t-1}$ keeps getting longer.
Idea: keep a summary and recursively update it



$$
\begin{aligned}
\text{Summary update rule: } \quad h_{t+1} &= tanh(W_{hh} h_t + W_{xh} x_{t+1}) \\
\text{Prediction: } \quad o_{t+1} &= W_{hy} h_{t+1} \\
\text{Summary initalization: } \quad h_0 &= \boldsymbol{b}_0
\end{aligned}
$$

1. Hidden layer h_t is a summary of the inputs seen till time t
2. Output layer o_{t-1} specifies parameters for conditional $p(x_t \mid x_{1:t-1})$
3. Parameterized by $\boldsymbol{b}_0$ (initialization), and matrices W_{hh}, W_{xh}, W_{hy}. Constant number of parameters w.r.t n!

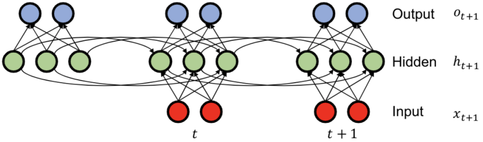
Example: Character RNN (from Andrej Karpathy)



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

$$\begin{aligned} p(x_2 = e|x_1 = h) &= softmax(o_1) = \frac{\exp(2.2)}{\exp(1.0) + \cdots + \exp(4.1)} \\ o_1 &= W_{hy} h_1 \\ h_1 &= tanh(W_{hh} h_0 + W_{xh} x_1) \end{aligned}$$

RNN: Recurrent Neural Nets



Pros:

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

Cons:

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

Example: Character RNN (from Andrej Karpathy)

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.

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

Example: Character RNN (from Andrej Karpathy)

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.

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

Example: Character RNN (from Andrej Karpathy)

Train on Wikipedia. Then sample from the model:

{ { cite journal — id=Cerling Nonforest Department—format=Newlymeslated—none } }
"www.e-complete".
"'See also"': [[List of ethical consent processing]]

== See also ==
*[[Iender dome of the ED]]
*[[Anti-autism]]

== External links==
* [http://www.biblegateway.nih.gov/entrepre/ Website of the World Festival. The labour of India-county defeats at the Ripper of California Road.]

Example: Character RNN (from Andrej Karpathy)

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

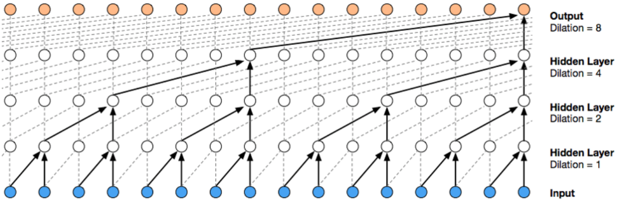
Rudi Levette Berice Lussa Hany Mareanne Chrestina Carissy Marylen Hammine Janye Marlise Jacacrie Hendred Romand Charienna Nenotto Ette Dorane Wallen Marly Darine Salina Elvyn Ersia Maralena Minoria Ellia Charmin Antley Nerille Chelon Walmor Evena Jeryly Stachon Charisa Allisa Anatha Cathanie Geetra Alexie 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

Lecture Outline

1. **Basic Autoregressive Models**
   - Sigmoid Belief Networks: Models Based on Logistic Regression
   - NADE: From Logistic Regression to Multi-Layer Perceptrons
   - Autoregressive Models Are Masked Autoencoders
2. Recurrent Neural Networks as Autoregressive Models
3. **Modern Autoregressive Models**
   - PixelRNN and PixelCNN
   - WaveNet

WaveNet (Oord et al., 2016)

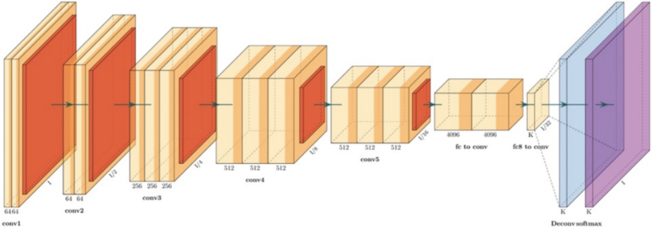
WaveNet is a sophisticated autoregressive generative model for raw audio.



- Its computational graph looks like a masked autoencoder—the output $\hat{x}$ (top) is a shifted version of the input x (bottom).
- The computational graph (black arrows) is sparse (not all nodes are connected to each other), and parameters are shared across the graph.
- It relies on a few technical ideas: causal convolutions and dilation.

Recall: Convolutional Neural Networks

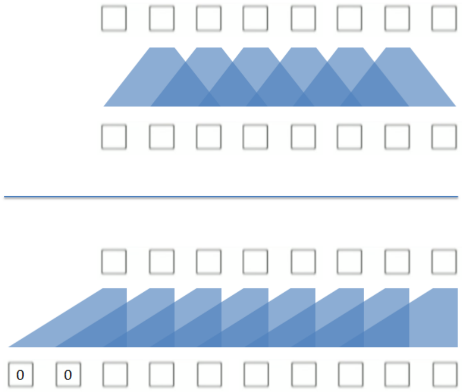
Convolutions are a translationally invariant operation commonly used in neural networks for image classification.



- WaveNet uses convolutions to parameterize a masked autoencoder mapping inputs x to model parameters $\hat{x}_i$.
- This means that the parameters to generate each $\hat{x}_i$ from $x_{<i}$ are the same for each i (i.e., all $p(x_i|x_{<i})$ have the same parameters).

Causal Convolutions

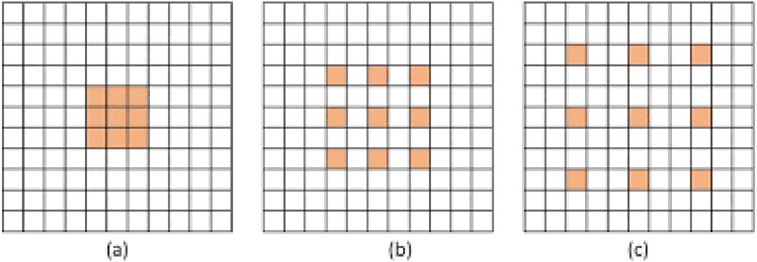
Regular 1D convolutions (top) have symmetrical receptive fields—this is a problem because x_{i+1} is part of the receptive field for predicting $\hat{x}_i$.



Causal convolutions (bottom) mask parts of the filter that touch the future

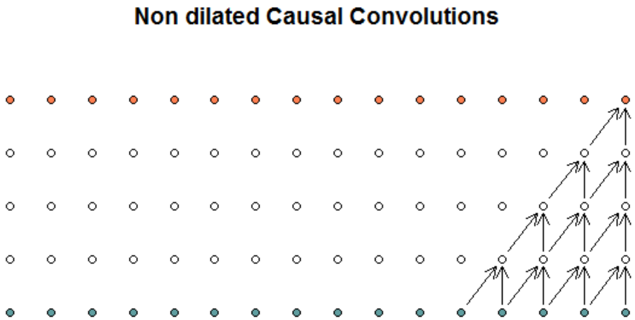
Dilated Convolutions

Dilated convolutions introduce "holes" into the convolution filters:



Dilated Convolutions

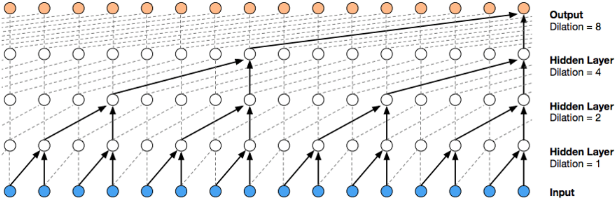
Normal convolutions in Wavenet would look like this:



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

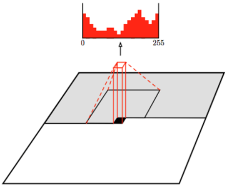
WaveNet (Oord et al., 2016)

State of the art model for speech:

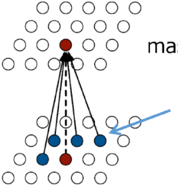


Dilated convolutions increase the receptive field: kernel only touches the signal at every 2^d entries.

PixelCNN (Oord et al., 2016)

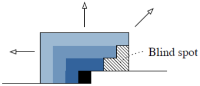


Idea: Use convolutional architecture to predict next pixel given context (a neighborhood of pixels).
Challenge: Has to be autoregressive. Masked convolutions preserve raster scan order. Additional masking for colors order.

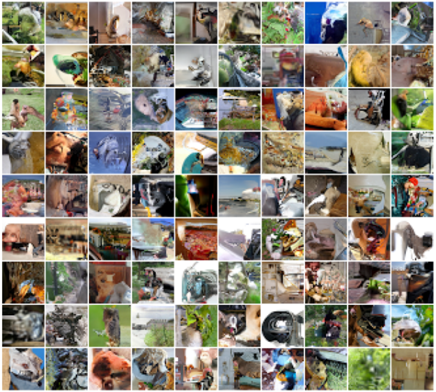


masked convolution

1	1	1
1	0	0
0	0	0



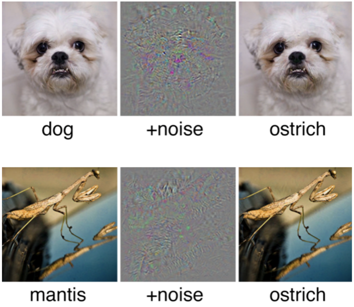
PixelCNN



Samples from the model trained on Imagenet (32×32 pixels).

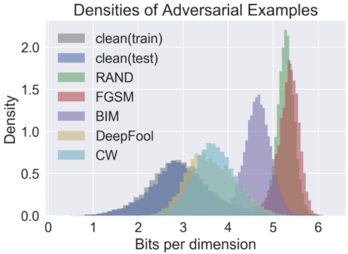
Application in Adversarial Attacks and Anomaly detection

Machine learning methods are vulnerable to adversarial examples



Can we detect them?

PixelDefend (Song et al., 2018)



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

Summary of Autoregressive Models

- Easy to sample from
  1. Sample $\overline{x}_0 \sim p(x_0)$
  2. Sample $\overline{x}_1 \sim p(x_1 \mid x_0 = \overline{x}_0)$
  3. $\cdots$
- Easy to compute probability $p(x = \overline{x})$
  1. Compute $p(x_0 = \overline{x}_0)$
  2. Compute $p(x_1 = \overline{x}_1 \mid x_0 = \overline{x}_0)$
  3. Multiply together (sum their logarithms)
  4. $\cdots$
  5. Ideally, can compute all these terms in parallel for fast training
- Easy to extend to continuous variables. For example, can choose Gaussian conditionals $p(x_t \mid x_{<t}) = \mathcal{N}(\mu_\theta(x_{<t}), \Sigma_\theta(x_{<t}))$ or mixture of logistics
- No natural way to get features, cluster points, do unsupervised learning
- Next: learning