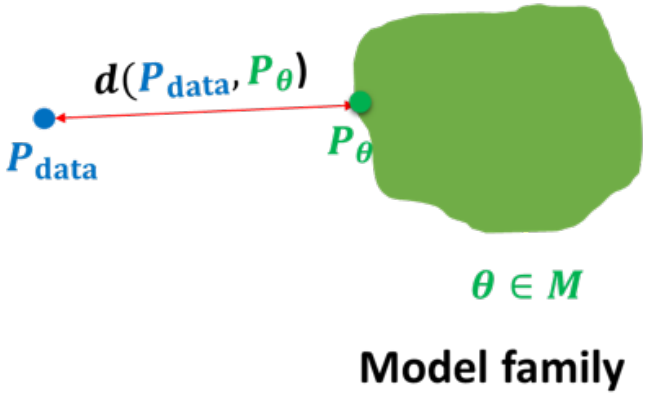
Learning a generative model

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

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



- We want to learn a probability distribution $p(x)$ over images x such that
  1. **Generation:** If we sample $x_{new} \sim p(x)$, x_{new} should look like a dog (*sampling*)
  2. **Density estimation:** $p(x)$ should be high if x looks like a dog, and low otherwise (*anomaly detection*)
  3. **Unsupervised representation learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc. (*features*)
- First question: how to represent $p(x)$. Second question: how to learn it.

Recap: Bayesian networks vs neural models

- Using Chain Rule

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

Fully General, no assumptions needed (exponential size, no free lunch)

- Bayes Net

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

Assumes conditional independencies; tabular representations via conditional probability tables (CPT)

- Neural Models

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

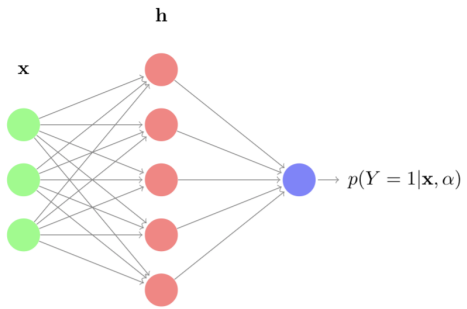
Assumes specific functional form for the conditionals. A sufficiently deep neural net can approximate any function.

Neural Models for classification

- Setting: binary classification of $Y \in \{0, 1\}$ given input features $X \in \{0, 1\}^n$
- For classification, we care about $p(Y \mid \mathbf{x})$, and assume that

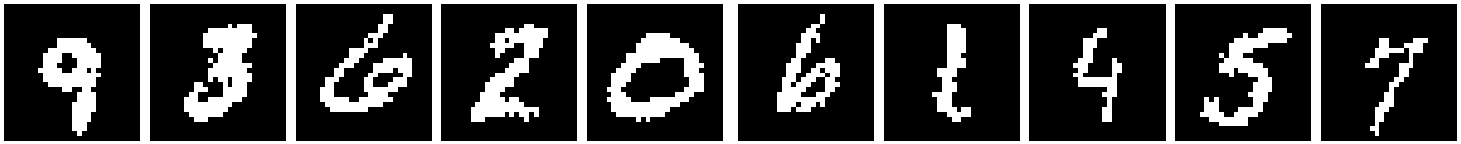
$$p(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = f(\mathbf{x}, \boldsymbol{\alpha})$$

- **Logistic regression**: let $z(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_0 + \sum_{i=1}^{n} \alpha_i x_i$.
  $p_{\text{logit}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}) = \sigma(z(\boldsymbol{\alpha}, \mathbf{x}))$, where $\sigma(z) = 1/(1 + e^{-z})$
- **Non-linear** dependence: let $\mathbf{h}(A, \mathbf{b}, \mathbf{x})$ be a non-linear transformation of the input features. $p_{\text{Neural}}(Y = 1 \mid \mathbf{x}; \boldsymbol{\alpha}, A, \mathbf{b}) = \sigma(\alpha_0 + \sum_{i=1}^{h} \alpha_i \mathbf{h}_i)$
  - More flexible
  - More parameters: $A, \mathbf{b}, \boldsymbol{\alpha}$
  - Repeat multiple times to get a multilayer perceptron (neural network)



Motivating Example: MNIST

- **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).
- **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]

Autoregressive Models

- We can pick an ordering of all the random variables, i.e., 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

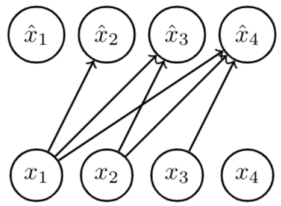
$$p(x_1, \cdots, x_{784}) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2) \cdots p(x_n \mid x_1, \cdots, x_{n-1})$$

- Some conditionals are too complex to be stored in tabular form. Instead, we **assume**

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

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

Fully Visible Sigmoid Belief Network (FVSBN)



FVSBN

- The conditional variables $X_i \mid X_1, \cdots, X_{i-1}$ are Bernoulli with parameters

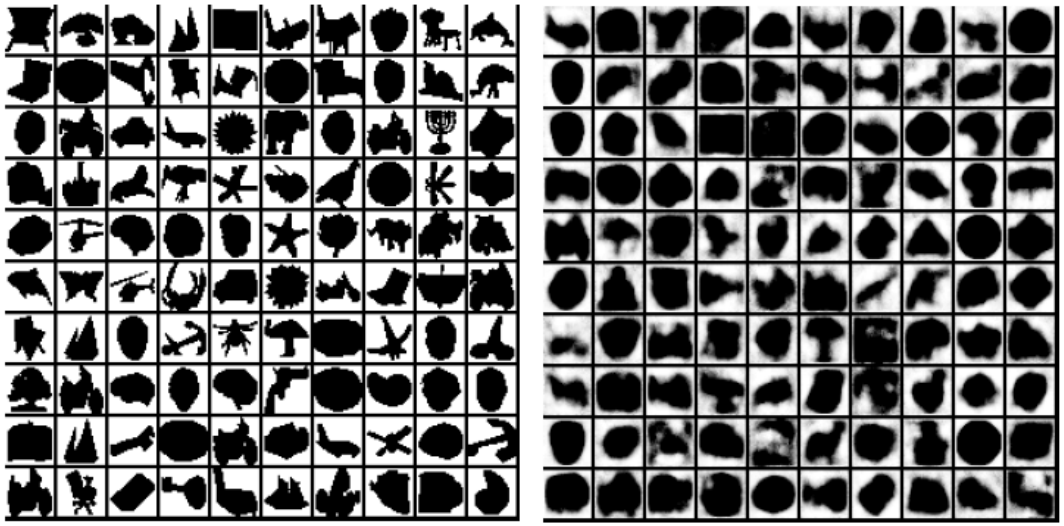
$$\hat{x}_i = p(X_i = 1 | x_1, \cdots, x_{i-1}; \boldsymbol{\alpha}^i) = p(X_i = 1 | x_{<i}; \boldsymbol{\alpha}^i) = \sigma(\alpha_0^i + \sum_{j=1}^{i-1} \alpha_j^i x_j)$$

- How to evaluate $p(x_1, \cdots, x_{784})$? Multiply all the conditionals (factors)
  - In the above example:

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

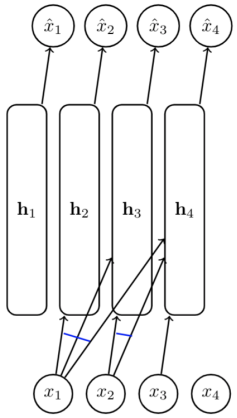
- How to sample from $p(x_1, \cdots, x_{784})$?
  1. Sample $\overline{x}_1 \sim p(x_1)$ (`np.random.choice([1,0],p=`$[\hat{x}_1, 1 - \hat{x}_1]$`)`)
  2. Sample $\overline{x}_2 \sim p(x_2 \mid x_1 = \overline{x}_1)$
  3. Sample $\overline{x}_3 \sim p(x_3 \mid x_1 = \overline{x}_1, x_2 = \overline{x}_2)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

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, 2015*.

NADE: Neural Autoregressive Density Estimation



NADE

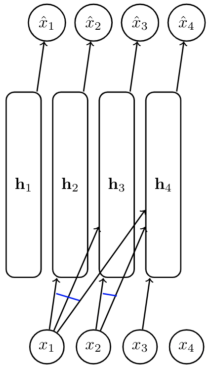
- To improve model: use one layer neural network instead of logistic regression

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

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

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

NADE: Neural Autoregressive Density Estimation



NADE

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

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

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

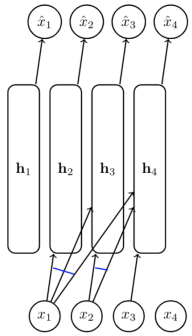
- For example $\mathbf{h}_2 = \sigma\left(\underbrace{\begin{pmatrix} \vdots \\ w_1 \\ \vdots \end{pmatrix}}_{W_{\cdot,<2}} x_1 + \mathbf{c}\right)$ $\mathbf{h}_3 = \sigma\left(\underbrace{\begin{pmatrix} \vdots & \vdots \\ w_1 & w_2 \\ \vdots & \vdots \end{pmatrix}}_{W_{\cdot,<3}} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right)$ $\mathbf{h}_4 = \sigma\left(\underbrace{\begin{pmatrix} \vdots & \vdots & \vdots \\ w_1 & w_2 & w_3 \\ \vdots & \vdots & \vdots \end{pmatrix}}_{W_{\cdot,<4}} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}\right)$

- 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 results

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

General discrete distributions



NADE

How to model non-binary discrete random variables $X_i \in \{1, \cdots, K\}$? E.g., pixel intensities varying from 0 to 255

One solution: Let $\hat{\boldsymbol{x}}_i$ parameterize a categorical distribution

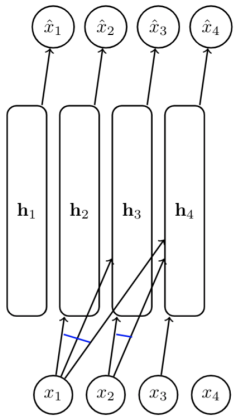
$$\mathbf{h}_i = \sigma(W_{\cdot,<i}\mathbf{x}_{<i} + \mathbf{c})$$
$$p(x_i|x_1, \cdots, x_{i-1}) = Cat(p_i^1, \cdots, p_i^K)$$
$$\hat{\boldsymbol{x}}_i = (p_i^1, \cdots, p_i^K) = softmax(A_i\mathbf{h}_i + \mathbf{b}_i)$$

Softmax generalizes the sigmoid/logistic function $\sigma(\cdot)$ and transforms a vector of K numbers into a vector of K *probabilities* (non-negative, sum to 1).

$$softmax(\mathbf{a}) = softmax(a^1, \cdots, a^K) = \left(\frac{\exp(a^1)}{\sum_i \exp(a^i)}, \cdots, \frac{\exp(a^K)}{\sum_i \exp(a^i)}\right)$$

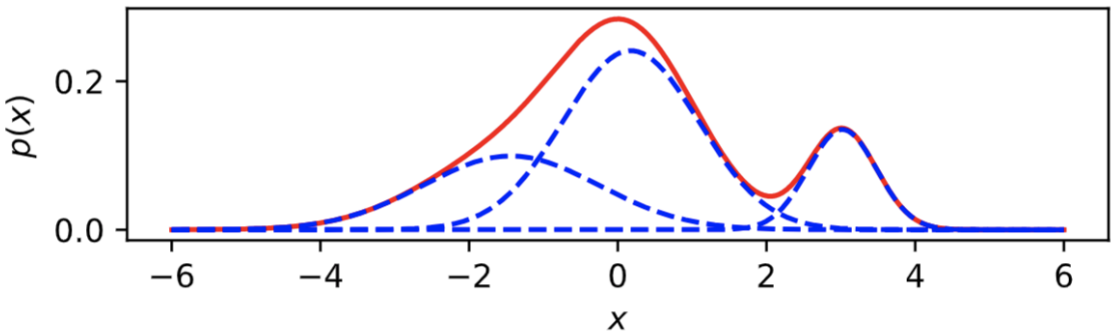
In numpy: `np.exp(a)/np.sum(np.exp(a))`

RNADE

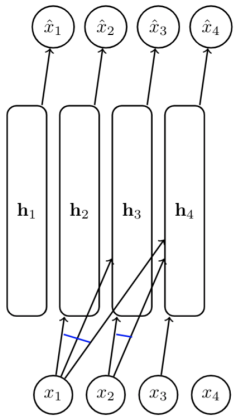


NADE

How to model continuous random variables $X_i \in \mathbb{R}$? E.g., speech signals
Solution: let $\hat{\boldsymbol{x}}_i$ parameterize a continuous distribution
E.g., uniform mixture of K Gaussians



RNADE



NADE

How to model continuous random variables $X_i \in \mathbb{R}$? E.g., speech signals
Solution: let $\hat{\boldsymbol{x}}_i$ parameterize a continuous distribution
E.g., In a mixture of K Gaussians,

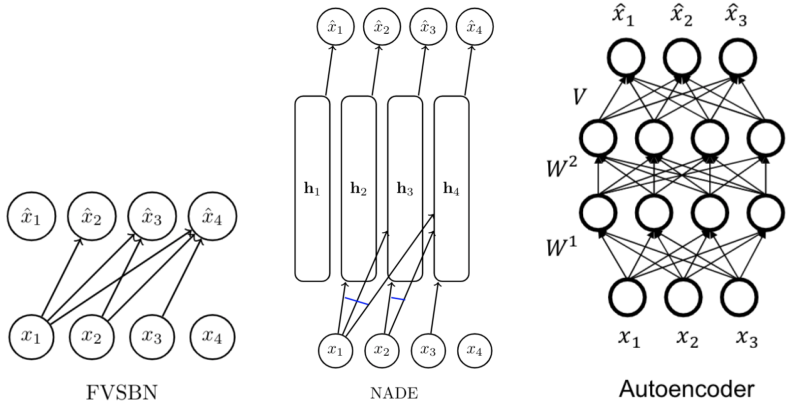
$$p(x_i|x_1, \cdots, x_{i-1}) = \sum_{j=1}^{K} \frac{1}{K} \mathcal{N}(x_i; \mu_i^j, \sigma_i^j)$$

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

$$\hat{\boldsymbol{x}}_i = (\mu_i^1, \cdots, \mu_i^K, \sigma_i^1, \cdots, \sigma_i^K) = f(\mathbf{h}_i)$$

$\hat{\boldsymbol{x}}_i$ defines the mean and standard deviation of each of the K Gaussians (μ_i^j, σ_i^j).
Can use exponential $\exp(\cdot)$ to ensure non-negativity

Autoregressive models vs. autoencoders



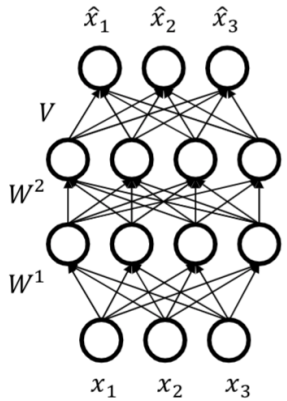
- On the surface, FVSBN and NADE look similar to an **autoencoder**:
- an **encoder** $e(\cdot)$. E.g., $e(x) = \sigma(W^2(W^1 x + b^1) + b^2)$
- a **decoder** such that $d(e(x)) \approx x$. E.g., $d(h) = \sigma(Vh + c)$.
- Loss function for dataset $\mathcal{D}$

$$\text{Binary r.v.:} \quad \min_{W^1, W^2, b^1, b^2, V, c} \sum_{x \in \mathcal{D}} \sum_i -x_i \log \hat{x}_i - (1 - x_i) \log(1 - \hat{x}_i)$$

$$\text{Continuous r.v.:} \quad \min_{W^1, W^2, b^1, b^2, V, c} \sum_{x \in \mathcal{D}} \sum_i (x_i - \hat{x}_i)^2$$

- 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.

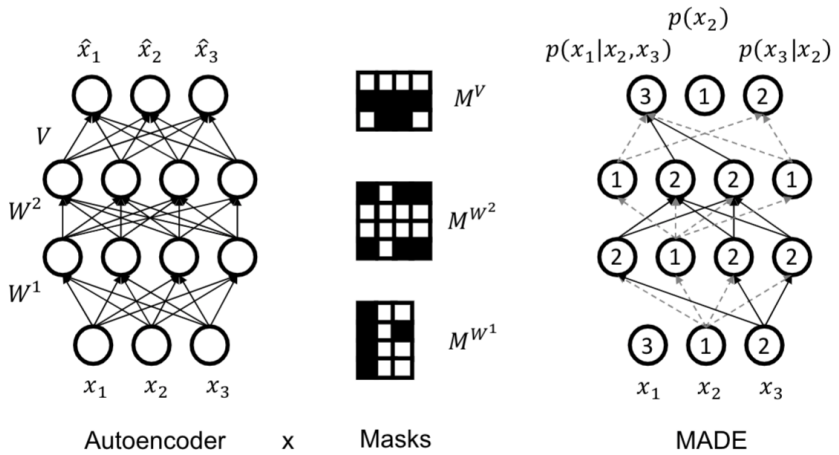
Autoregressive autoencoders



Autoencoder

- On the surface, FVSBN and NADE look similar to an **autoencoder**. Can we get a generative model from an autoencoder?
- We need to make sure it corresponds to a valid Bayesian Network (DAG structure), i.e., we need an *ordering* for chain rule. If ordering is $1, 2, 3$, then:
  - $\hat{x}_1$ cannot depend on any input $x = (x_1, x_2, x_3)$. Then at generation time we don't need any input to get started
  - $\hat{x}_2$ can only depend on x_1
  - $\dots$
- **Bonus**: we can use a single neural network (with n inputs and outputs) to produce all the parameters $\hat{x}$ in a single pass. In contrast, NADE requires n passes. Much more efficient on modern hardware.

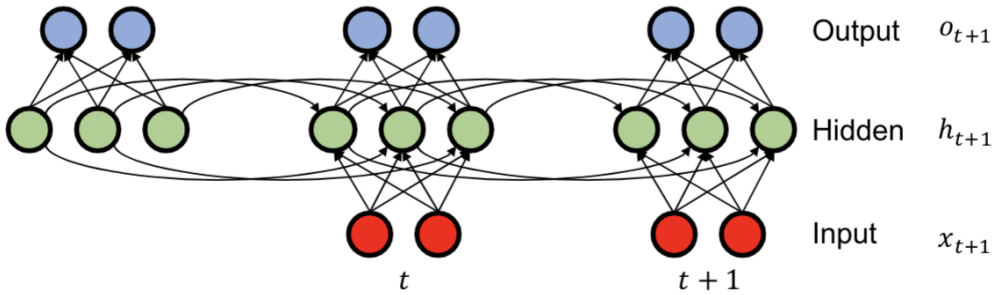
MADE: Masked Autoencoder for Distribution Estimation



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_2, x_3, x_1, so $p(x_1, x_2, x_3) = p(x_2)p(x_3 \mid x_2)p(x_1 \mid x_2, x_3)$.
   1. The unit producing the parameters for $\hat{x}_2 = p(x_2)$ is not allowed to depend on any input. Unit for $p(x_3|x_2)$ only on x_2. And so on...
   2. For each unit in a hidden layer, pick a random integer i in $[1, n-1]$. That unit is allowed to depend only on the first i inputs (according to the chosen ordering).
   3. Add mask to preserve this invariant: connect to all units in previous layer with smaller or equal assigned number (strictly $<$ in final layer)

RNN: Recurrent Neural Nets

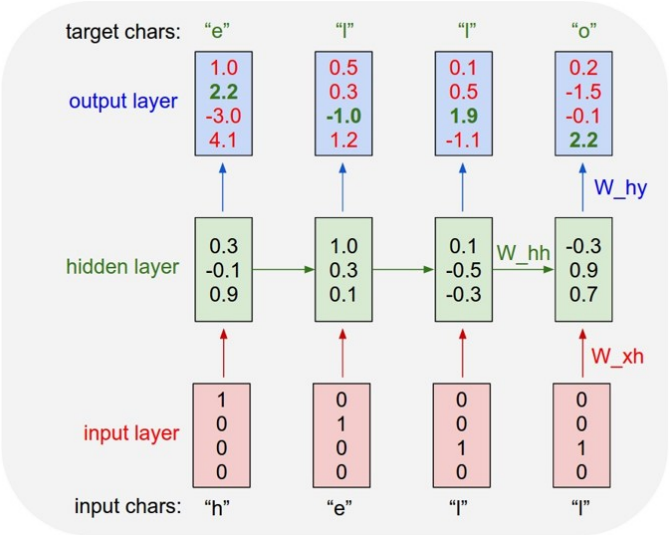
Challenge: model $p(x_t|x_{1:t-1}; \alpha^t)$. "History" $x_{1:t-1}$ keeps getting longer.
Idea: keep a summary and recursively update it



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

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)



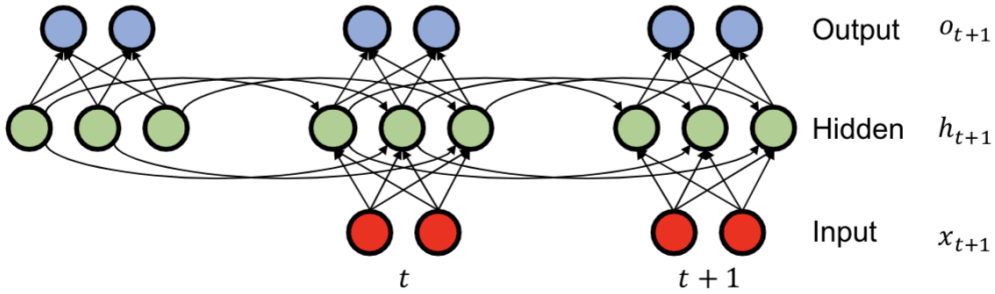
1. Suppose $x_i \in \{h, e, l, o\}$. Use one-hot encoding:
   - h encoded as $[1, 0, 0, 0]$, e encoded as $[0, 1, 0, 0]$, etc.
2. **Autoregressive**: $p(x = hello) = p(x_1 = h)p(x_2 = e|x_1 = h)p(x_3 = l|x_1 = h, x_2 = e) \cdots p(x_5 = o|x_1 = h, x_2 = e, x_3 = l, x_4 = l)$
3. For example,

$$p(x_2 = e|x_1 = h) = softmax(o_1) = \frac{\exp(2.2)}{\exp(1.0) + \cdots + \exp(4.1)}$$

$$o_1 = W_{hy} h_1$$

$$h_1 = tanh(W_{hh} h_0 + W_{xh} x_1)$$

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)

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 ==
*[[lender dome of the ED]]
*[[Anti-autism]]

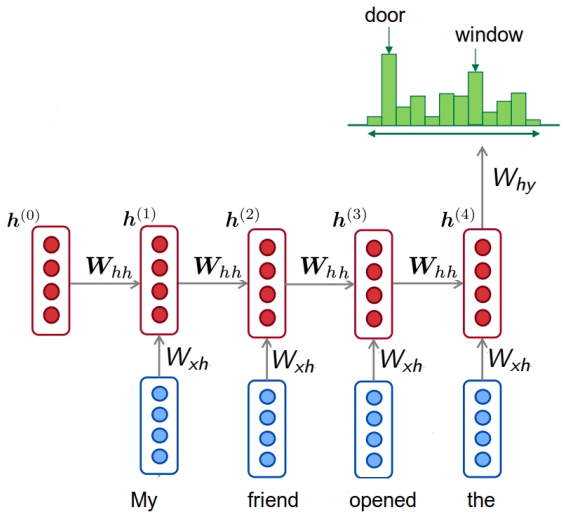
== External links==
* [http://www.biblegateway.nih.gov/entrepre/ Website of the World Festival. The labour of India-county defeats at the Ripper of California Road.]

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

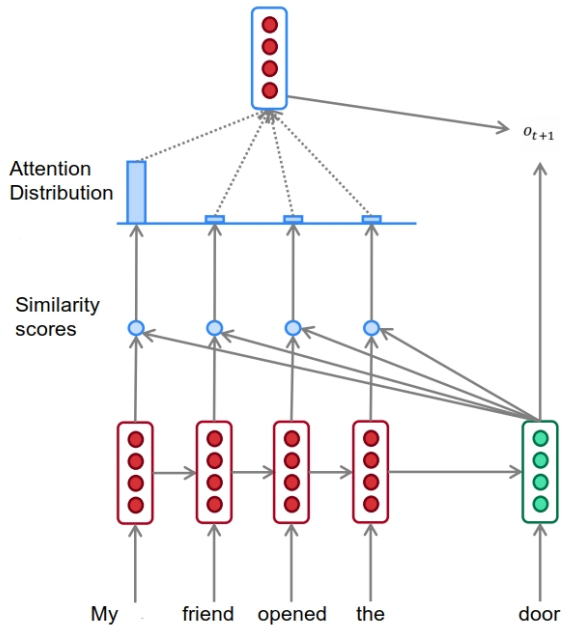
Issues with RNNs



Issues with RNN models

- A single hidden vector needs to summarize all the (growing) history. For example, $h^{(4)}$ needs to summarize the meaning of "My friend opened the".
- Sequential evaluation, cannot be parallelized
- Exploding/vanishing gradients when accessing information from many steps back

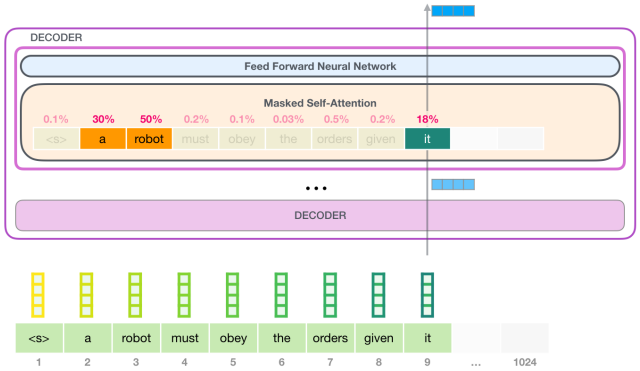
Attention based models



Attention mechanism to compare a *query* vector to a set of *key* vectors

1. Compare current hidden state (query) to all past hidden states (keys), e.g., by taking a dot product
2. Construct attention distribution to figure out what parts of the history are relevant, e.g., via a softmax
3. Construct a summary of the history, e.g., by weighted sum
4. Use summary and current hidden state to predict next token/word

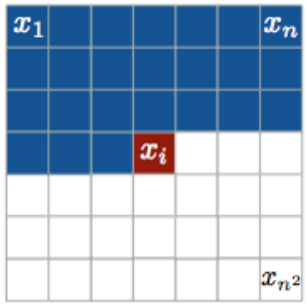
Generative Transformers



Current state of the art (GPTs): replace RNN with Transformer

- Attention mechanisms to adaptively focus only on relevant context
- Avoid recursive computation. Use only self-attention to enable parallelization
- Needs **masked** self-attention to preserve autoregressive structure
- Demo: `https://transformer.huggingface.co/doc/gpt2-large`
- Demo: `https://huggingface.co/spaces/huggingface-projects/llama-2-13b-chat`

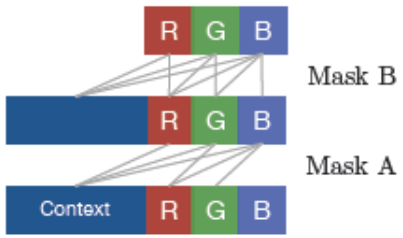
Pixel RNN (Oord et al., 2016)



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

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

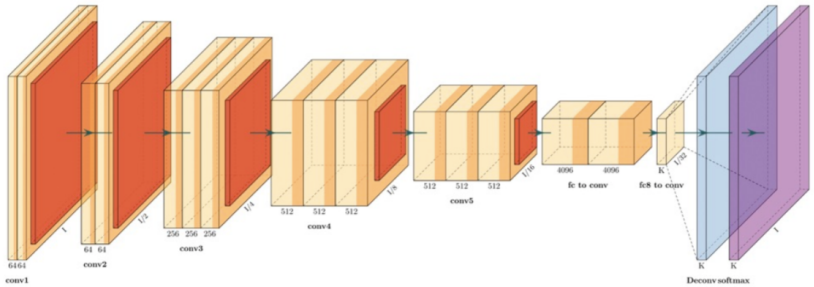
   and each conditional is a categorical random variable with 256 possible values
3. Conditionals modeled using RNN variants. LSTMs + masking (like MADE)



Pixel RNN

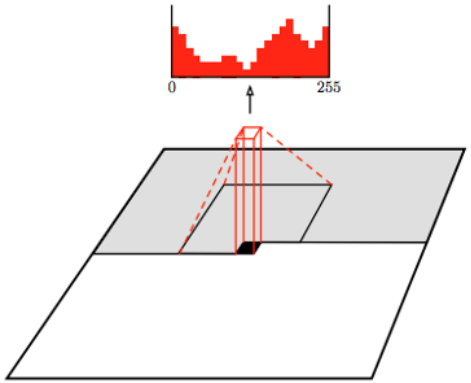
Results on downsampled ImageNet. Very slow: sequential likelihood evaluation.

Convolutional Architectures

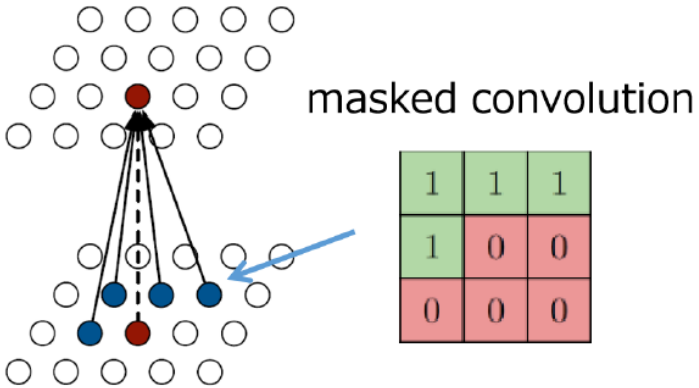


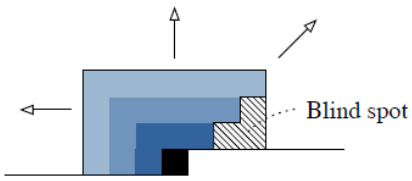
Convolutions are natural for image data and easy to parallelize on modern hardware.

PixelCNN (Oord et al., 2016)

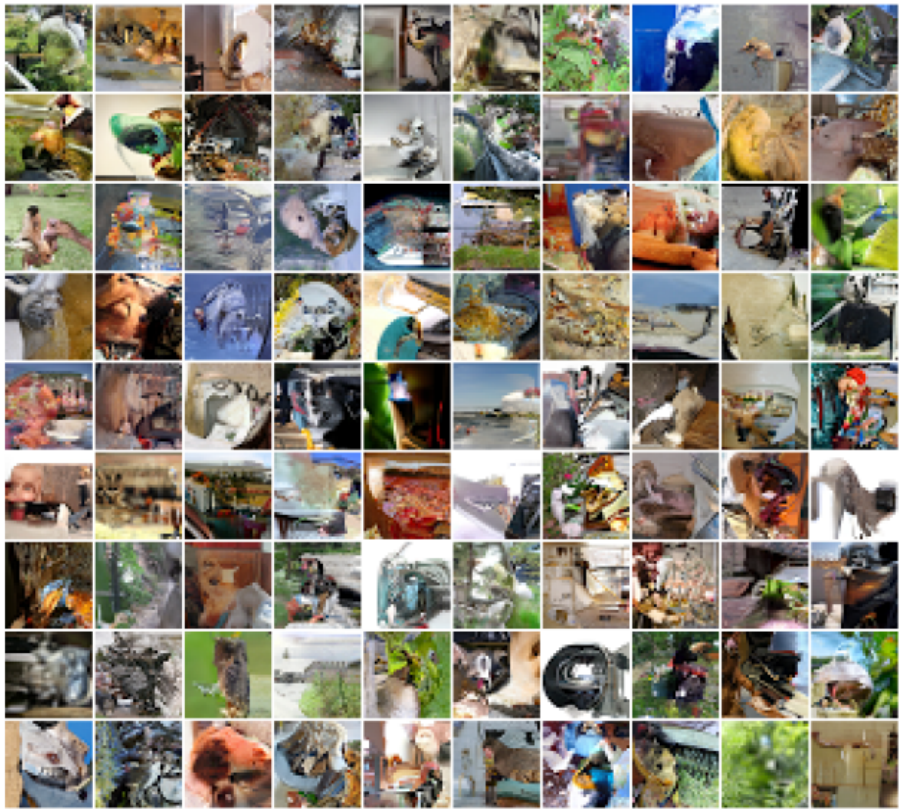


Idea: Use convolutional architecture to predict next pixel given context (a neighborhood of pixels).
Challenge: Has to be autoregressive. Masked convolutions preserve raster scan order. Additional masking for colors order.





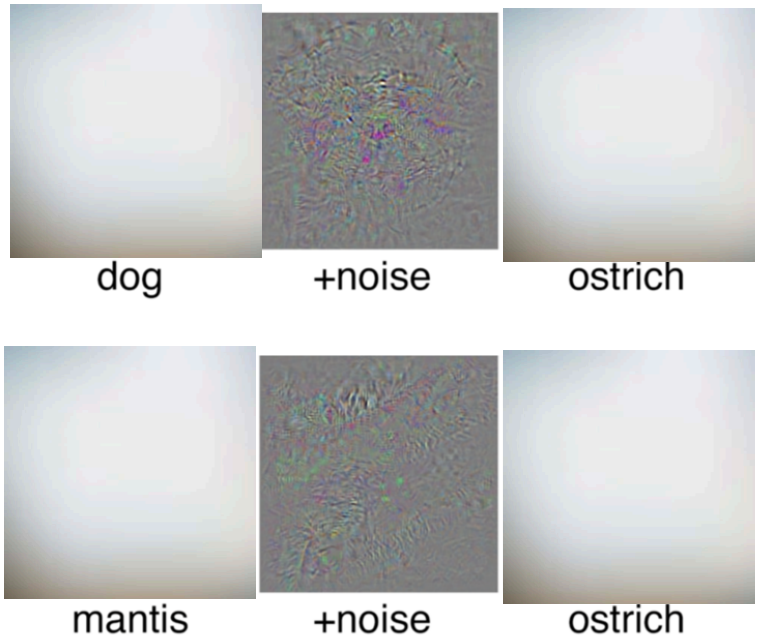
PixelCNN



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

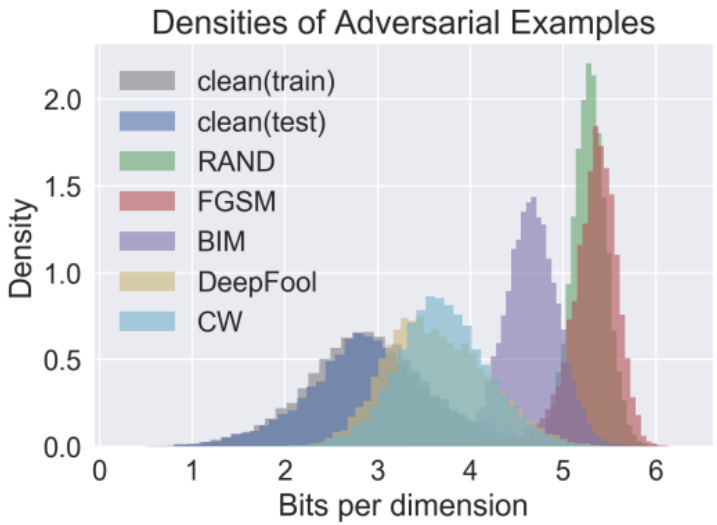
Application in Adversarial Attacks and Anomaly detection

Machine learning methods are vulnerable to adversarial examples



Can we detect them?

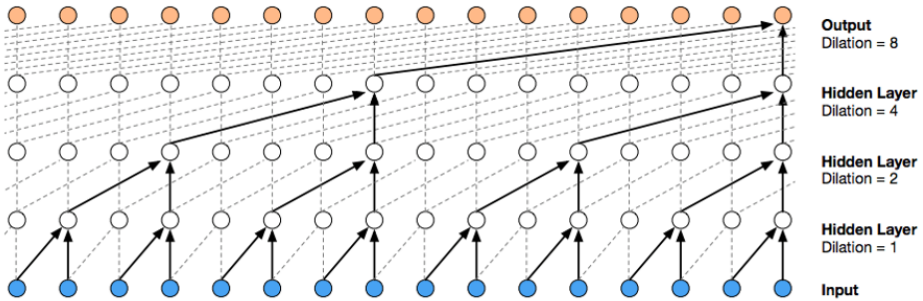
PixelDefend (Song et al., 2018)



- 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 $p(x)$

WaveNet (Oord et al., 2016)

Very effective model for speech:



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

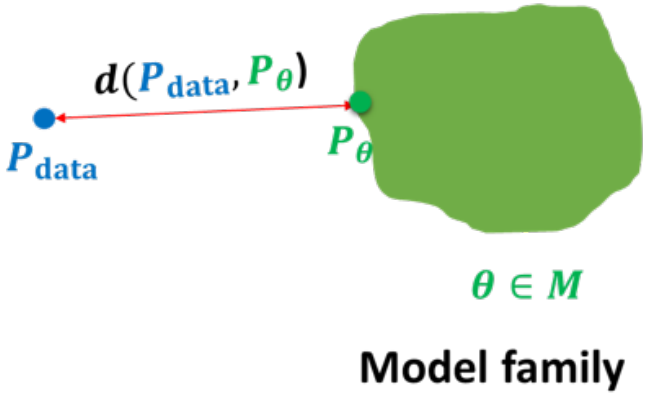
Summary of Autoregressive Models

- 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. $\ldots$
- 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. $\ldots$
  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

Learning a generative model

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

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



- We want to learn 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 (*sampling*)
  - **Density estimation:** $p(x)$ should be high if x looks like a dog, and low otherwise (*anomaly detection*)
  - **Unsupervised representation learning:** We should be able to learn what these images have in common, e.g., ears, tail, etc. (*features*)
- First question: how to represent $p_\theta(x)$. Second question: **how to learn it**.

Setting

- Lets 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 (a subset of) the variables, e.g., $(X_{\text{bank}} = 1, X_{\text{dollar}} = 0, ..., Y = 1)$ 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" distribution in this set:
  - For example, $\mathcal{M}$ could be all Bayes nets with a given graph structure, for all possible choices of the CPD tables
  - For example, a FVSBN for all possible choices of the logistic regression parameters , $\theta =$ concatenation of all logistic regression coefficients

Goal of learning

- The goal of learning is to return a model P_θ 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
  - computational reasons
- Example. Suppose we represent each image with a vector X of 784 binary variables (black vs. white pixel). How many possible states ($=$ possible images) in the model? $2^{784} \approx 10^{236}$. Even 10^7 training examples provide *extremely* sparse coverage!
- We want to select P_θ to construct the "best" approximation to the underlying distribution P_{data}
- What is "best"?

What is "best"?

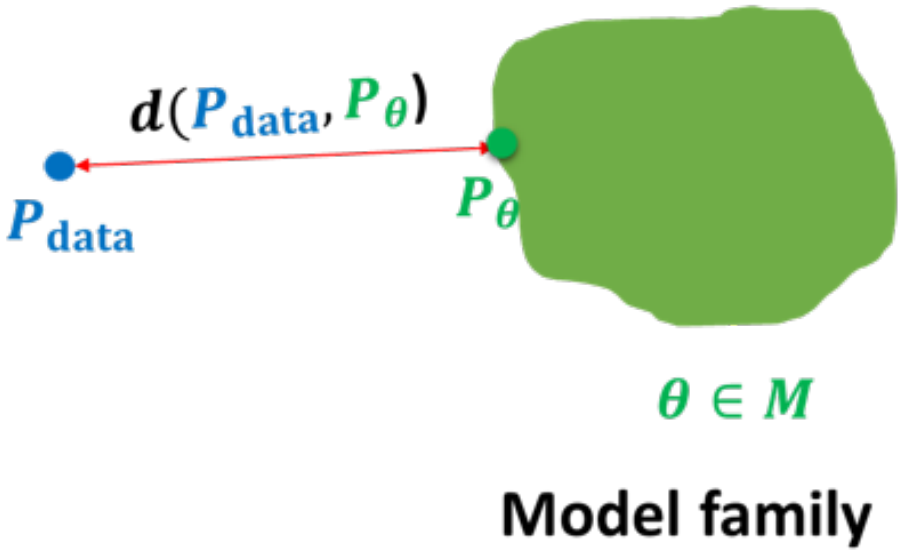
This depends on what we want to do

1. Density estimation: we are interested in the full distribution (so later we can compute whatever conditional probabilities we want)
2. Specific prediction tasks: we are using the distribution to make a prediction
   - Is this email spam or not?
   - **Structured prediction:** Predict next frame in a video, or caption given an image
3. Structure or knowledge discovery: we are interested in the model itself
   - How do some genes interact with each other?
   - What causes cancer?
   - Take CS 228

Learning as density estimation

- We want to learn the full distribution so that later we can answer *any* probabilistic inference query
- In this setting we can view the learning problem as **density estimation**
- We want to construct P_θ as "close" as possible to P_{data} (recall we assume we are given a dataset $\mathcal{D}$ of samples from P_{data})

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



- How do we evaluate "closeness"?

KL-divergence

- How should we measure distance between distributions?
- The **Kullback-Leibler divergence** (KL-divergence) between two distributions p and q is defined as

$$D(p\|q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}.$$

- $D(p \,\|\, q) \geq 0$ for all p, q, with equality if and only if $p = q$. Proof:

$$\mathbf{E}_{\mathbf{x}\sim p}\left[-\log \frac{q(\mathbf{x})}{p(\mathbf{x})}\right] \geq -\log\left(\mathbf{E}_{\mathbf{x}\sim p}\left[\frac{q(\mathbf{x})}{p(\mathbf{x})}\right]\right) = -\log\left(\sum_{\mathbf{x}} p(\mathbf{x})\frac{q(\mathbf{x})}{p(\mathbf{x})}\right) = 0$$

- Notice that KL-divergence is **asymmetric**, i.e., $D(p\|q) \neq D(q\|p)$
- Measures the expected number of extra bits required to describe *samples from* $p(\mathbf{x})$ using a compression code based on q instead of p

Detour on KL-divergence

- To compress, it is useful to know the probability distribution the data is sampled from
- For example, let $X_1, \cdots, X_{100}$ be samples of an unbiased coin. Roughly 50 heads and 50 tails. Optimal compression scheme is to record heads as 0 and tails as 1. In expectation, use 1 bit per sample, and cannot do better
- Suppose the coin is biased, and $P[H] \gg P[T]$. Then it's more efficient to uses fewer bits on average to represent heads and more bits to represent tails, e.g.
  - Batch multiple samples together
  - Use a short sequence of bits to encode $HHHH$ (common) and a long sequence for $TTTT$ (rare).
  - Like Morse code: $E = \bullet$, $A = \bullet -$, $Q = - - \bullet -$
- KL-divergence: if your data comes from p, but you use a scheme optimized for q, the divergence $D_{KL}(p||q)$ is the number of *extra* bits you'll need on average

Learning as density estimation

- We want to learn the full distribution so that later we can answer *any* probabilistic inference query
- In this setting we can view the learning problem as **density estimation**
- We want to construct P_θ as "close" as possible to P_{data} (recall we assume we are given a dataset $\mathcal{D}$ of samples from P_{data})
- How do we evaluate "closeness"?
- **KL-divergence** is one possibility:

$$\mathbf{D}(P_{\text{data}}||P_\theta) = \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log\left(\frac{P_{\text{data}}(\mathbf{x})}{P_\theta(\mathbf{x})}\right)\right] = \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \frac{P_{\text{data}}(\mathbf{x})}{P_\theta(\mathbf{x})}$$

- $\mathbf{D}(P_{\text{data}}||P_\theta) = 0$ iff the two distributions are the same.
- It measures the "compression loss" (in bits) of using P_θ instead of P_{data}.

Expected log-likelihood

- We can simplify this somewhat:

$$\begin{aligned}\mathbf{D}(P_{\text{data}}||P_\theta) &= \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log\left(\frac{P_{\text{data}}(\mathbf{x})}{P_\theta(\mathbf{x})}\right)\right] \\ &= \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{data}}(\mathbf{x})\right] - \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right]\end{aligned}$$

- The first term does not depend on P_θ.
- Then, *minimizing* KL divergence is equivalent to *maximizing* the **expected log-likelihood**

$$\arg\min_{P_\theta} \mathbf{D}(P_{\text{data}}||P_\theta) = \arg\min_{P_\theta} -\mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right] = \arg\max_{P_\theta} \mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right]$$

  - Asks that P_θ assign high probability to instances sampled from P_{data}, so as to reflect the true distribution
  - Because of log, samples $\mathbf{x}$ where $P_\theta(\mathbf{x}) \approx 0$ weigh heavily in objective
- Although we can now compare models, since we are ignoring $\mathbf{H}(P_{\text{data}}) = -\mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{data}}(\mathbf{x})\right]$, we don't know how close we are to the optimum
- Problem: In general we do not know P_{data}.

Maximum likelihood

- Approximate the expected log-likelihood

$$\mathbf{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_\theta(\mathbf{x})\right]$$

  with the *empirical log-likelihood*:

$$\mathbf{E}_{\mathcal{D}}\left[\log P_\theta(\mathbf{x})\right] = \frac{1}{|\mathcal{D}|}\sum_{\mathbf{x}\in\mathcal{D}} \log P_\theta(\mathbf{x})$$

- **Maximum likelihood learning** is then:

$$\max_{P_\theta} \frac{1}{|\mathcal{D}|}\sum_{\mathbf{x}\in\mathcal{D}} \log P_\theta(\mathbf{x})$$

- Equivalently, maximize likelihood of the data $P_\theta(\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}) = \prod_{\mathbf{x}\in\mathcal{D}} P_\theta(\mathbf{x})$

Main idea in Monte Carlo Estimation

1. **Express the quantity of interest as the expected value of a random variable.**

$$E_{x\sim P}[g(x)] = \sum_x g(x)P(x)$$

2. Generate T samples $\mathbf{x}^1, \ldots, \mathbf{x}^T$ from the distribution P with respect to which the expectation was taken.
3. Estimate the expected value from the samples using:

$$\hat{g}(\mathbf{x}^1, \cdots, \mathbf{x}^T) \triangleq \frac{1}{T}\sum_{t=1}^{T} g(\mathbf{x}^t)$$

where $\mathbf{x}^1, \ldots, \mathbf{x}^T$ are independent samples from P. Note: $\hat{g}$ is a random variable. Why?

Properties of the Monte Carlo Estimate

- **Unbiased:**

$$E_P[\hat{g}] = E_P[g(x)]$$

- **Convergence:** By law of large numbers

$$\hat{g} = \frac{1}{T}\sum_{t=1}^{T} g(x^t) \to E_P[g(x)] \text{ for } T \to \infty$$

- **Variance:**

$$V_P[\hat{g}] = V_P\left[\frac{1}{T}\sum_{t=1}^{T} g(x^t)\right] = \frac{V_P[g(x)]}{T}$$

Thus, variance of the estimator can be reduced by increasing the number of samples.

Example

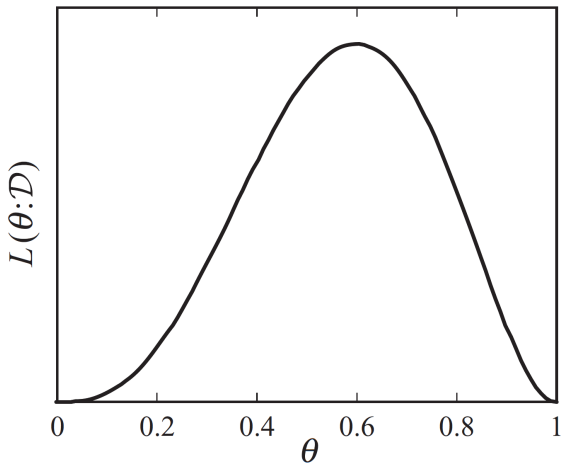
Single variable example: A biased coin

- Two outcomes: *heads* (H) and *tails* (T)
- Data set: Tosses of the biased coin, e.g., $\mathcal{D} = \{H, H, T, H, T\}$
- Assumption: the process is controlled by a probability distribution $P_{\text{data}}(x)$ where $x \in \{H, T\}$
- Class of models $\mathcal{M}$: all probability distributions over $x \in \{H, T\}$.
- Example learning task: How should we choose $P_\theta(x)$ from $\mathcal{M}$ if 3 out of 5 tosses are heads in $\mathcal{D}$?

MLE scoring for the coin example

We represent our model: $P_\theta(x = H) = \theta$ and $P_\theta(x = T) = 1 - \theta$

- Example data: $\mathcal{D} = \{H, H, T, H, T\}$
- Likelihood of data $= \prod_i P_\theta(x_i) = \theta \cdot \theta \cdot (1 - \theta) \cdot \theta \cdot (1 - \theta)$



- Optimize for θ which makes $\mathcal{D}$ most likely. What is the solution in this case? $\theta = 0.6$, optimization problem can be solved in closed-form

Extending the MLE principle to autoregressive models

Given an autoregressive model with n variables and factorization

$$P_\theta(\mathbf{x}) = \prod_{i=1}^{n} p_{\text{neural}}(x_i | \mathbf{x}_{<i}; \theta_i)$$

$\theta = (\theta_1, \cdots, \theta_n)$ are the parameters of all the conditionals. Training data $\mathcal{D} = \{\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(m)}\}$. Maximum likelihood estimate of the parameters θ?

- Decomposition of Likelihood function

$$L(\theta, \mathcal{D}) = \prod_{j=1}^{m} P_\theta(\mathbf{x}^{(j)}) = \prod_{j=1}^{m} \prod_{i=1}^{n} p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

- Goal : maximize $\arg\max_\theta L(\theta, \mathcal{D}) = \arg\max_\theta \log L(\theta, \mathcal{D})$
- We no longer have a closed form solution

MLE Learning: Gradient Descent

$$L(\theta, \mathcal{D}) = \prod_{j=1}^{m} P_\theta(\mathbf{x}^{(j)}) = \prod_{j=1}^{m} \prod_{i=1}^{n} p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

Goal : maximize $\arg\max_\theta L(\theta, \mathcal{D}) = \arg\max_\theta \log L(\theta, \mathcal{D})$

$$\ell(\theta) = \log L(\theta, \mathcal{D}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize $\theta^0 = (\theta_1, \cdots, \theta_n)$ at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

Non-convex optimization problem, but often works well in practice

MLE Learning: Stochastic Gradient Descent

$$\ell(\theta) = \log L(\theta, \mathcal{D}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize θ^0 at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

What is the gradient with respect to θ_i?

$$\nabla_{\theta_i} \ell(\theta) = \sum_{j=1}^{m} \nabla_{\theta_i} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) = \sum_{j=1}^{m} \nabla_{\theta_i} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

Each conditional $p_{\text{neural}}(x_i | \mathbf{x}_{<i}; \theta_i)$ can be optimized separately if there is no parameter sharing. In practice, parameters θ_i are shared (e.g., NADE, PixelRNN, PixelCNN, etc.)

MLE Learning: Stochastic Gradient Descent

$$\ell(\theta) = \log L(\theta, \mathcal{D}) = \sum_{j=1}^{m} \sum_{i=1}^{n} \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

1. Initialize θ^0 at random
2. Compute $\nabla_\theta \ell(\theta)$ (by back propagation)
3. $\theta^{t+1} = \theta^t + \alpha_t \nabla_\theta \ell(\theta)$

$$\nabla_\theta \ell(\theta) = \sum_{j=1}^{m} \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$$

What if $m = |\mathcal{D}|$ is huge?

$$\begin{aligned} \nabla_\theta \ell(\theta) &= m \sum_{j=1}^{m} \frac{1}{m} \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) \\ &= m E_{x^{(j)} \sim \mathcal{D}} \left[\sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i) \right] \end{aligned}$$

Monte Carlo: Sample $x^{(j)} \sim \mathcal{D}; \nabla_\theta \ell(\theta) \approx m \sum_{i=1}^{n} \nabla_\theta \log p_{\text{neural}}(x_i^{(j)} | \mathbf{x}_{<i}^{(j)}; \theta_i)$

Empirical Risk and Overfitting

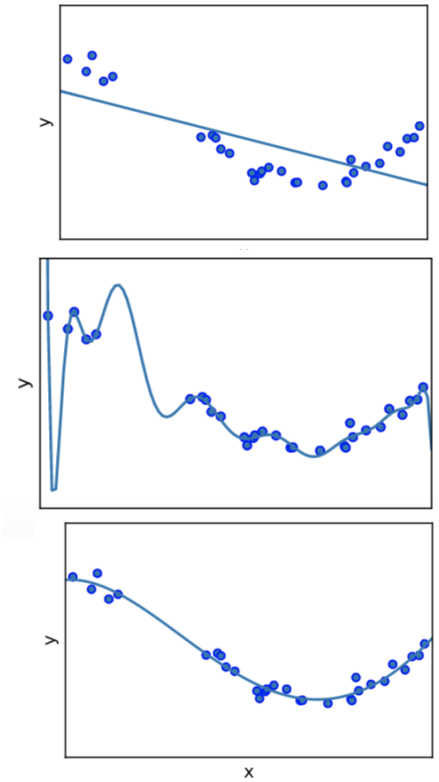
- Empirical risk minimization can easily **overfit** the data
  - Extreme example: The data is the model (remember all training data).
- Generalization: the data is a sample, usually there is vast amount of samples that you have never seen. Your model should generalize well to these "never-seen" samples.
- Thus, we typically restrict the **hypothesis space** of distributions that we search over

Bias-Variance trade off

- If the hypothesis space is very limited, it might not be able to represent P_{data}, even with unlimited data
  - This type of limitation is called **bias**, as the learning is limited on how close it can approximate the target distribution
- If we select a highly expressive hypothesis class, we might represent better the data
  - When we have small amount of data, multiple models can fit well, or even better than the true model. Moreover, small perturbations on $\mathcal{D}$ will result in very different estimates
  - This limitation is call the **variance**.

Bias-Variance trade off

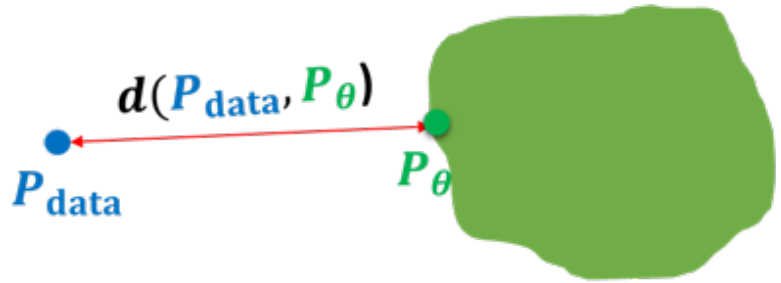
- There is an inherent **bias-variance trade off** when selecting the hypothesis class. Error in learning due to both things: bias and variance.
- Hypothesis space: linear relationship
  - Does it fit well? Underfits
- Hypothesis space: high degree polynomial
  - Overfits
- Hypothesis space: low degree polynomial
  - Right tradeoff



How to avoid overfitting?

- Hard constraints, e.g. by selecting a less expressive model family:
  - Smaller neural networks with less parameters
  - Weight sharing

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



- Soft preference for "simpler" models: **Occam Razor**.
- Augment the objective function with **regularization**:

$$objective(\mathbf{x}, \mathcal{M}) = loss(\mathbf{x}, \mathcal{M}) + R(\mathcal{M})$$

- Evaluate generalization performance on a held-out validation set