Lecture 18: HMM & Deep Learning

Winter 2018

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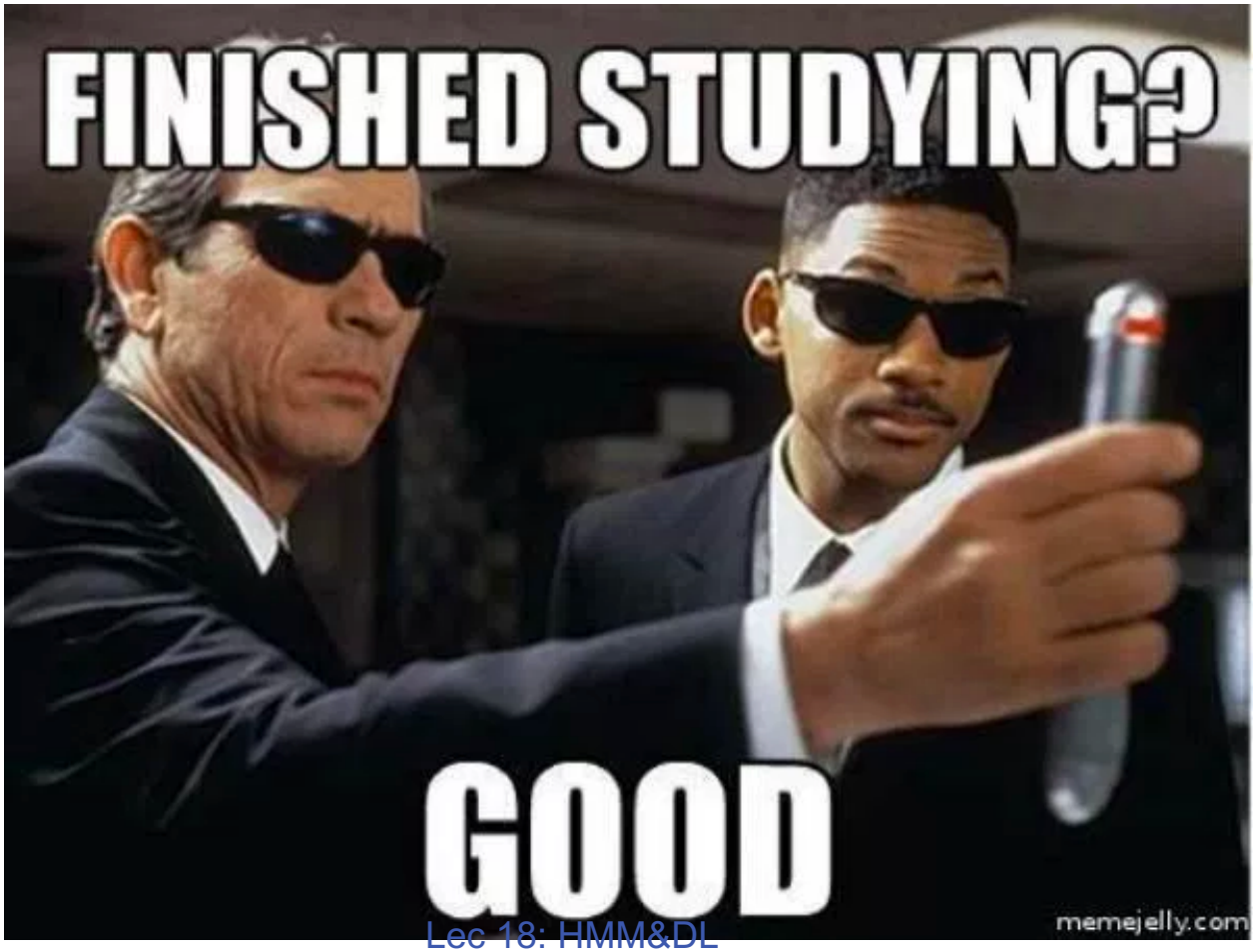
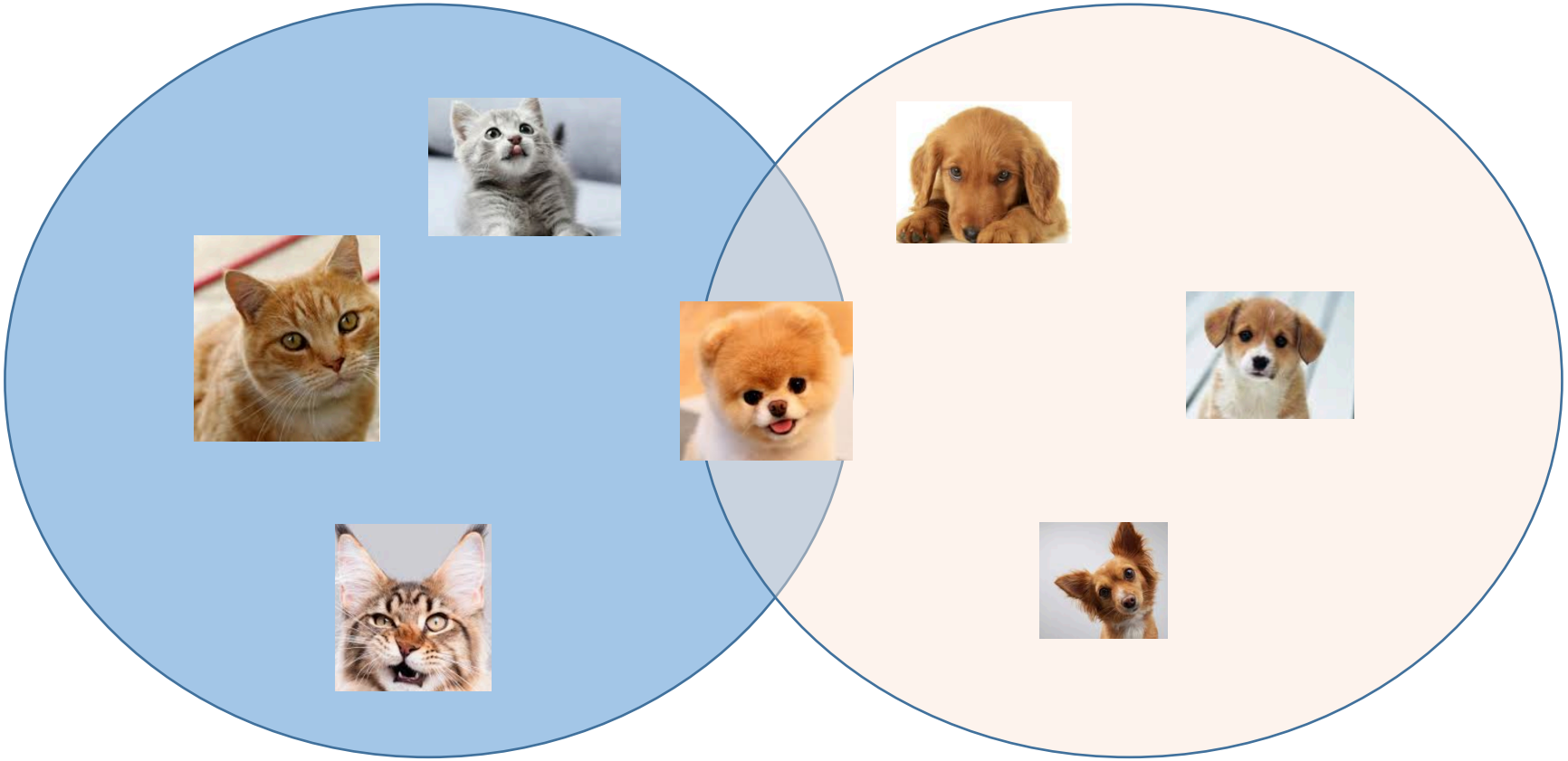
Final Exam 3/22, 11:30am-2:00pm

- Franz Hall: 1178 , 150min exam



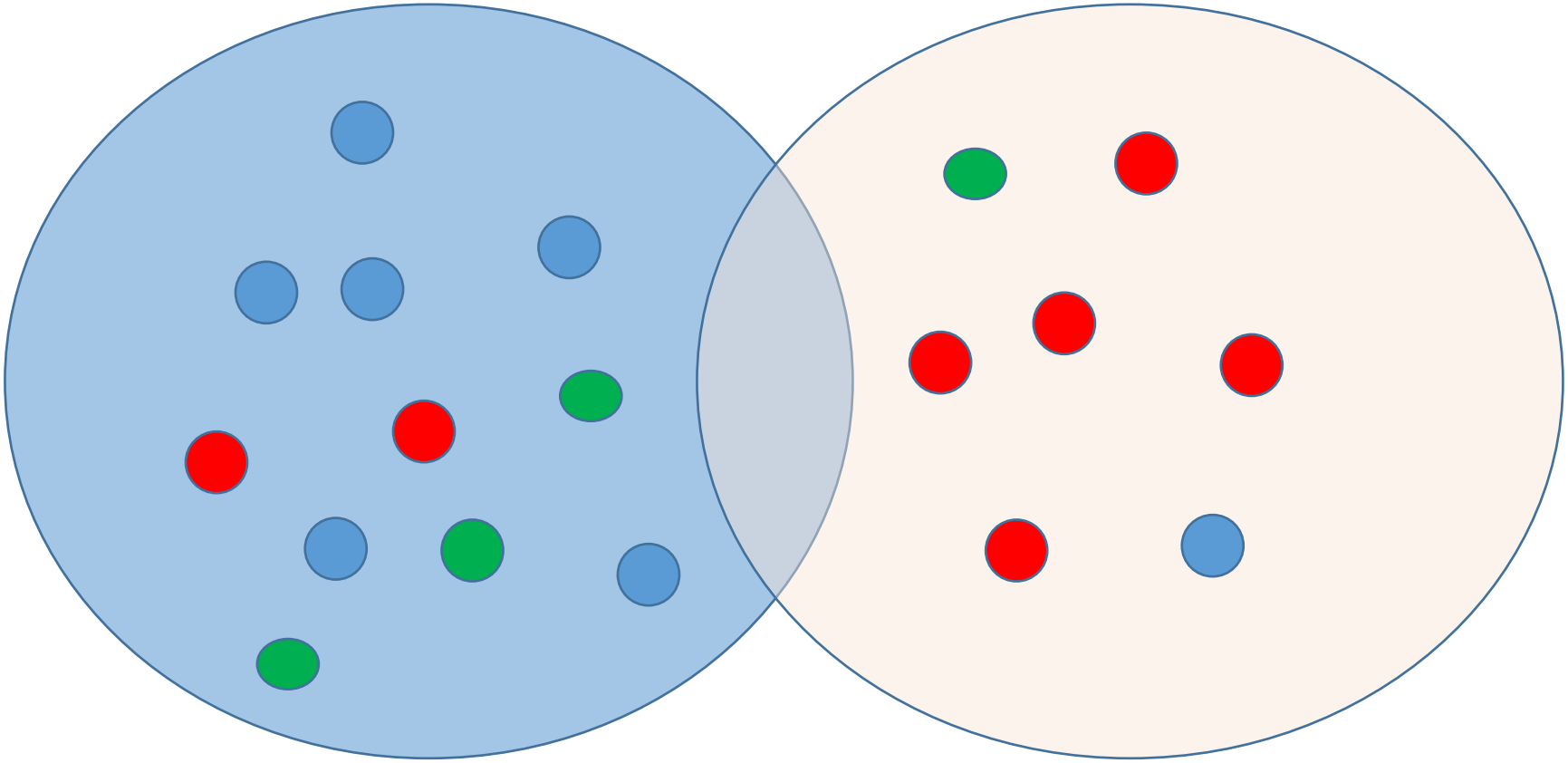
Generative model

- Idea: build a probabilistic model to measure how likely we would see the observations



Generative model

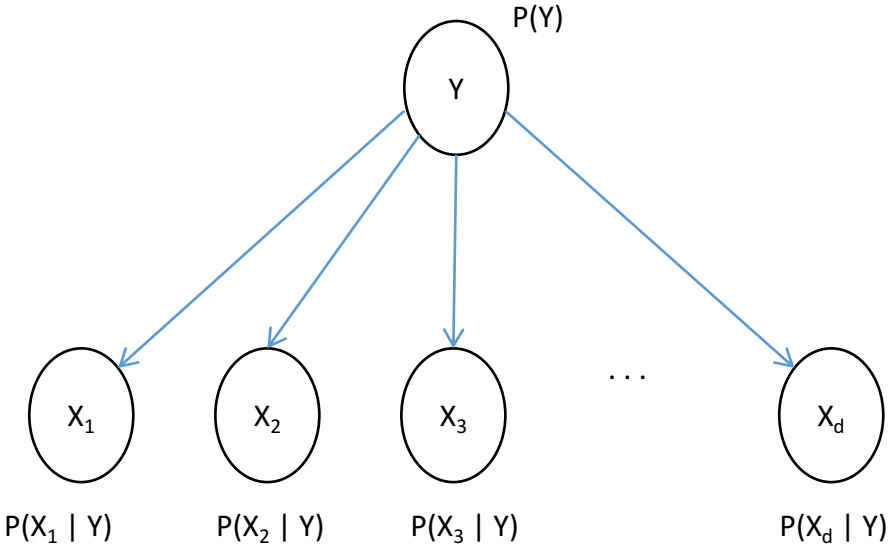
- Idea: build a probabilistic model to measure how likely we would see the observations



Prediction under a generative Model

Given the label, sample the features independently from the conditional distributions

Cat? or Dog?



$$\underset{y}{\operatorname{argmax}} P(y) \prod_j P(x_j|y)$$

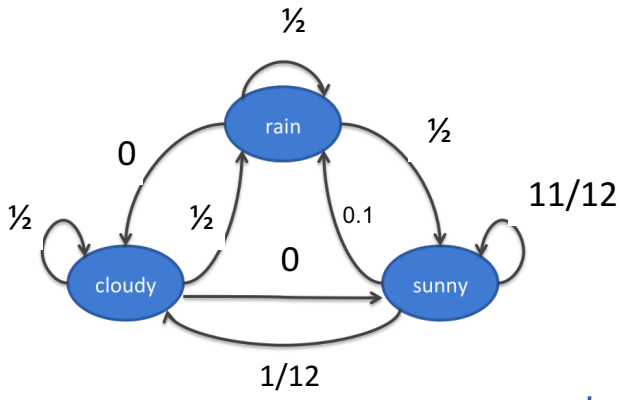
Weather Forecast by Markov Chain

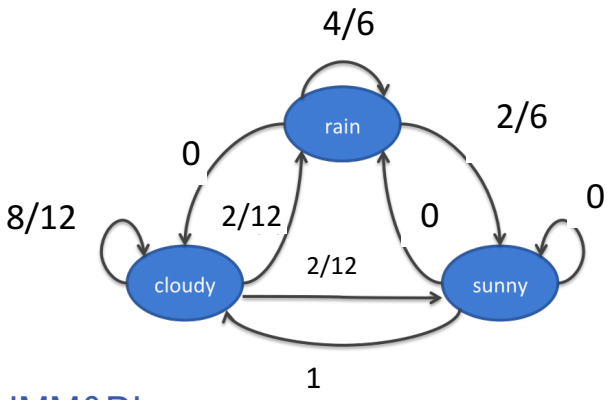
- Observing a sequence of weather events, predict the weather tomorrow

S: Sunny, C: Cloudy, R: rainy

Los Angeles (winter): S S S S S S S S C C R R S S S S S S S S

Seattle (winter): C C C C C C R R C S C C S C R R R R C C C





Discrete Markov Process

- State at time t is x_t
- First-order Markov assumption

  The state of the system at any time is ***independent*** of the full sequence history given the previous state

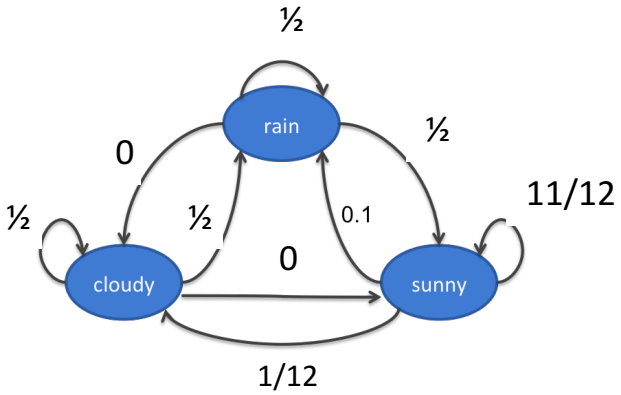
$$P(x_1, x_2, \cdots, x_n) = \prod_{i=1}^{n} P(x_i | x_{i-1})$$

  - Defined by two sets of probabilities:
    - Initial state distribution: $P(x_1 = S_j)$
    - State transition probabilities: $P(x_i = S_j \mid x_{i-1} = S_k)$

Example: The weather

- Three states: rain, cloudy, sunny

State transitions:



- Observations are Markov chains:

Eg: *cloudy sunny sunny rain*

Probability of the sequence =

P(cloudy) P(sunny|cloudy) P(sunny | sunny) P(rain | sunny)

Initial probability

Transition probabilities

Weather Forecast by Markov Chain

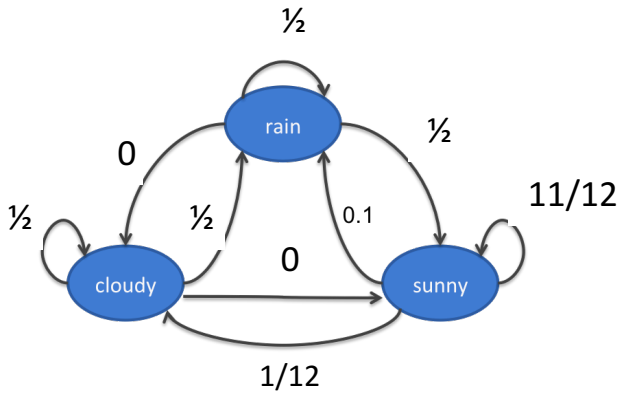
- Maximum Likelihood estimation:

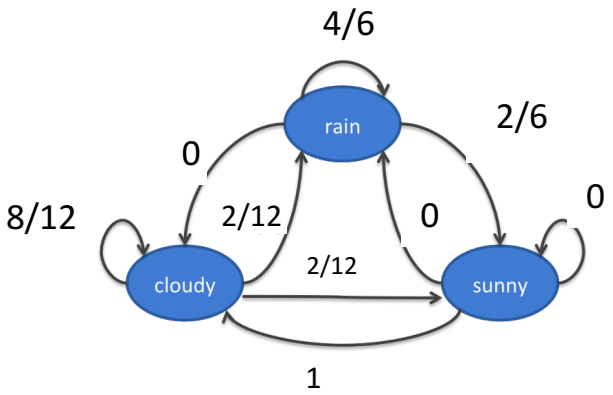
$$P(y_t = \text{Rain} \mid y_{t-1} = \text{Sunny}) = \frac{\#\, S\, R}{\#\, S}$$

S: Sunny, C: Cloudy, R: rainy

Los Angeles (winter): S S S S S S S S C C R R S S S S S S S S S

Seattle (winter): C C C C C C R R C S C C S C R R R R C C C





Example: Another language model

It was a bright cold day in April

$$P(\text{It was a bright cold day in April}) =$$
$$P(\text{It}) \times$$
$$P(\text{was}|\text{It}) \times$$
$$P(\text{a}|\text{was}) \times$$
$$P(\text{bright}|\text{a}) \times$$
$$P(\text{cold}|\text{bright}) \times$$
$$P(\text{day}|\text{cold}) \times \cdots$$

Probability of a word starting a sentence

Probability of a word following "It"

Probability of a word following "was"

Probability of a word following "a"

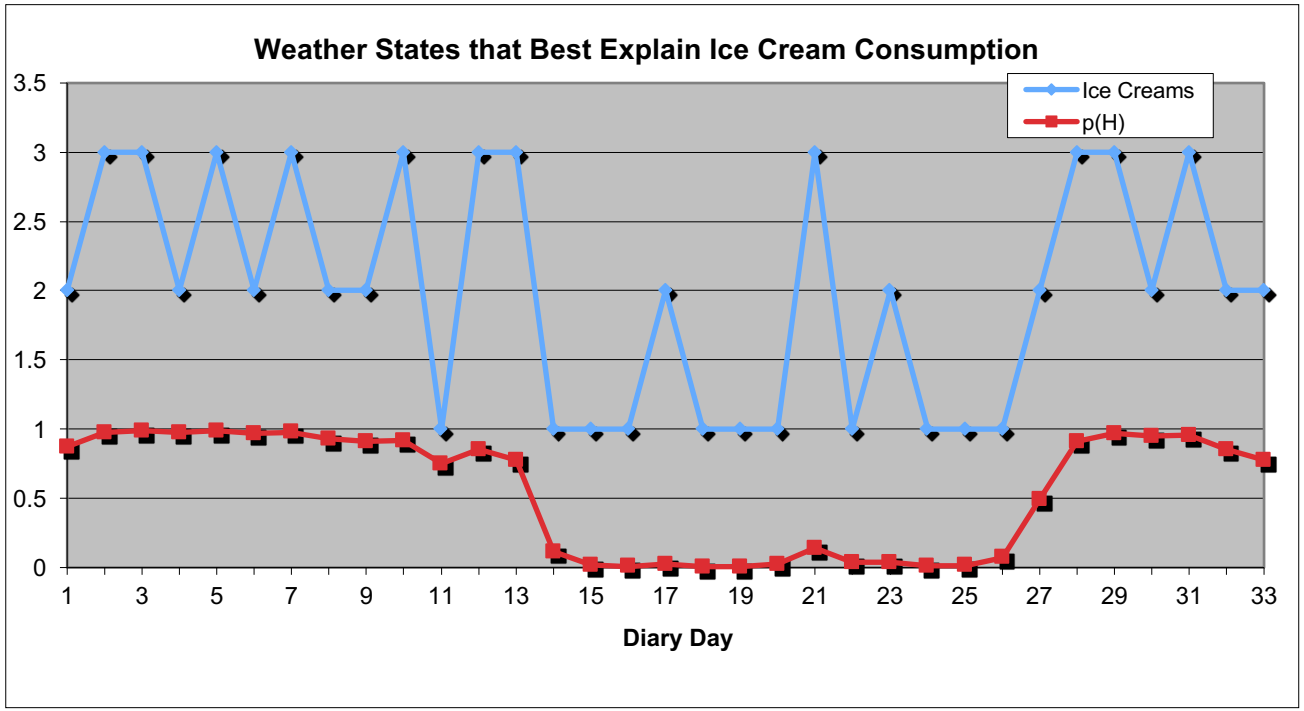
If there are K tokens/states, how many parameters do we need? $O(K^2)$

Hidden Markov Model

(C)old day v.s. (H)ot day

#cones

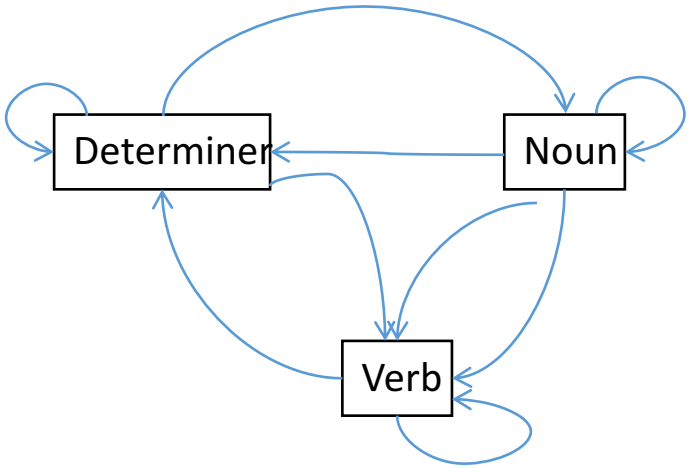
	p(…|C)	p(…|H)	p(…|START)
(1|…)	0.7	0.1	
(2|…)	0.2	0.2	
(3|…)	0.1	0.7	
(C|…)	0.8	0.1	0.5
(H|…)	0.1	0.8	0.5
…)	0.1	0.1	0



Toy part-of-speech example

The Fed raises interest rates

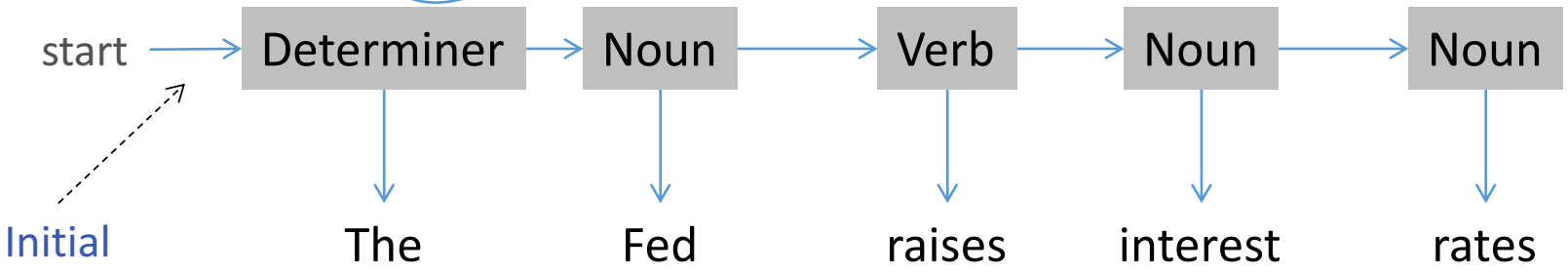
Transitions



Emissions

P(The | Determiner) = 0.5
P(A | Determiner) = 0.3
P(An | Determiner) = 0.1
P(Fed | Determiner) = 0
…

P(Fed| Noun) = 0.001
P(raises| Noun) = 0.04
P(interest| Noun) = 0.07
P(The| Noun) = 0
…



Joint model over states and observations

- Notation
  - Number of states = K, Number of observations = M
  - π: Initial probability over states (K dimensional vector)
  - A: Transition probabilities (K×K matrix)
  - B: Emission probabilities (K×M matrix)

- Probability of states and observations
  - Denote states by $y_1, y_2, \cdots$ and observations by $x_1, x_2, \cdots$

$$P(x_1, x_2, \cdots, x_n, y_1, y_2, \cdots y_n) = P(y_1) \prod_{i=1}^{n-1} P(y_{i+1}|y_i) \prod_{i=1}^{n} P(x_i|y_i)$$

$$= \pi_{y_1} \prod_{i=1}^{n-1} A_{y_i, y_{i+1}} \prod_{i=1}^{n} B_{y_i, x_i}$$

Key questions for HMMs

[Rabiner 1999]

1. Given an observation sequence, $x_1, x_2, \cdots, x_n$ and a model (π, A, B), how to efficiently calculate the most probable state sequence?

   Inference

2. How to calculate (π, A, B) from observations?

   Learning

Outline

- *Sequence models*
- Hidden Markov models
  - Inference with HMM
  - Supervised Learning for HMM

Most likely state sequence

- Input:
  - A hidden Markov model (π, A, B)
  - An observation sequence $\mathbf{x} = (x_1, x_2, \cdots, x_n)$

- Output: A state sequence $\mathbf{y} = (y_1, y_2, \cdots, y_n)$ that corresponds to
  - Maximum *a posteriori* inference (MAP inference)

$$\arg\max_{\mathbf{y}} P(\mathbf{y}|\mathbf{x}, \pi, A, B)$$

- Computationally: combinatorial optimization

MAP inference

- We want $\arg\max_{\mathbf{y}} P(\mathbf{y}|\mathbf{x}, \pi, A, B)$
- We have defined

$$P(x_1, x_2, \cdots, x_n, y_1, y_2, \cdots y_n) = P(y_1) \prod_{i=1}^{n-1} P(y_{i+1}|y_i) \prod_{i=1}^{n} P(x_i|y_i)$$

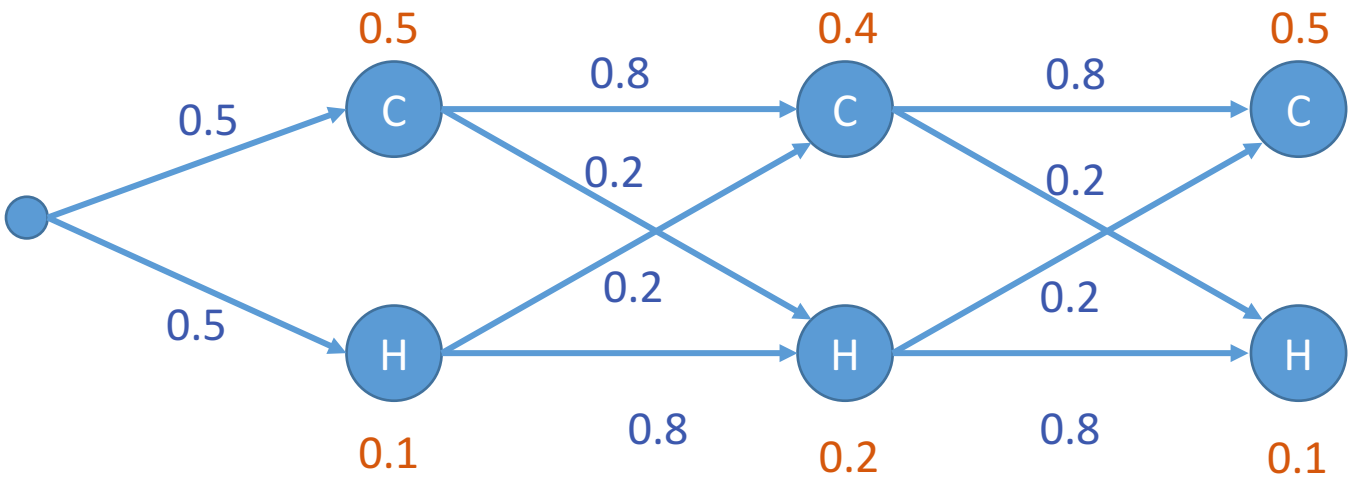
- But $P(\mathbf{y}|\mathbf{x}, \pi, A, B) \propto P(\mathbf{x}, \mathbf{y}|\pi, A, B)$
  - And we don't care about P(**x**) we are maximizing over **y**
- So, $\arg\max_{\mathbf{y}} P(\mathbf{y}|\mathbf{x}, \pi, A, B) = \arg\max_{\mathbf{y}} P(\mathbf{y}, \mathbf{x}|\pi, A, B)$

Jason's ice cream

#cones

	p(…|C)	p(…|H)	p(…|START)
(1|…)	**0.5**	**0.1**	
(2|…)	**0.4**	**0.2**	
(3|…)	**0.1**	**0.7**	
(C|…)	**0.8**	**0.2**	**0.5**
(H|…)	**0.2**	**0.8**	**0.5**

- Best tag sequence for P("1,2,1")?



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(H|…)	**0.2**	**0.8**	**0.5**

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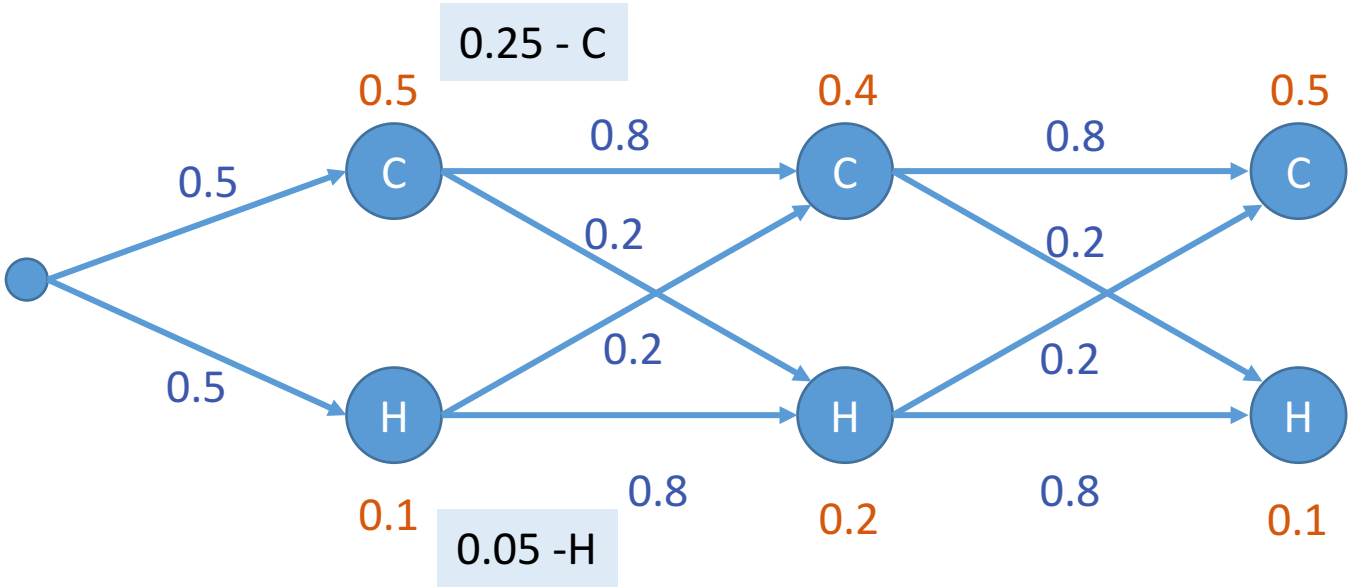

Jason's ice cream

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	p(…|C)	p(…|H)	p(…|START)
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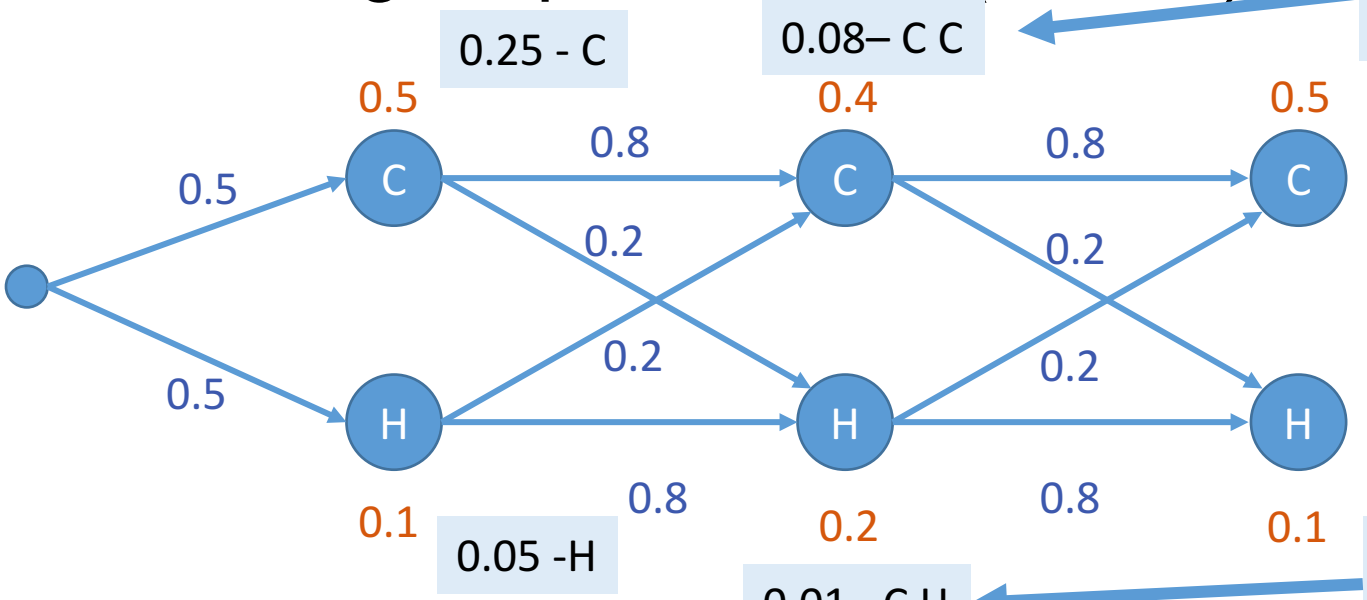
(3|…)	**0.1**	**0.7**	
(C|…)	**0.8**	**0.2**	**0.5**
(H|…)	**0.2**	**0.8**	**0.5**

- Best tag sequence for P("1,2,1")?

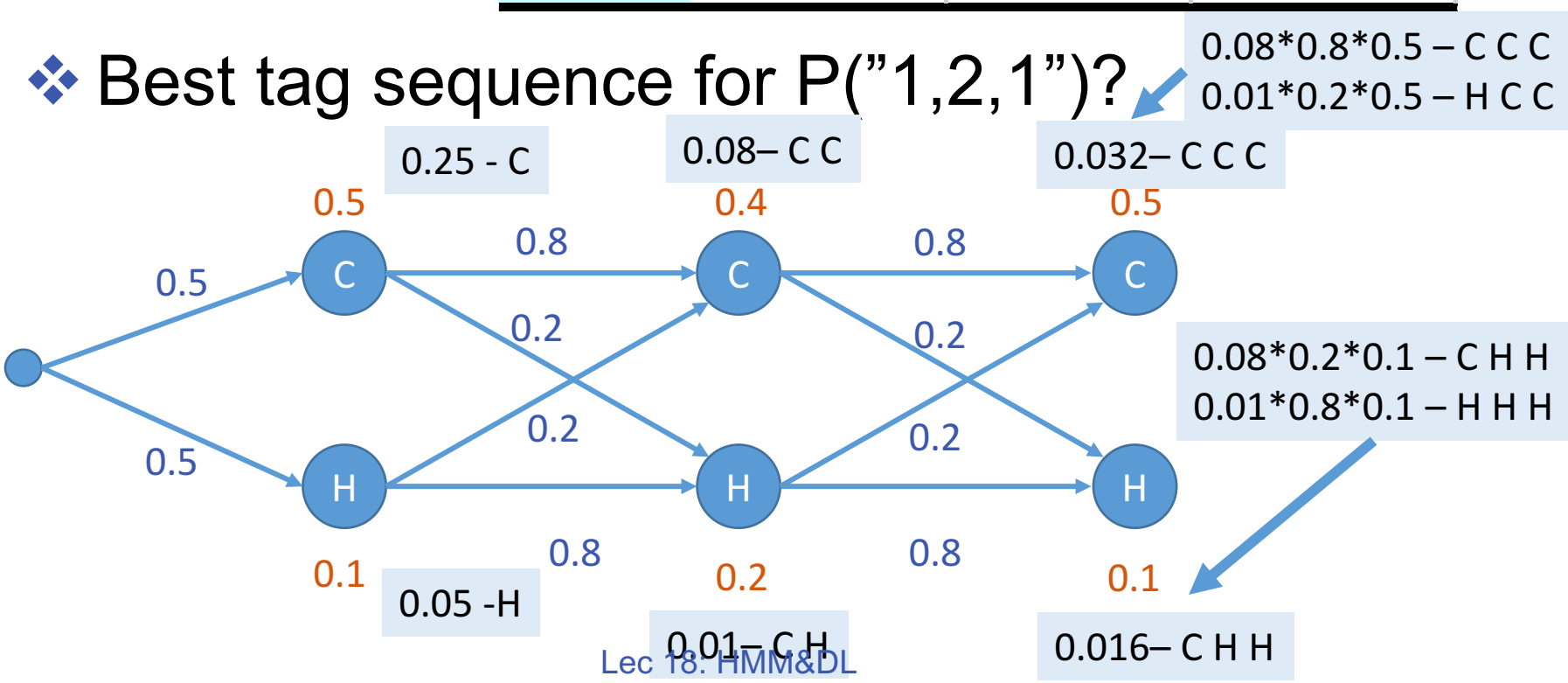


Jason's ice cream

#cones

	p(…|C)	p(…|H)	p(…|START)
(1|…)	**0.5**	**0.1**	
(2|…)	**0.4**	**0.2**	
(3|…)	**0.1**	**0.7**	
(C|…)	**0.8**	**0.2**	**0.5**
(H|…)	**0.2**	**0.8**	**0.5**

- Best tag sequence for P("1,2,1")?

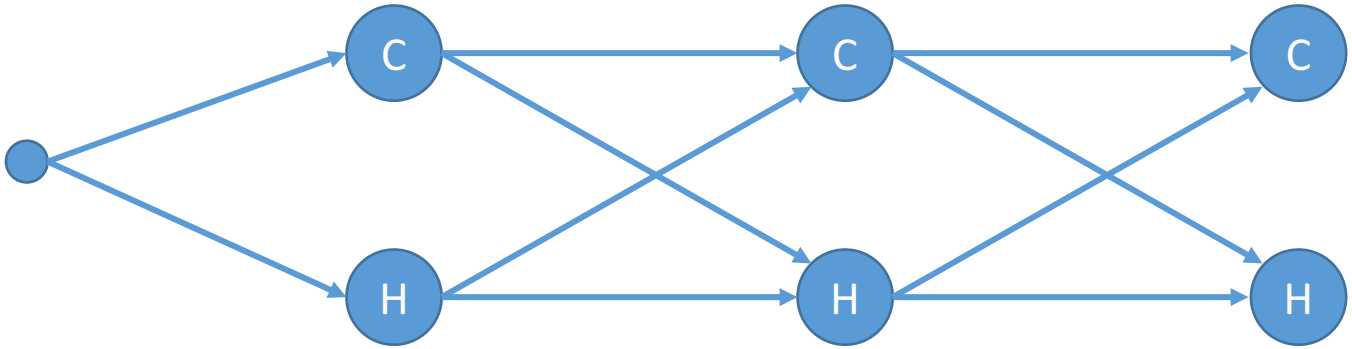


Your turn

#cones

	p(…|C)	p(…|H)	p(…|START)
(1|…)	**0.5**	**0.1**	
(2|…)	**0.4**	**0.2**	
(3|…)	**0.1**	**0.7**	
(C|…)	**0.8**	**0.2**	**0.5**
(H|…)	**0.2**	**0.8**	**0.5**

- Best tag sequence for P(”3,3,2”)?



Viterbi algorithm

π: Initial probabilities
A: Transitions
B: Emissions

Max-product algorithm for first order sequences

1. Initial: For each state s, calculate

$$\text{score}_1(s) = P(s)P(x_1|s) = \pi_s B_{x_1,s}$$

1. Recurrence: For i = 2 to n, for every state s, calculate

$$\begin{aligned}\text{score}_i(s) &= \max_{y_{i-1}} P(s|y_{i-1})P(x_i|s)\text{score}_{i-1}(y_{i-1}) \\ &= \max_{y_{i-1}} A_{y_{i-1},s}B_{s,x_i}\text{score}_{i-1}(y_{i-1})\end{aligned}$$

1. Final state: calculate

$$\max_{\mathbf{y}} P(\mathbf{y}, \mathbf{x}|\pi, A, B) = \max_s \text{score}_n(s)$$

This only calculates the max. To get final answer (*argmax*),

- keep track of which state corresponds to the max at each step
- build the answer using these back pointers

Questions?

General idea

- Dynamic programming
  - The best solution for the full problem relies on best solution to sub-problems
  - Memoize partial computation

- Examples
  - Viterbi algorithm
  - Dijkstra's shortest path algorithm
  - …

Complexity of inference

- Complexity parameters
  - Input sequence length: n
  - Number of states: K
- Memory
  - Storing the table: nK (scores for all states at each position)
- Runtime
  - At each step, go over pairs of states
  - $O(nK^2)$

Outline

- *Sequence models*
- Hidden Markov models
  - Inference with HMM
  - Supervised Learning for HMM

Learning HMM parameters

- Assume we know the number of states in the HMM
- Two possible scenarios
  1. We are given a data set D = {<$\mathbf{x}_i$, $\mathbf{y}_i$>} of sequences labeled with states

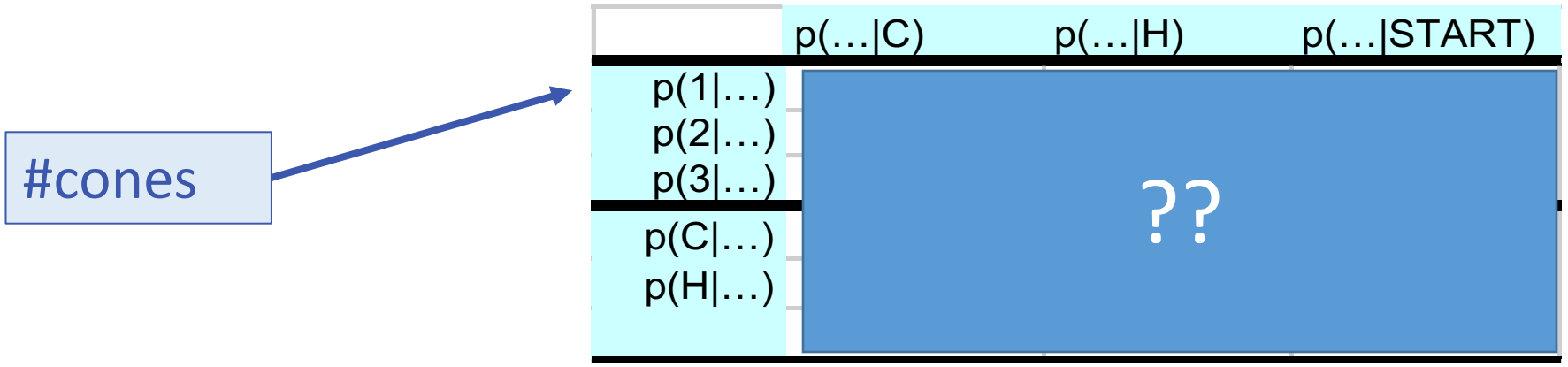
     And we have to learn the parameters of the HMM (π, A, B)

     Supervised learning with complete data
  2. We are given only a collection of sequences D = {$\mathbf{x}_i$}

     And we have to learn the parameters of the HMM (π, A, B)

     Unsupervised learning, with incomplete data

Jason's ice cream



- Can we figure out (π, A, B) from history records?

#cones	1	2	1	1	2	3	3	3	3	2	3	1	2
Hot/Cold	C	C	C	C	H	H	H	H	C	C	H	H	H

#cones	3	2	2	2	2	3	1	1	1	2	3	2	2
Hot/Cold	H	H	H	C	C	H	H	C	C	H	H	H	C

Supervised learning of HMM

- We are given a dataset D = {<$\mathbf{x}_i$, $\mathbf{y}_i$>}
  - Each $\mathbf{x}_i$ is a sequence of observations and $\mathbf{y}_i$ is a sequence of states that correspond to $\mathbf{x}_i$

  Goal: Learn initial, transition, emission distributions (π, A, B)

- How do we learn the parameters of the probability distribution?
  - The maximum likelihood principle

Where have we seen this before?

$$(\hat{\pi}, \hat{A}, \hat{B}) = \max_{\pi,A,B} P(D|\pi, A, B) = \max_{\pi,A,B} \prod_i P(\mathbf{x}_i, \mathbf{y}_i|\pi, A, B)$$

And we know how to write this in terms of the parameters of the HMM

Supervised learning details

$$(\hat{\pi}, \hat{A}, \hat{B}) = \max_{\pi,A,B} P(D|\pi, A, B) = \max_{\pi,A,B} \prod_i P(\mathbf{x}_i, \mathbf{y}_i|\pi, A, B)$$

π, A, B can be estimated separately just by counting

- Makes learning simple and fast

[Exercise: Derive the following using derivatives of the log likelihood.]

Number of instances where the first state is s

$$\pi_s = \frac{\text{count}(\text{start} \rightarrow s)}{n}$$

Number of examples

Initial probabilities

$$A_{s',s} = \frac{\text{count}\,(s \rightarrow s')}{\text{count}\,(s)}$$

Transition probabilities

$$B_{s,x} = \frac{\text{count}\begin{pmatrix} s \\ \downarrow \\ x \end{pmatrix}}{\text{count}\,(s)}$$

Emission probabilities

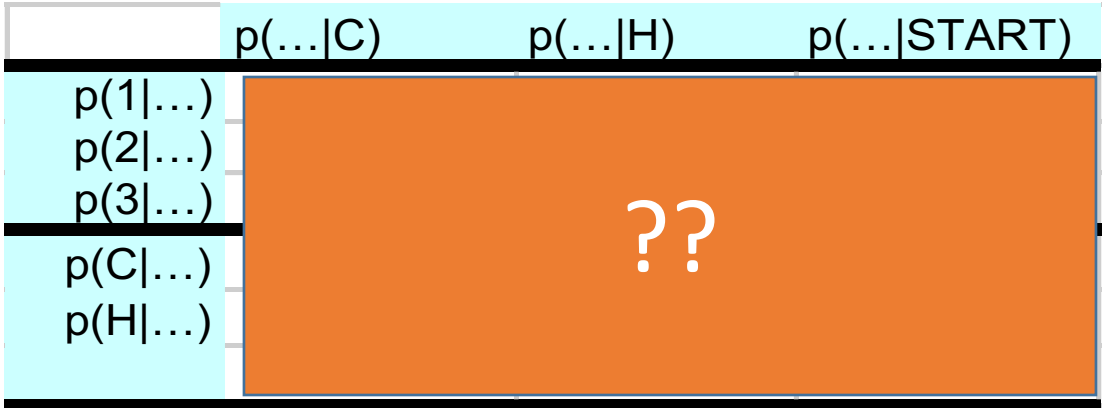
Priors and smoothing

- Maximum likelihood estimation works best with lots of annotated data
  - Never the case
- Priors inject information about the probability distributions
- Effectively additive smoothing
  - Add small constants to the counts

Question we will not answer in this lecture

- Can we figure out (π, A, B) from just observation

#cones



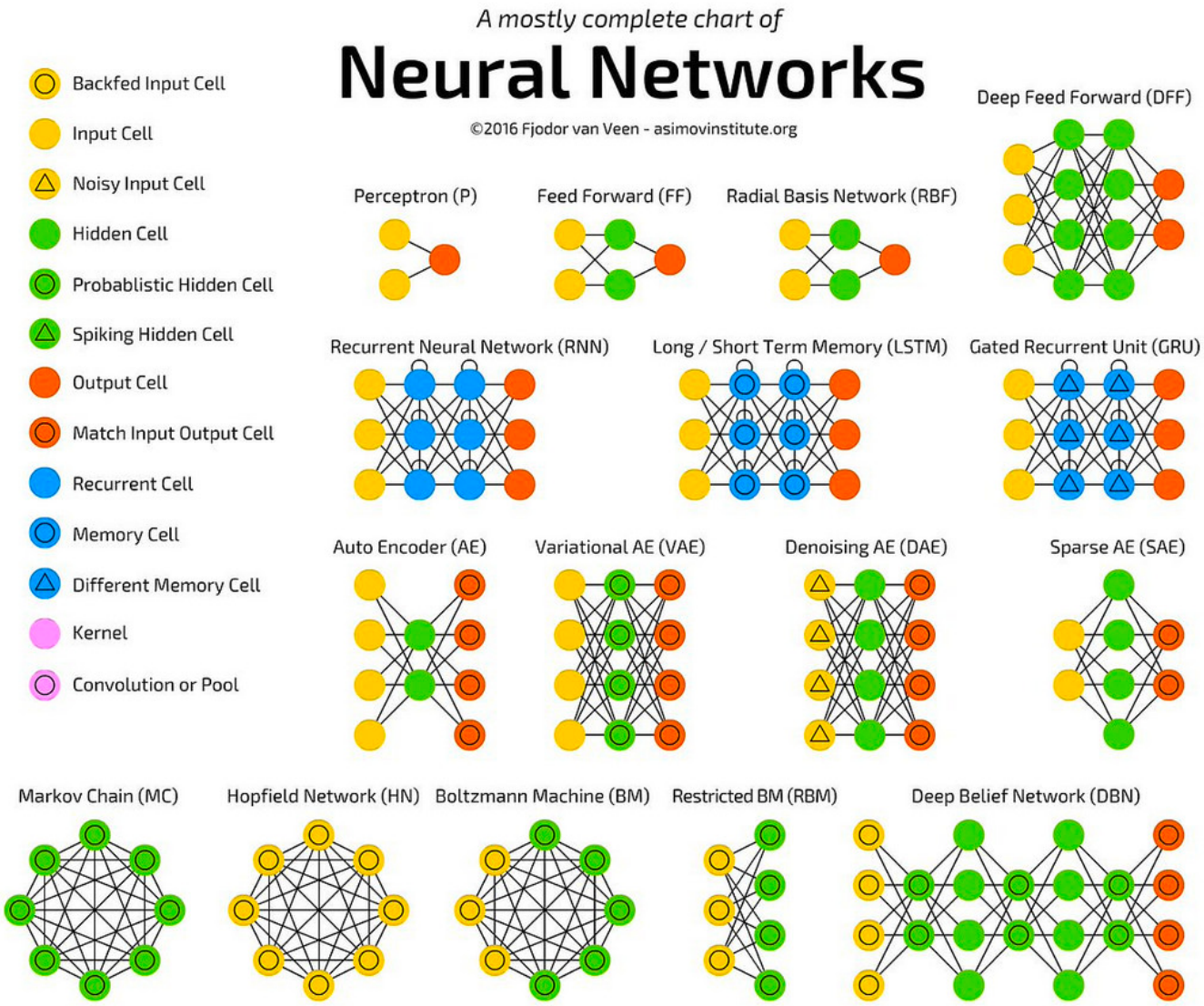
#cones	1	2	1	1	2	3	3	3	3	2	3	1	2
Hot/Cold	??												

#cones	3	2	2	2	2	3	1	1	1	2	3	2	2
Hot/Cold	??												

Hidden Markov Models summary

- Predicting sequences
  - As many output states as observations
- Markov assumption helps decompose the score
- Several algorithmic questions
  - Most likely state (decoding)
  - Learning parameters
    - Supervised, Unsupervised

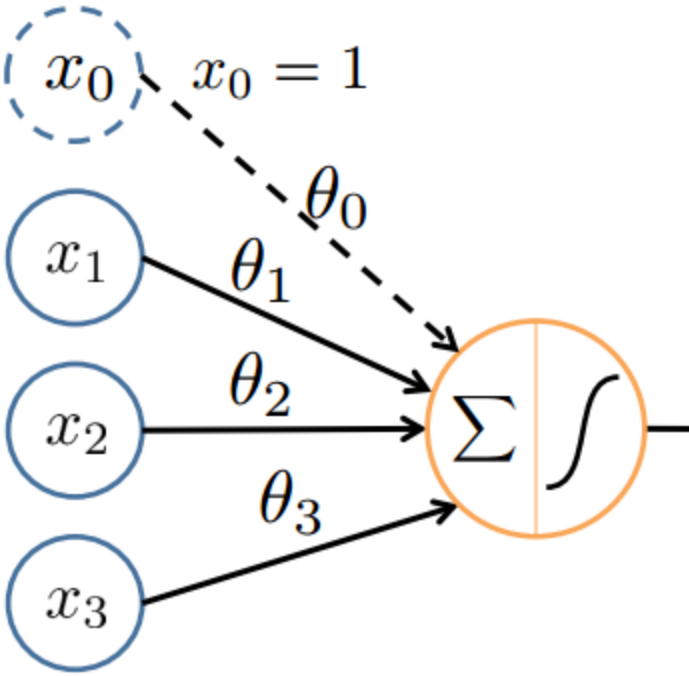
Neural Network



This lecture

- Neural Network
- Recurrent Neural Network

Neural Network

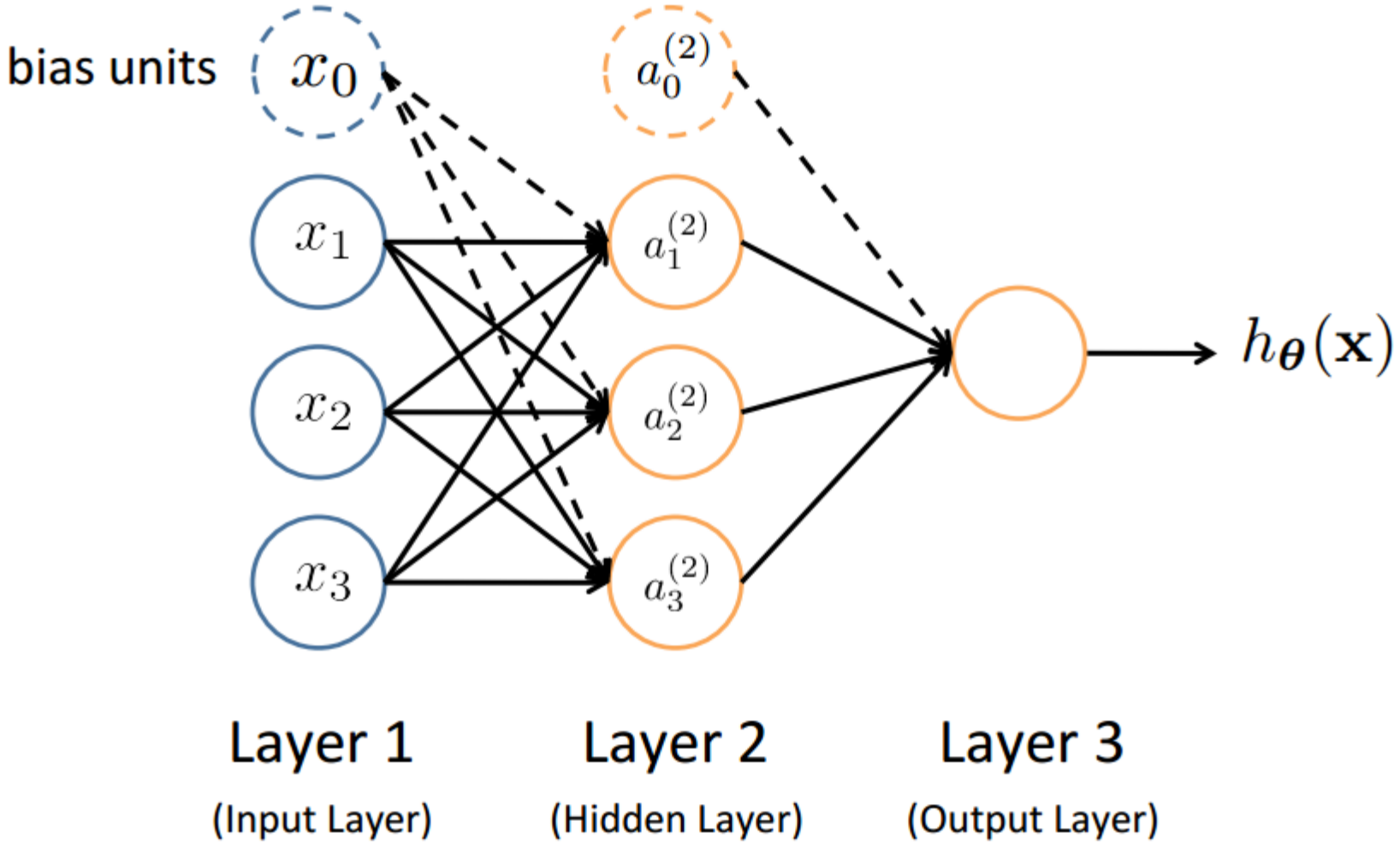


$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}\right) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}}}$$

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

Neural Network (feed forward)



Slide by Andrew Ng

Feed-Forward Process

- Input layer units are features (e.g., words)
  - Usually, one-hot vector or word embedding
- Working forward through the network, the **input function** is applied to compute the input value
  - E.g., weighted sum of the input
- The **activation function** transforms this input function into a final value
  - Typically a **nonlinear** function (e.g, **sigmoid**)

Based on slide by T. Finin, M. desJardins, L Getoor, R. Par

Activation functions

Also called transfer functions

$$output = activation(\boldsymbol{w}^T \boldsymbol{x} + b)$$

Name of the neuron	Activation function: $activation(z)$
Linear unit	z
Threshold/sign unit	$sign(z)$
Sigmoid unit	$\frac{1}{1+\exp(-z)}$
Rectified linear unit (ReLU)	$\max(0, z)$
Tanh unit	$\tanh(z)$

Many more activation functions exist (sinusoid, sinc, gaussian, polynomial…)

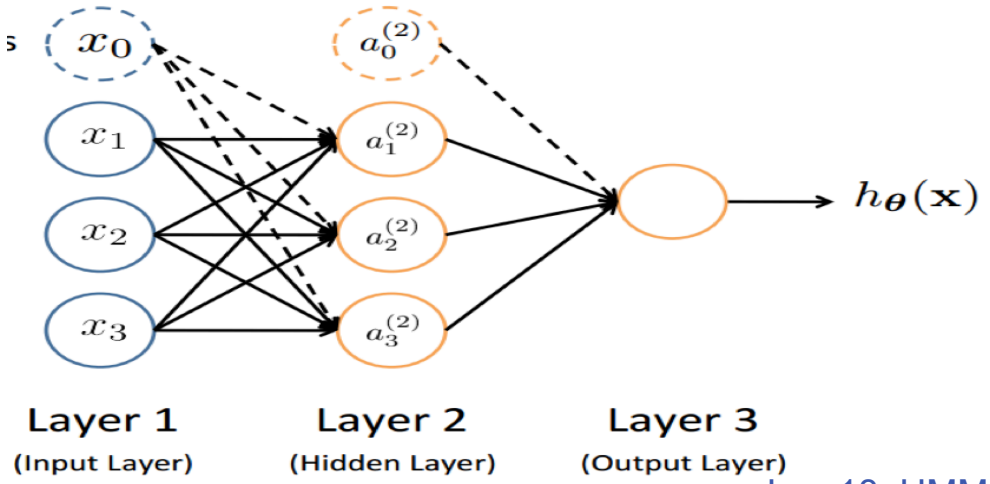
Vector Representation

$$a_1^{(2)} = g\left(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3\right) = g\left(z_1^{(2)}\right)$$

$$a_2^{(2)} = g\left(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3\right) = g\left(z_2^{(2)}\right)$$

$$a_3^{(2)} = g\left(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3\right) = g\left(z_3^{(2)}\right)$$

$$h_\Theta(\mathbf{x}) = g\left(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)}\right) = g\left(z_1^{(3)}\right)$$



Feed-Forward Steps:

$$\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{x}$$

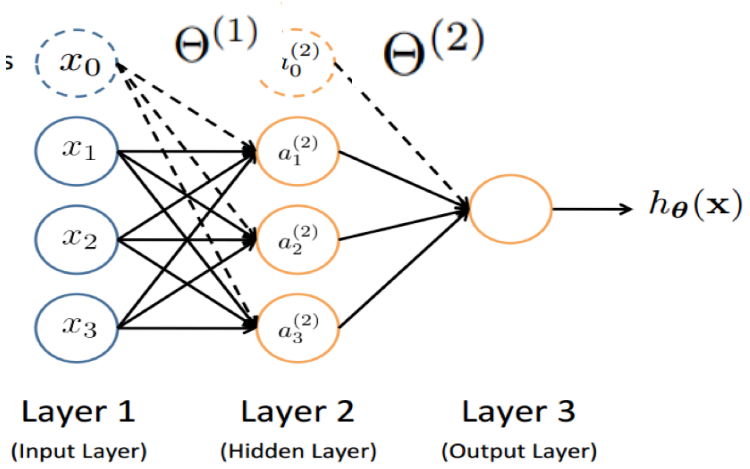
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

$$\text{Add } a_0^{(2)} = 1$$

$$\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$$

$$h_\Theta(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

Based on slide by Andrew Ng



$a_i^{(j)}$ = "activation" of unit i in layer j

$\Theta^{(j)}$ = weight matrix controlling function mapping from layer j to layer $j+1$

$$a_1^{(2)} = g(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)})$$

If network has s_j units in layer j *and* s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$.

$$\Theta^{(1)} \in \mathbb{R}^{3\times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times 4}$$

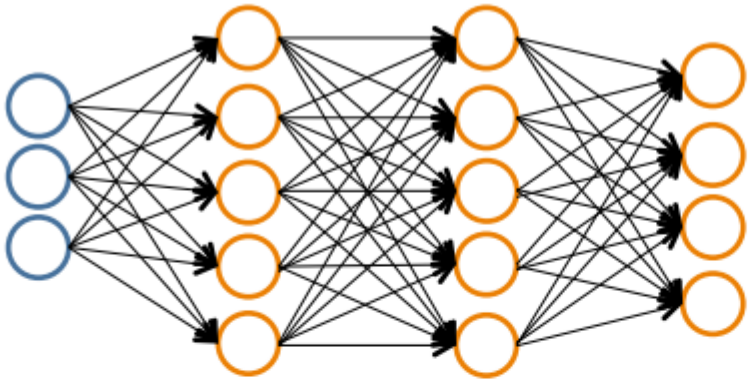
Can extend to multi-class

Pedestrian

Car

Motorcycle

Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

We want:

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$ when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$ when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$ when motorcycle

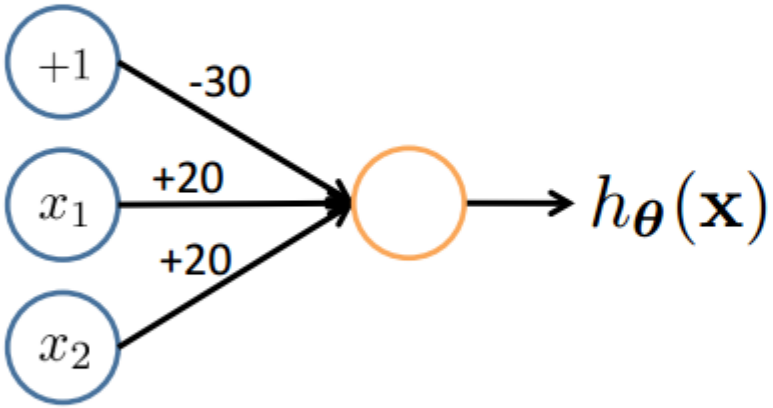
$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$ when truck

Why staged predictions?

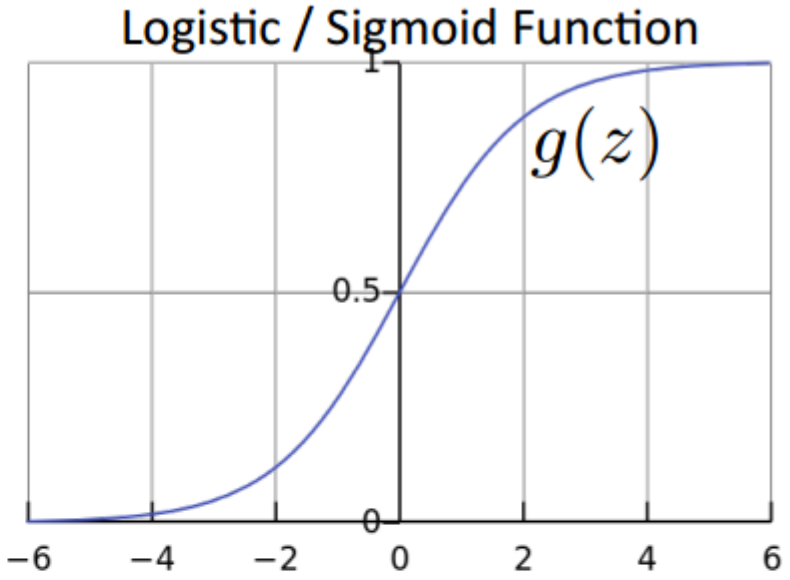
Simple example: AND

$x_1, x_2 \in \{0, 1\}$

$y = x_1$ AND x_2

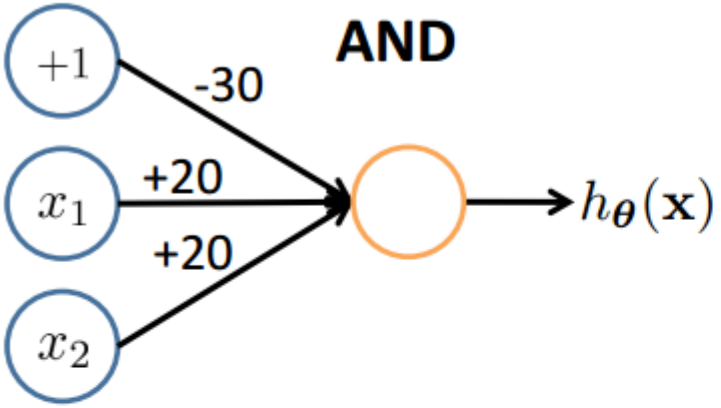


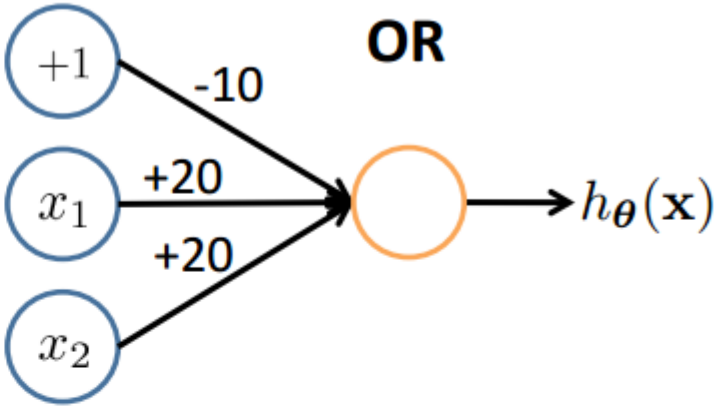
$\mathrm{h}_\Theta(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$

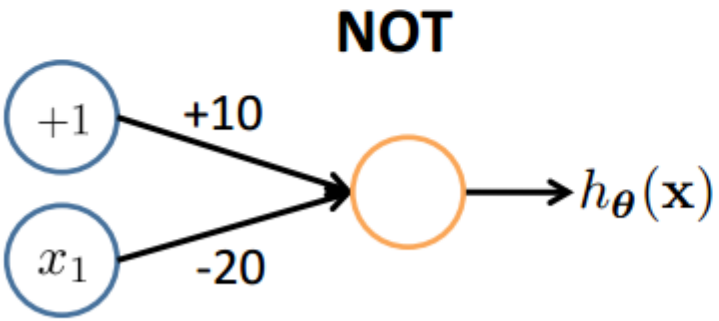


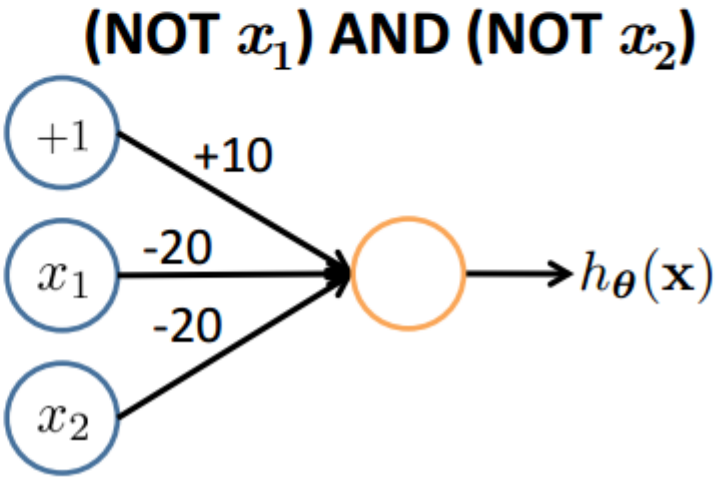
x_1	x_2	$\mathrm{h}_\Theta(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

Based on slide and example by Andrew Ng

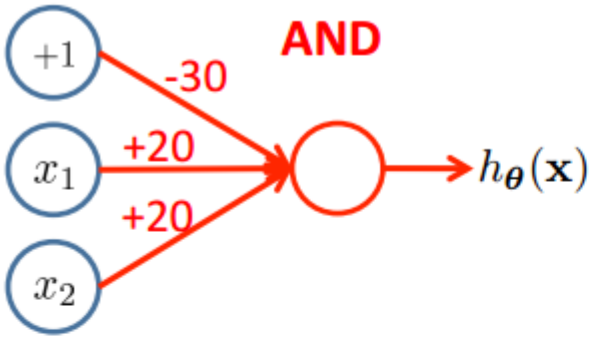

AND
+1
x_1
x_2
-30
+20
+20
$h_\theta(\mathbf{x})$

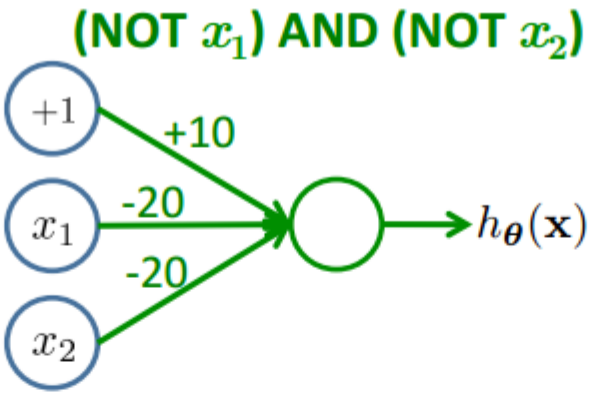

OR
+1
x_1
x_2
-10
+20
+20
$h_\theta(\mathbf{x})$

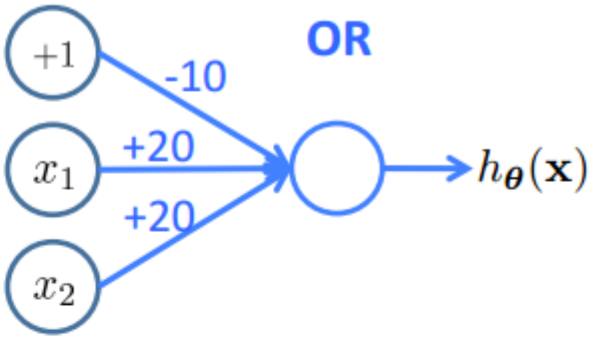

NOT
+1
x_1
+10
-20
$h_\theta(\mathbf{x})$

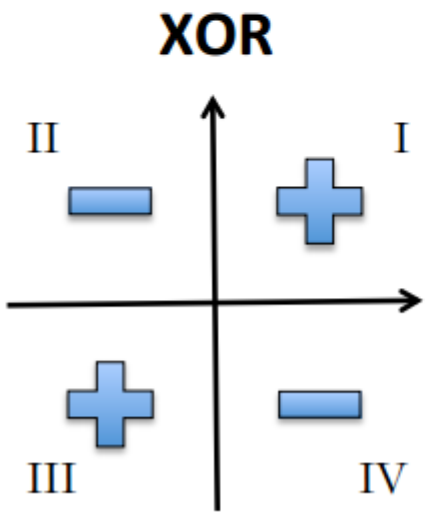

(NOT x_1) AND (NOT x_2)
+1
x_1
x_2
+10
-20
-20
$h_\theta(\mathbf{x})$

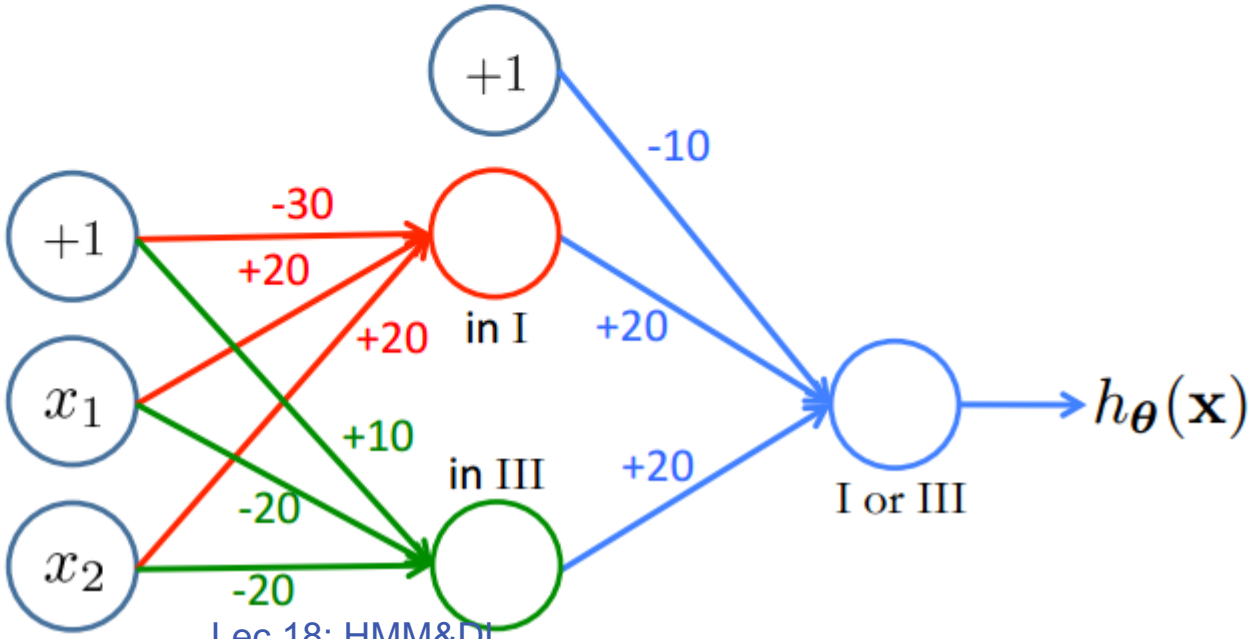
Combining Representations to Create Non-Linear Functions







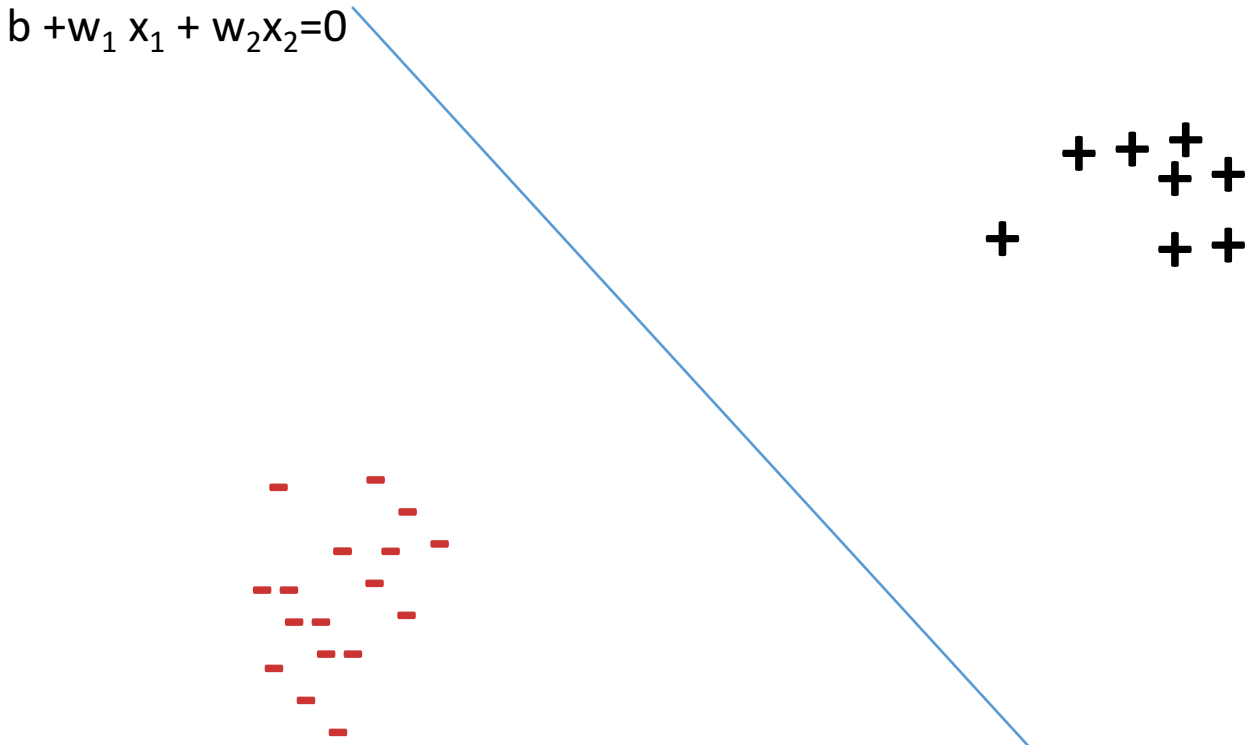




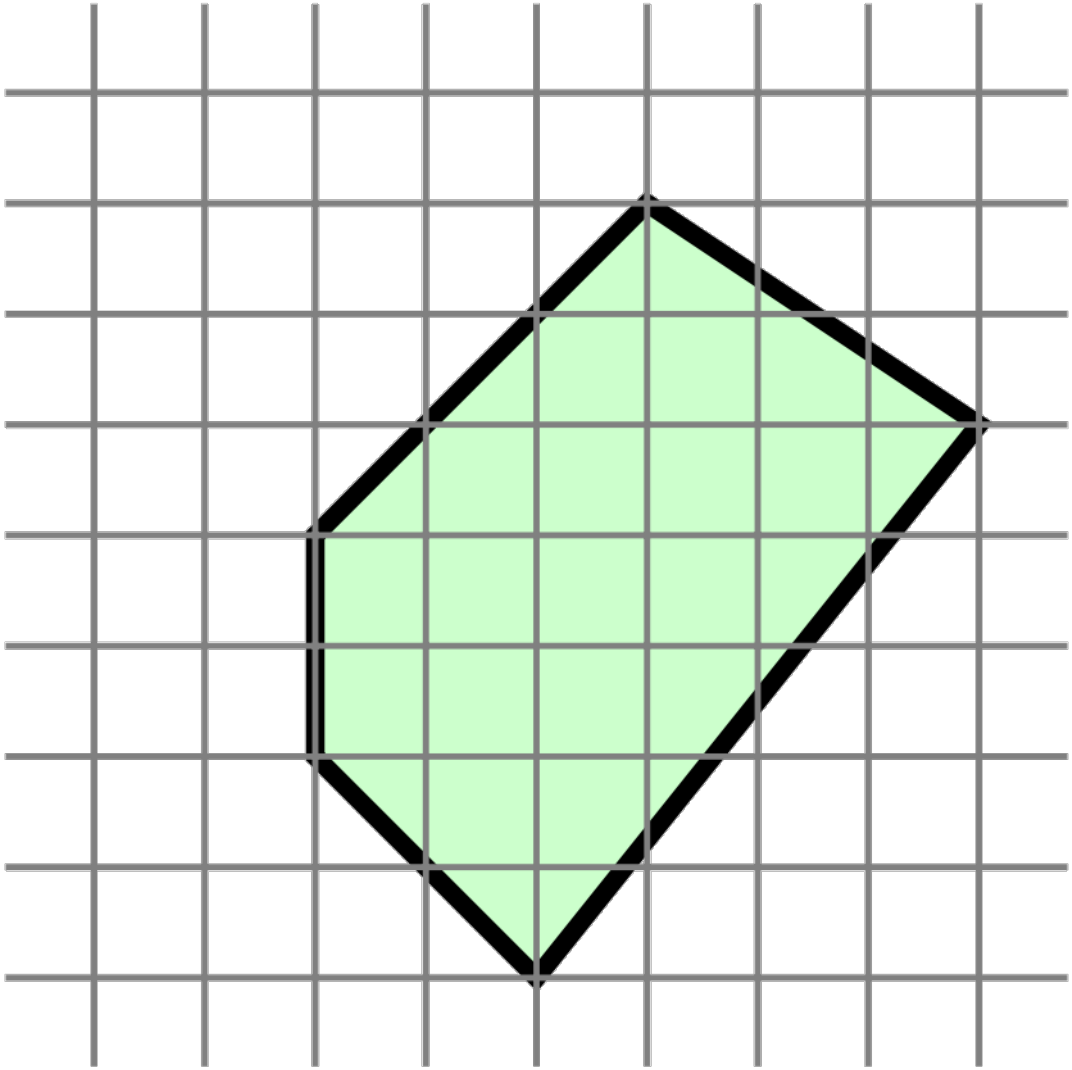
Based on example by Andrew Ng

A single neuron with threshold activation

Prediction = *sgn*$(b + w_1 x_1 + w_2 x_2)$



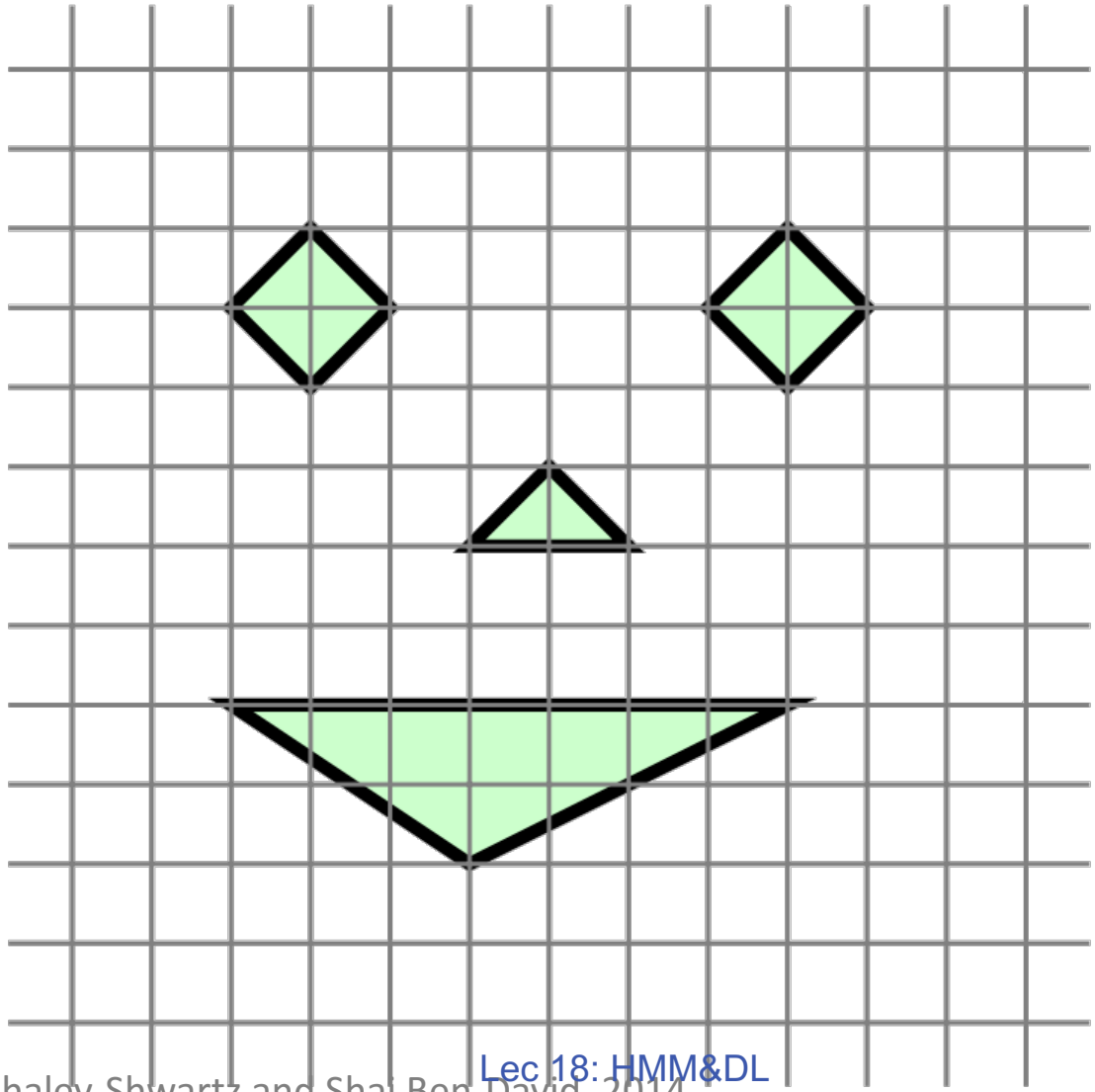
Two layers, with threshold activations



In general, convex polygons

Figure from Shai Shalev-Shwartz and Shai Ben-David, 2014

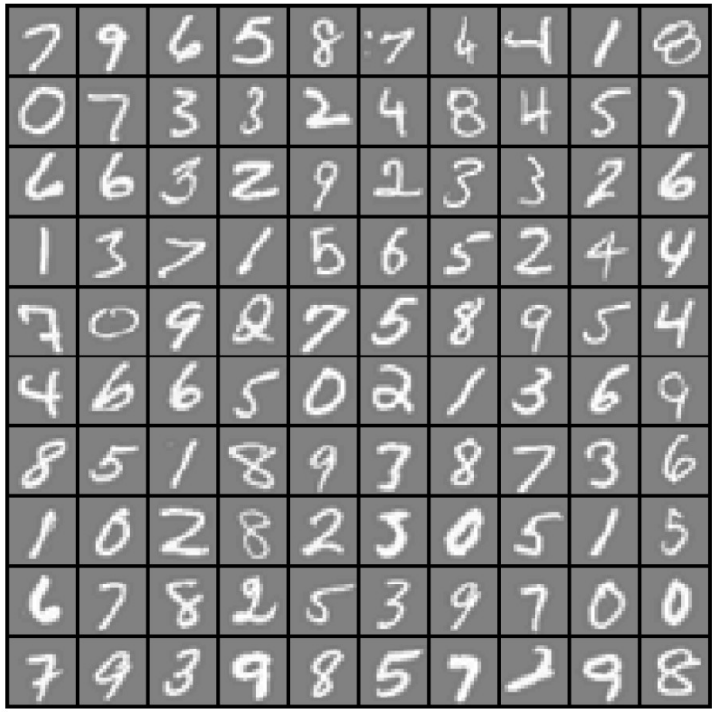
Three layers with threshold activations

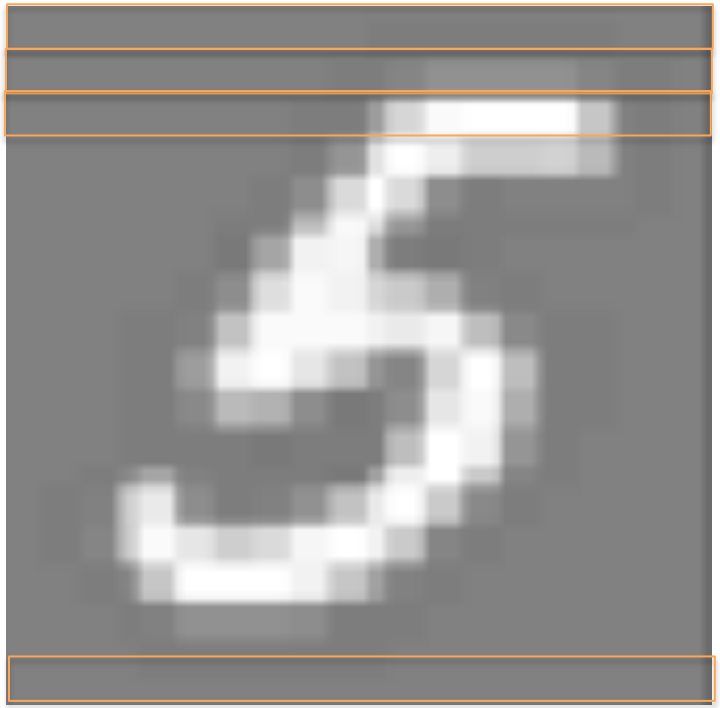


In general, unions of convex polygons

Figure from Shai Shalev-Shwartz and Shai Ben-David, 2014

Layering Representations





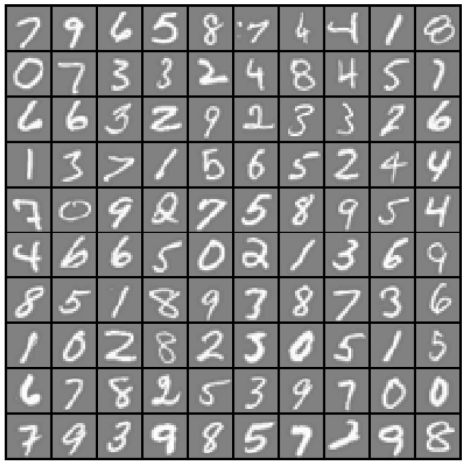
$x_1 \dots x_{20}$
$x_{21} \dots x_{40}$
$x_{41} \dots x_{60}$

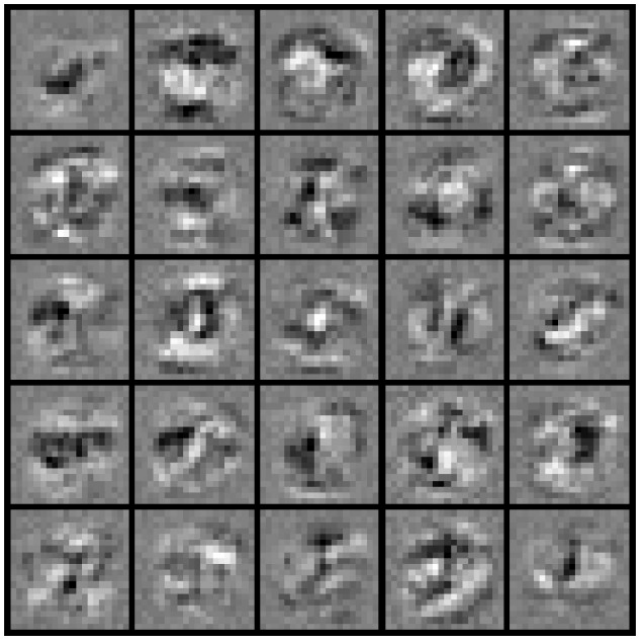
$x_{381} \dots x_{400}$

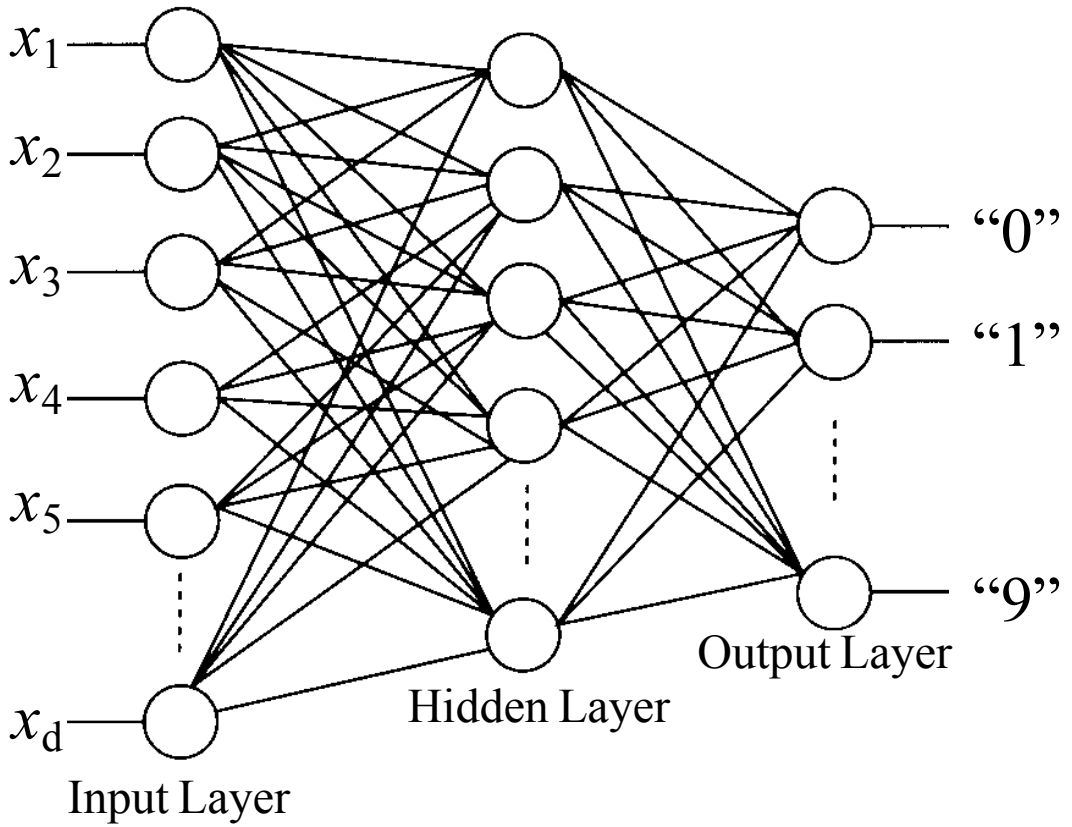
20 × 20 pixel images
$d = 400$ 10 classes

Each image is "unrolled" into a vector x of pixel intensities

Layering Representations







Visualization of Hidden Layer

This lecture

- Review: Neural Network
  - Learning NN
- Recursive and Recurrent NN

Why we need to learn this:
https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b

Recall: Learning as loss minimization

We have a classifier *NN* that is completely defined by its weights

Learn the weights by minimizing a loss L

$$\min_{\boldsymbol{w}} \sum_{i} L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$$

Perhaps with a *regularizer*

So far, we saw that this strategy worked for:

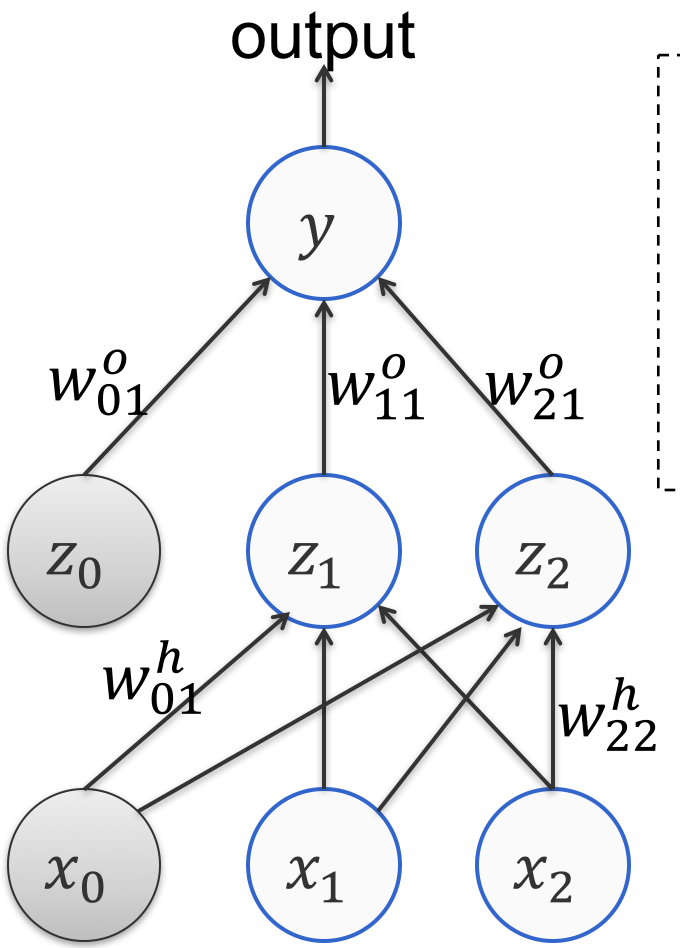
1. Logistic Regression
2. Support Vector Machines
3. Perceptron
4. LMS regression

Each minimizes a different loss function

All of these are linear models

Same idea for non-linear models too!

Back to our running example



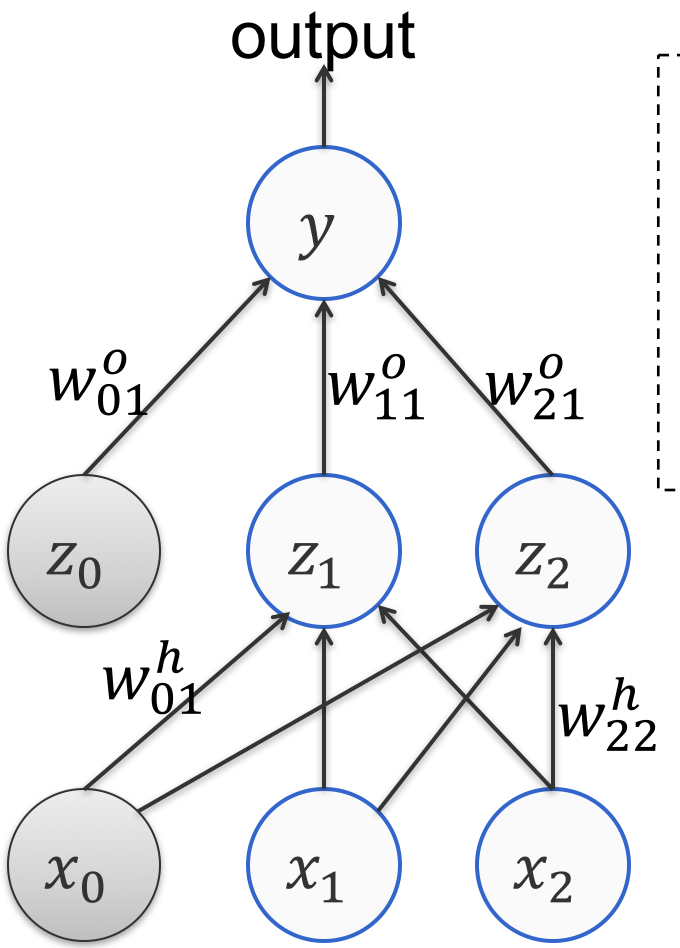
Given an input **x**, how is the output predicted

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

Back to our running example



Given an input **x**, how is the output predicted

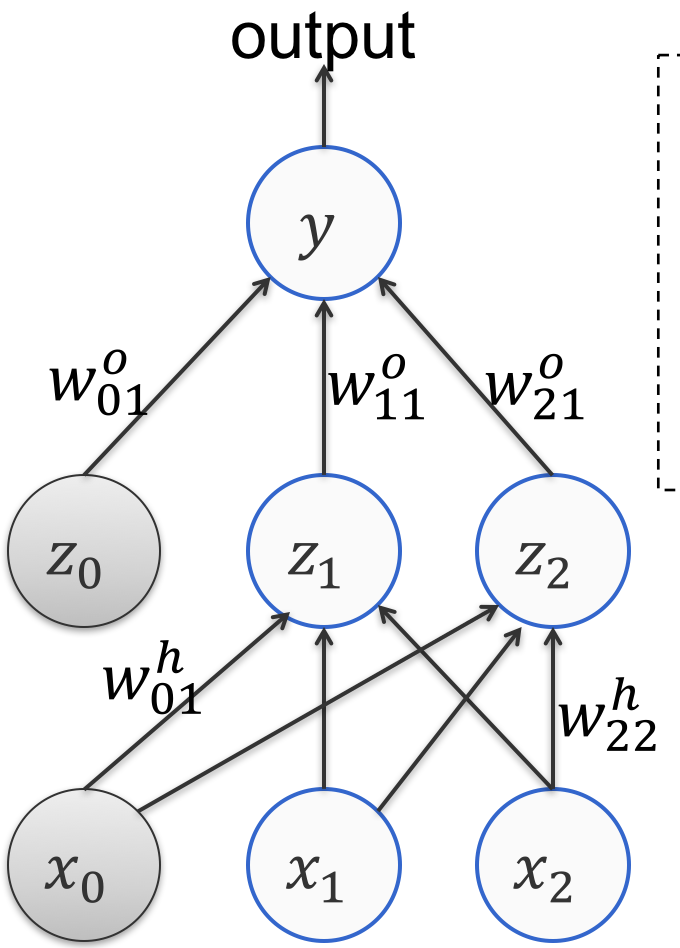
output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

$$z_1 = \sigma(w_{01}^h + w_{11}^h x_1 + w_{21}^h x_2)$$

Suppose the true label for this example is a number y^*

Back to our running example



Given an input **x**, how is the output predicted

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

$$z_1 = \sigma(w_{01}^h + w_{11}^h x_1 + w_{21}^h x_2)$$

Suppose the true label for this example is a number y^*

We can write the *square loss* for this example as:

$$L = \frac{1}{2}(y - y^*)^2$$

Learning as loss minimization

We have a classifier *NN* that is completely defined by its weights

Learn the weights by minimizing a loss L

$$\min_{\boldsymbol{w}} \sum_{i} L(NN(x_i, w), y_i)$$

Perhaps with a *regularizer*

How do we solve the optimization problem?

Stochastic gradient descent

$$\min_{w} \sum_{i} L(NN(x_i, w), y_i)$$

Given a training set S = $\{(\mathbf{x}_i, y_i)\}$

1. Initialize parameters w
2. For epoch = 1 … T:
   1. Shuffle the training set
   2. For each training example $(\mathbf{x}_i, y_i)$:
      - Treat this example as the entire dataset
        Compute the gradient of the loss $\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$
      - Update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \gamma_t \nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i))$
3. Return w

γ_t: learning rate, many tweaks possible

Stochastic gradient descent

$$\min_{w} \sum_{i} L(NN(x_i, w), y_i)$$

Given a training set S = $\{(\mathbf{x}_i, y_i)\}$, $\mathbf{x}$

1. Initialize parameters w
2. For epoch = 1 … T:
   1. Shuffle the training set
   2. For each training example $(\mathbf{x}_i, y_i)$:
      - Treat this example as the entire dataset
        Compute the gradient of the loss $\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$
      - Update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \gamma_t \nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i))$
3. Return w

The objective is not convex. Initialization can be important

γ_t: learning rate, many tweaks possible

Have we solved everything?

The derivative of the loss function?

$$\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$$

If the neural network is a differentiable function, we can find the gradient

- Or maybe its sub-gradient
- This is decided by the activation functions and the loss function

It was easy for SVMs and logistic regression

- Only one layer

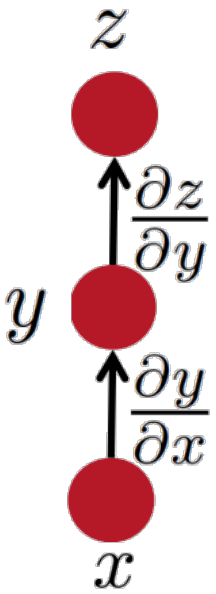
But how do we find the sub-gradient of a more complex function?

- Eg: A recent paper used a ~150 layer neural network for image classification!

We need an efficient algorithm: Backpropagation

Reminder: Chain rule for derivatives

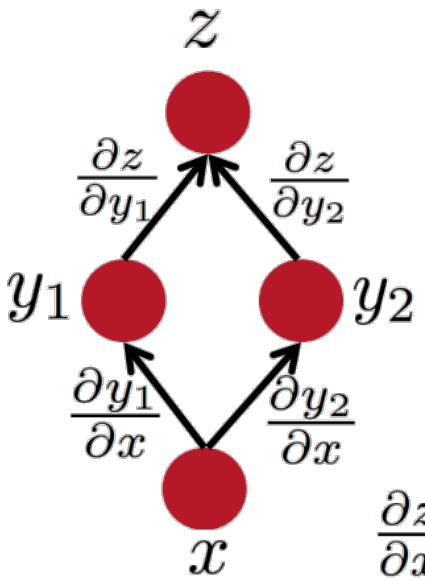
- If z is a function of y and y is a function of x
  - Then z is a function of x, as well
- Question: how to find $\frac{\partial z}{\partial x}$



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

Reminder: Chain rule for derivatives

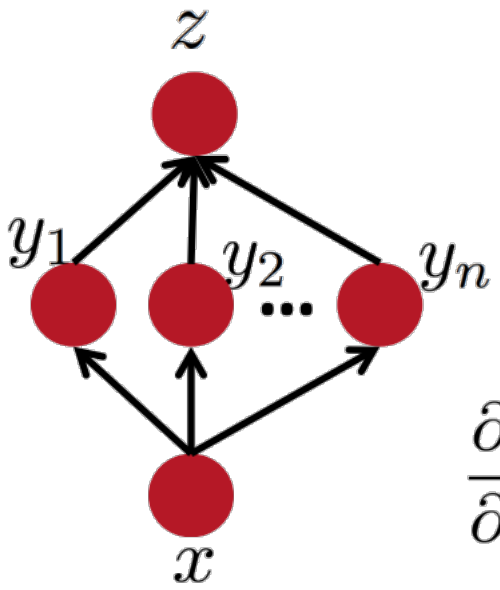
- If $z =$ a function of y_1 + a function of y_2, and the y_i's are functions of x
  - Then z is a function of x, as well
- Question: how to find $\frac{\partial z}{\partial x}$



$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

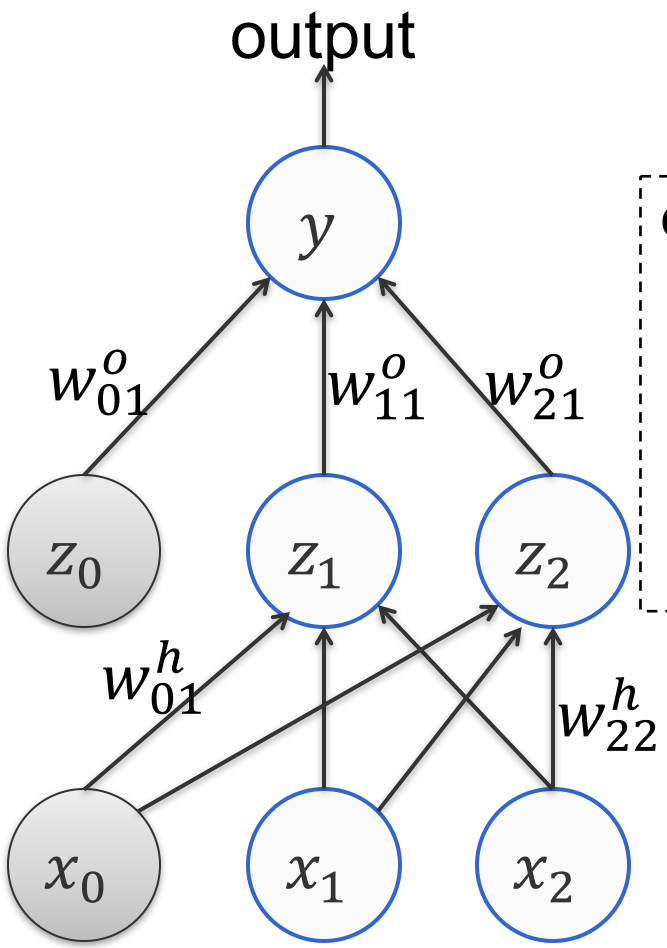
Reminder: Chain rule for derivatives

- If z is a sum of functions of y_i's, and the y_i's are functions of x
  - Then z is a function of x, as well
- Question: how to find $\frac{\partial z}{\partial x}$



$$\frac{\partial z}{\partial x} = \sum_{i=1}^{n} \frac{\partial z}{\partial y_i} \frac{\partial y_i}{\partial x}$$

Backpropagation



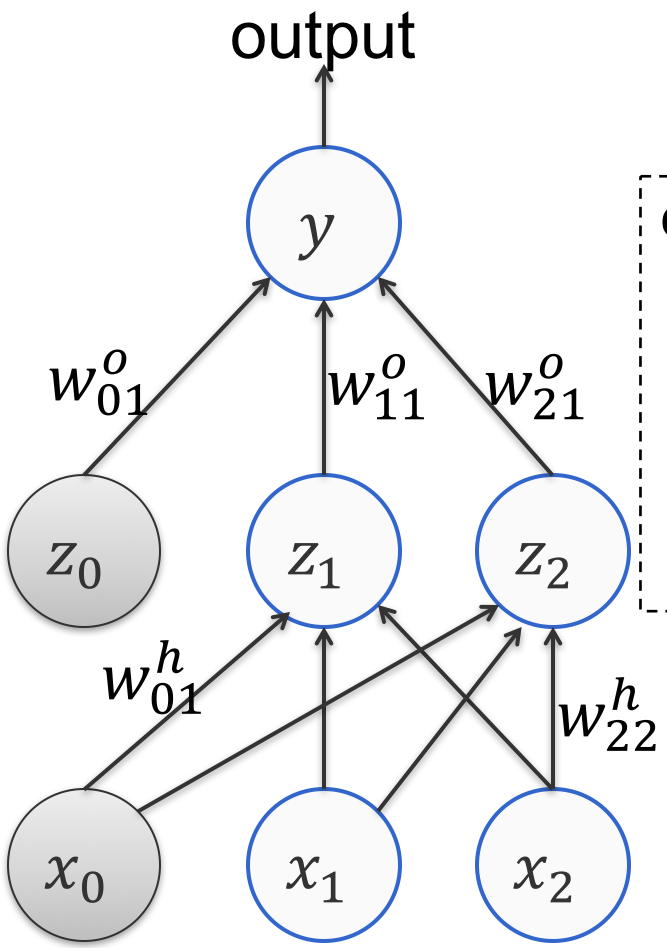
$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

Backpropagation



$$L = \frac{1}{2}(y - y^*)^2$$

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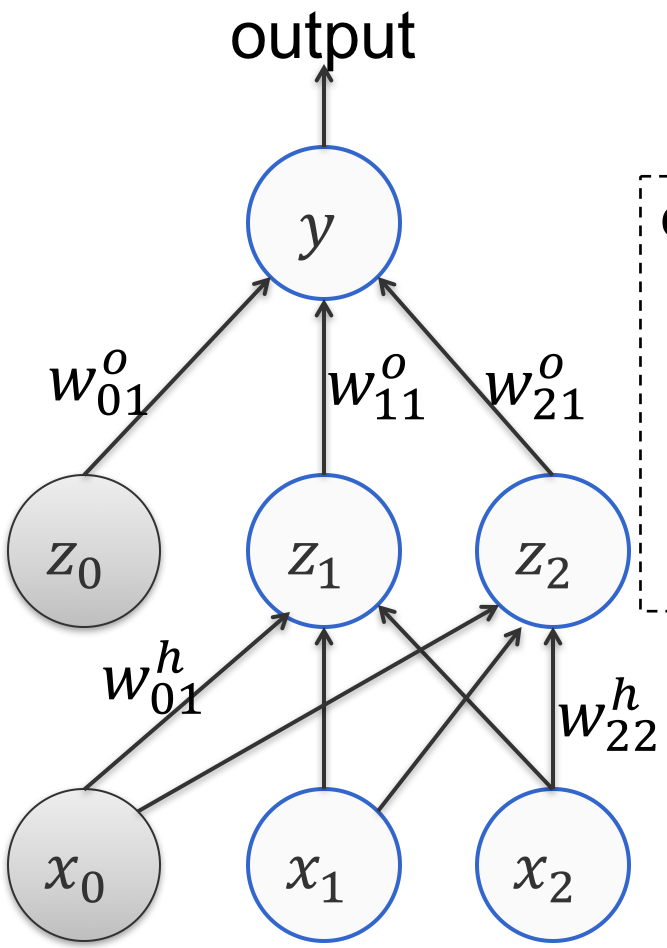
$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

We want to compute $\frac{\partial L}{\partial w_{ij}^{o}}$ and $\frac{\partial L}{\partial w_{ij}^{h}}$

Backpropagation

Applying the chain rule to compute the gradient (And remembering partial computations along the way to speed up things)



$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

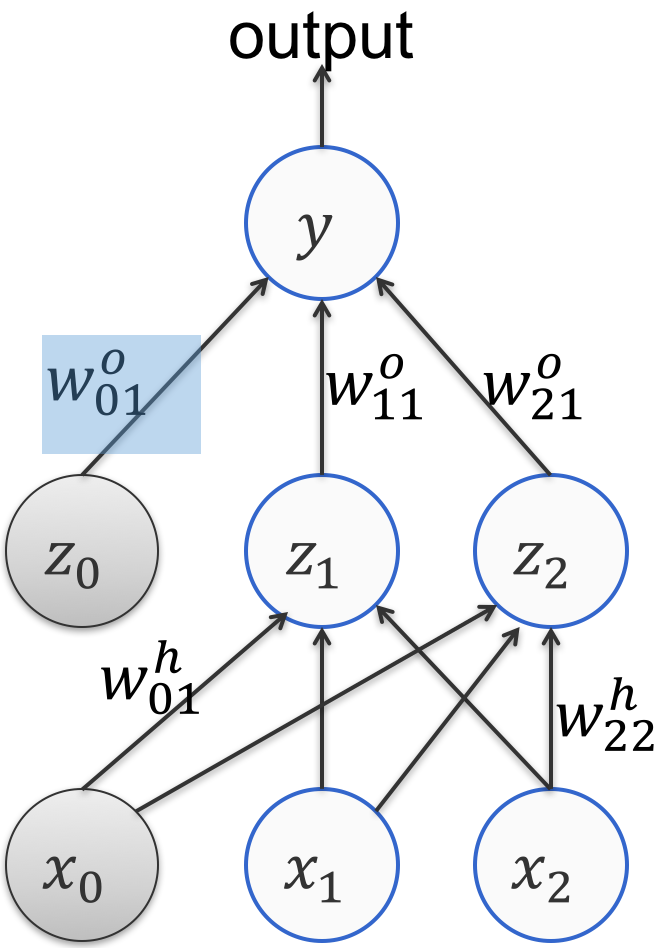
$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

We want to compute $\frac{\partial L}{\partial w_{ij}^{o}}$ and $\frac{\partial L}{\partial w_{ij}^{h}}$

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer

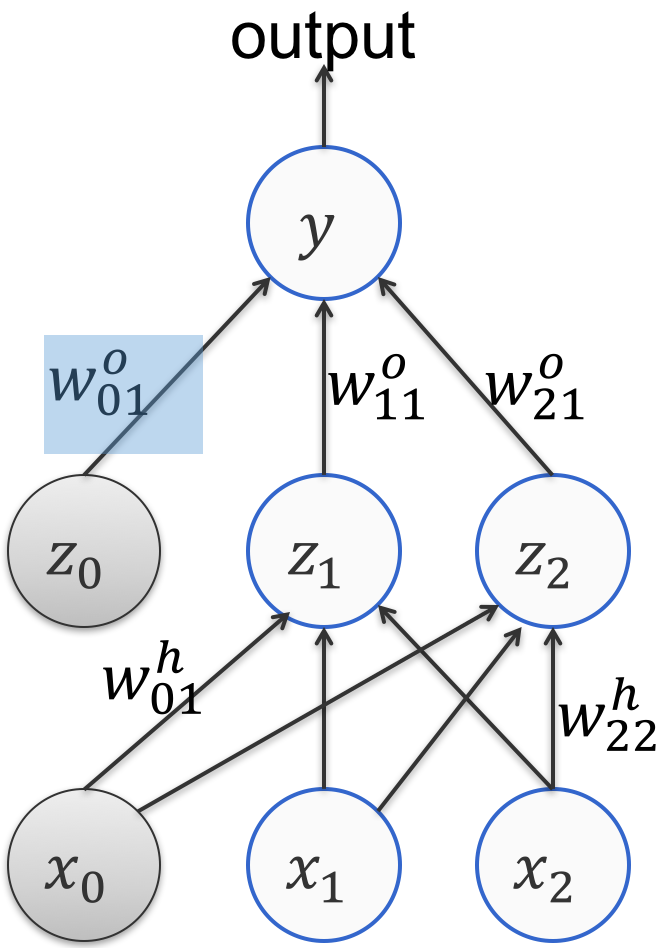


$$\frac{\partial L}{\partial w_{01}^o}$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer

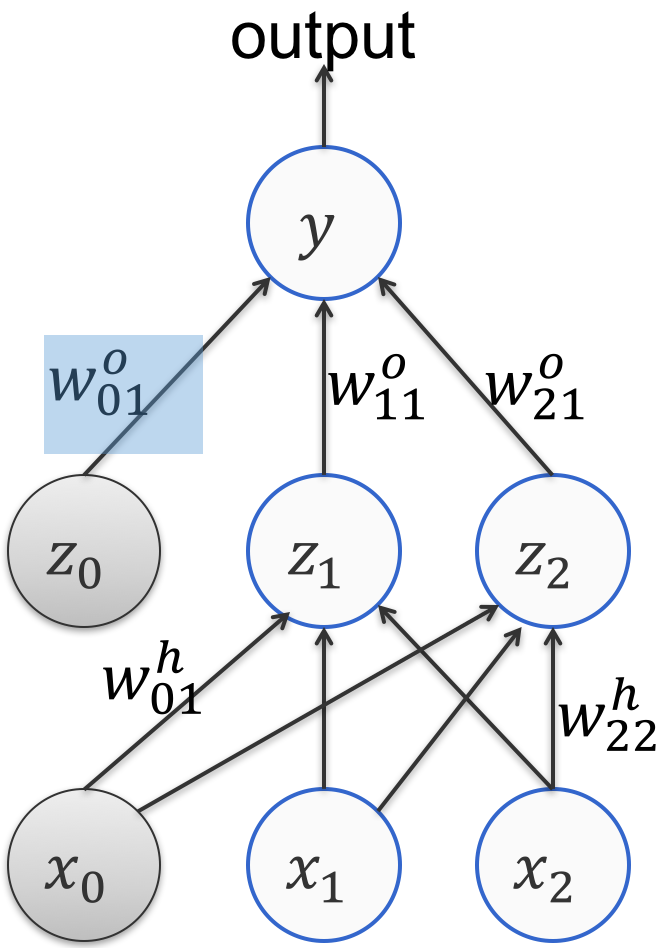


$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{01}^o}$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer



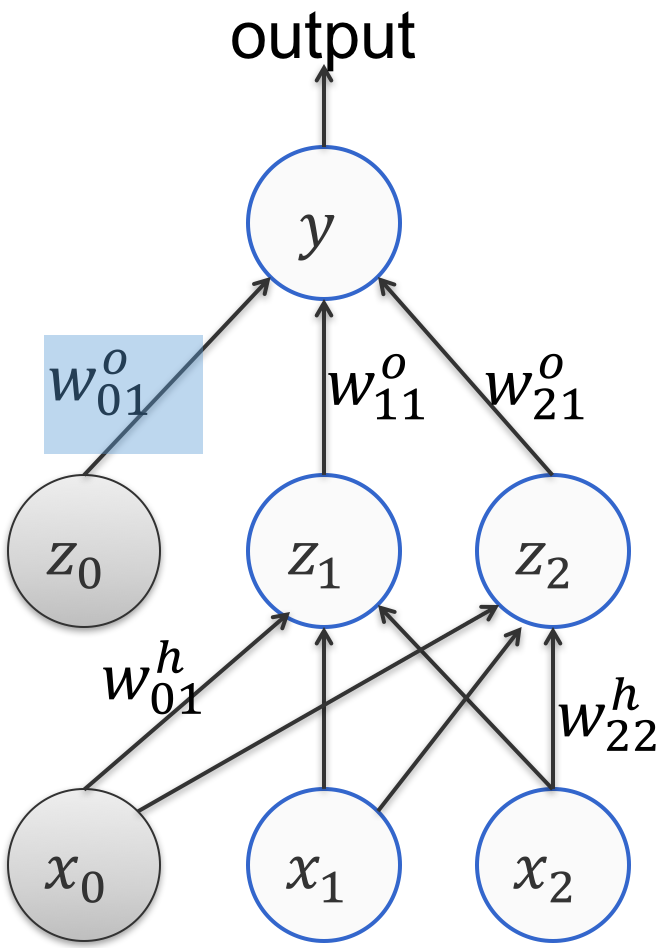
$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{01}^o}$$

$$\frac{\partial L}{\partial y} = y - y^*$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer



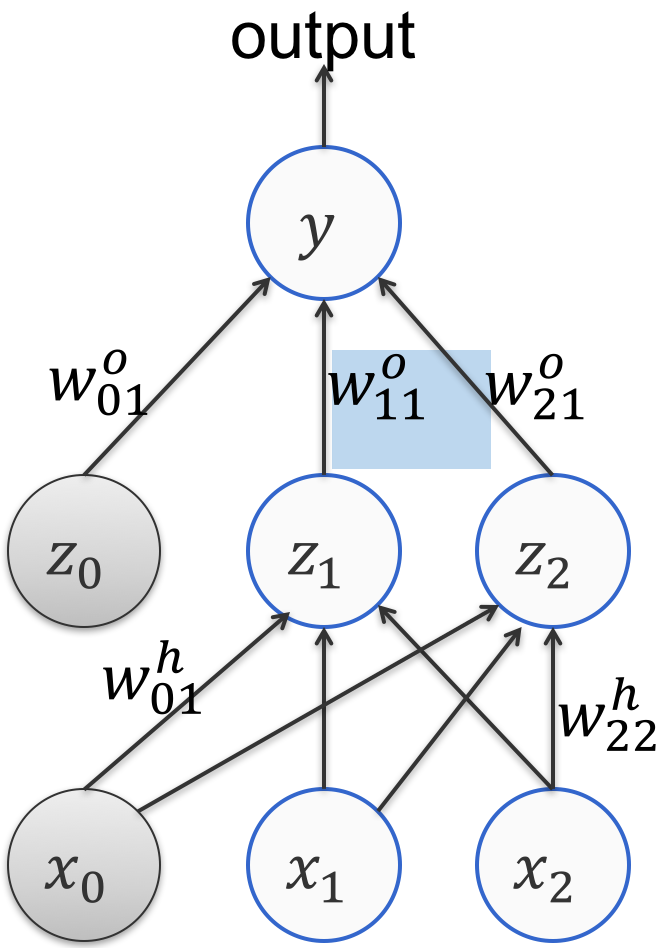
$$\frac{\partial L}{\partial w_{01}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{01}^o}$$

$$\frac{\partial L}{\partial y} = y - y^* \qquad \frac{\partial y}{\partial w_{01}^o} = 1$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $\quad y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer

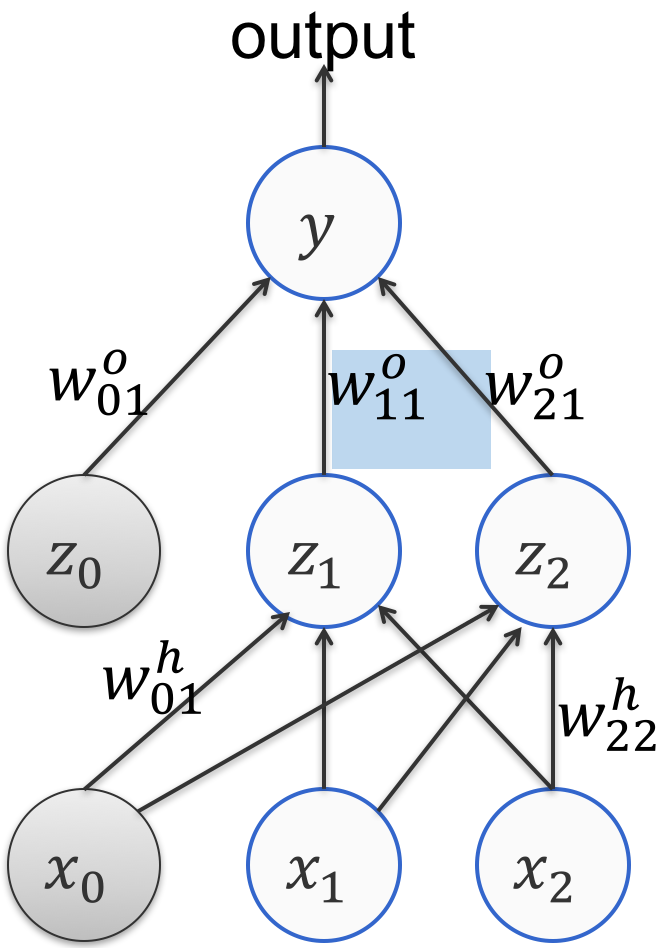


$$\frac{\partial L}{\partial w_{11}^o}$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer

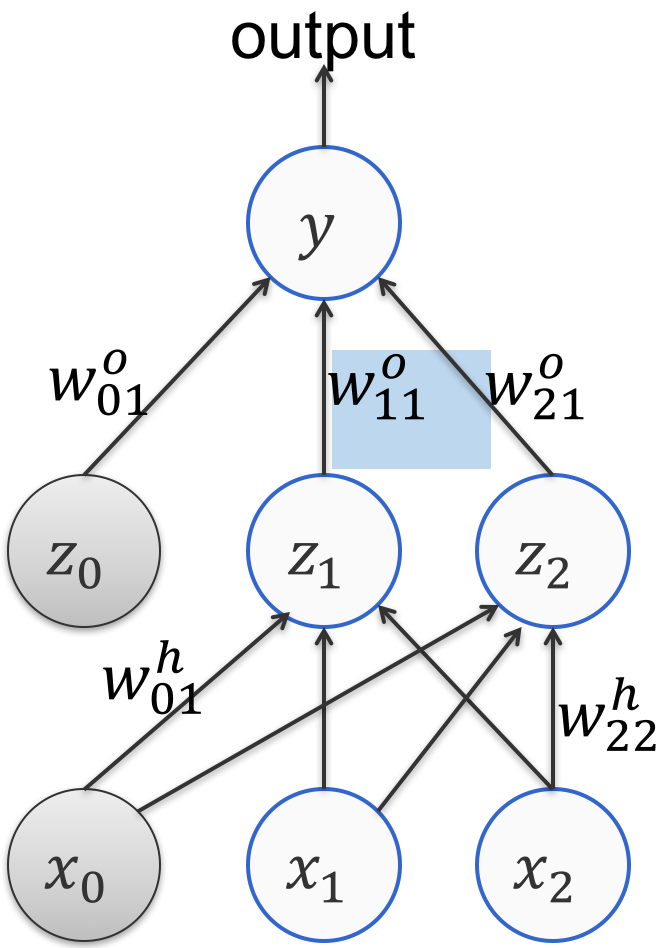


$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^0}$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer



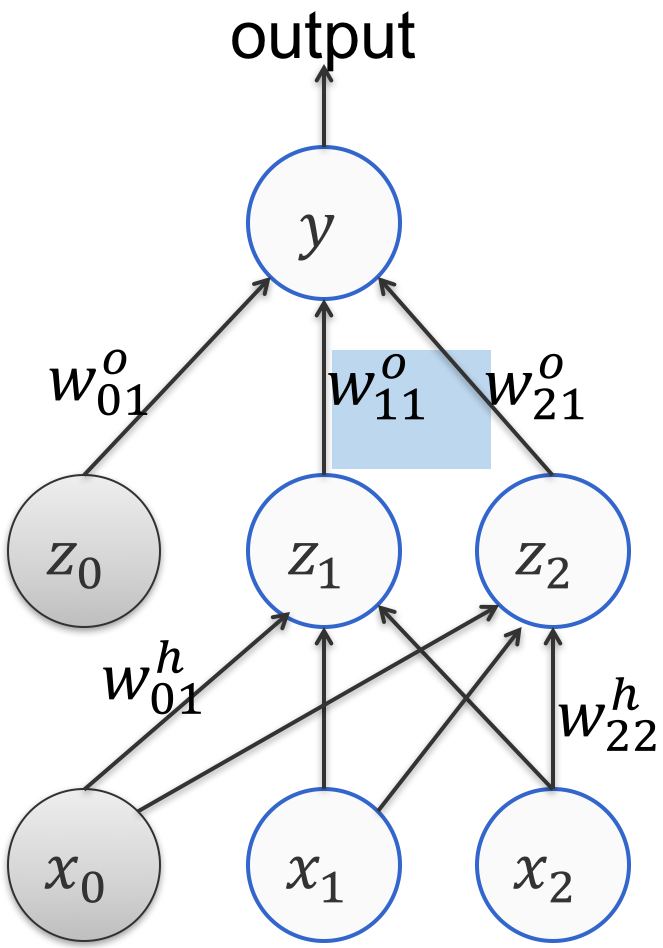
$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^0}$$

$$\frac{\partial L}{\partial y} = y - y^*$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer



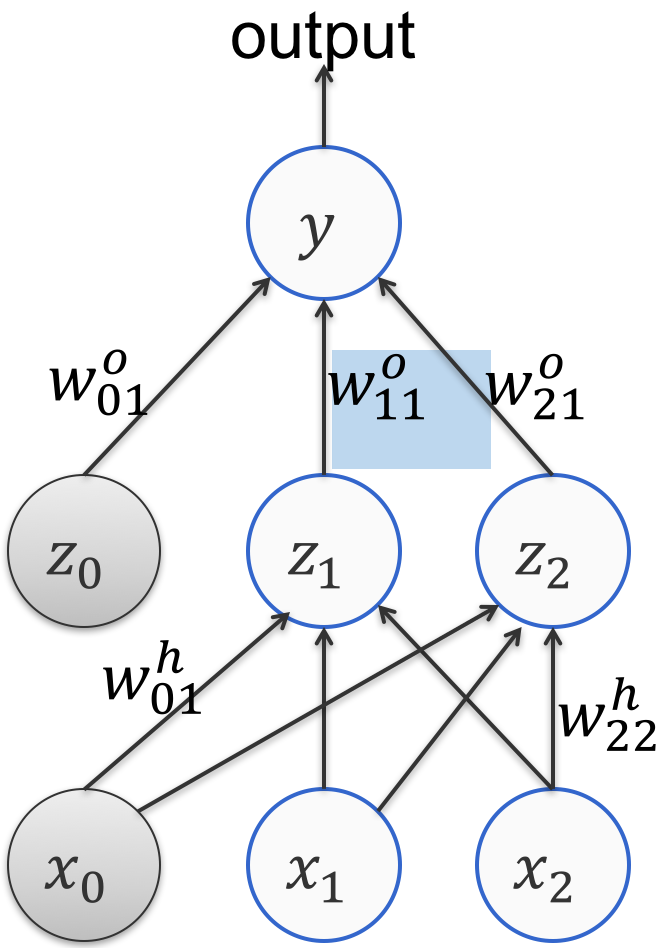
$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^o}$$

$$\frac{\partial L}{\partial y} = y - y^* \qquad \frac{\partial y}{\partial w_{01}^o} = z_1$$

$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2$

Output layer



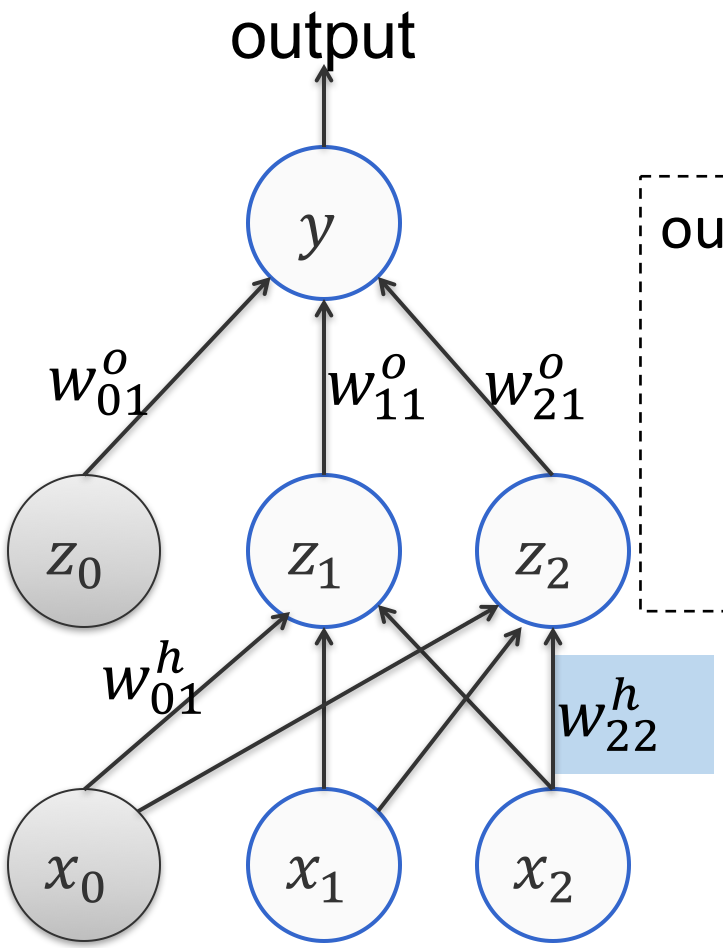
$$\frac{\partial L}{\partial w_{11}^o} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{11}^o}$$

$$\frac{\partial L}{\partial y} = y - y^* \qquad \frac{\partial y}{\partial w_{01}^o} = z_1$$

We have already computed this partial derivative for the previous case

Cache to speed up!

Hidden layer derivatives



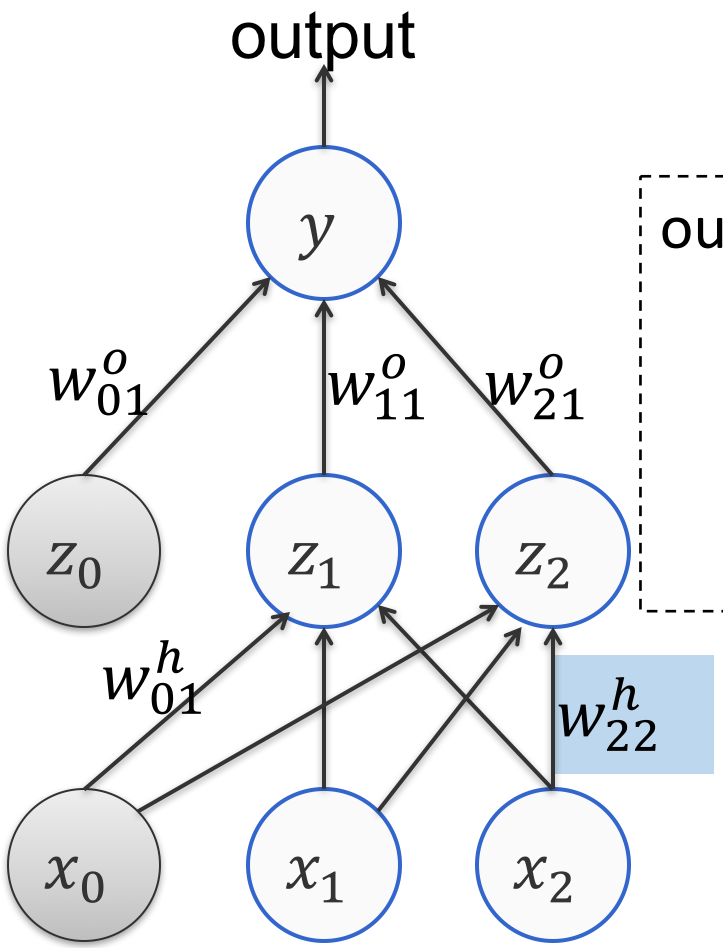
$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

Hidden layer derivatives



$$L = \frac{1}{2}(y - y^*)^2$$

output $y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$

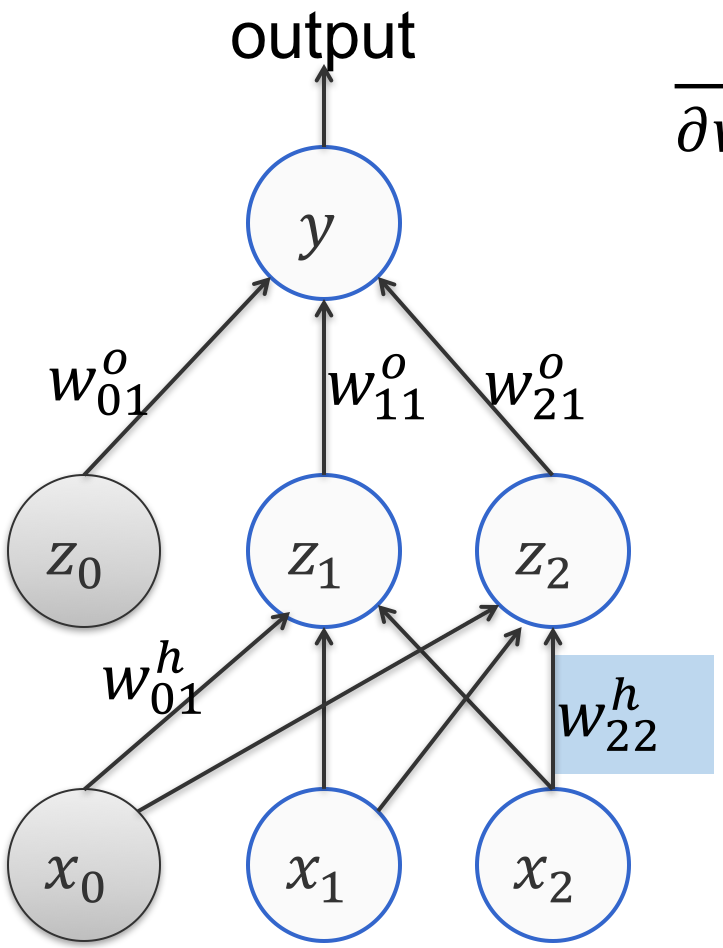
$$z_2 = \sigma(w_{02}^{h} + w_{12}^{h} x_1 + w_{22}^{h} x_2)$$

$$z_1 = \sigma(w_{01}^{h} + w_{11}^{h} x_1 + w_{21}^{h} x_2)$$

We want $\frac{\partial L}{\partial w_{22}^{h}}$

$$L = \frac{1}{2}(y - y^*)^2$$

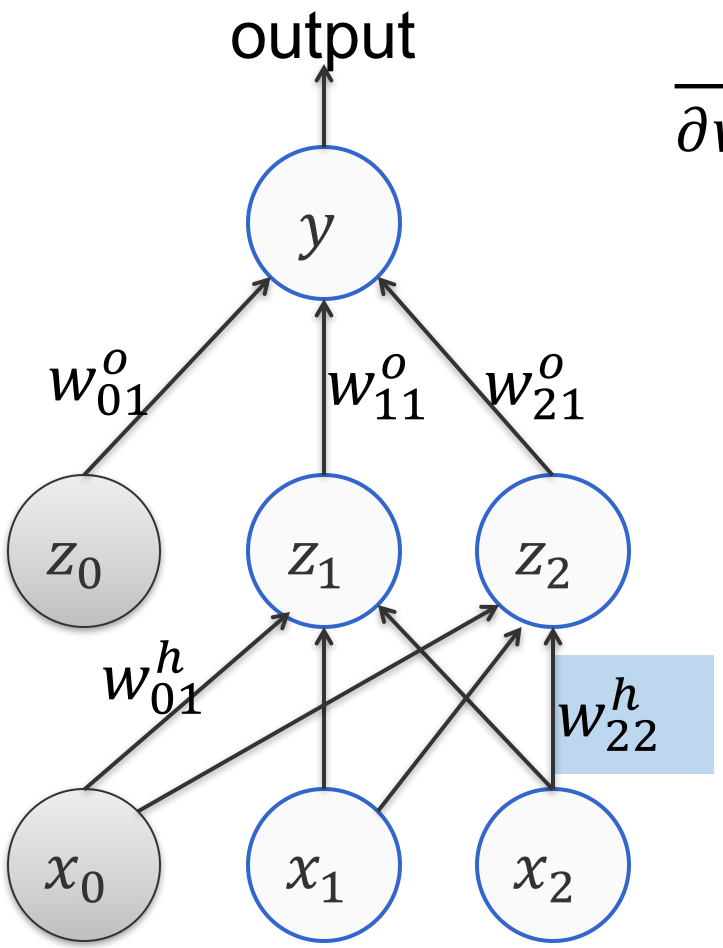
Hidden layer derivatives



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

$$y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$$

Hidden layer

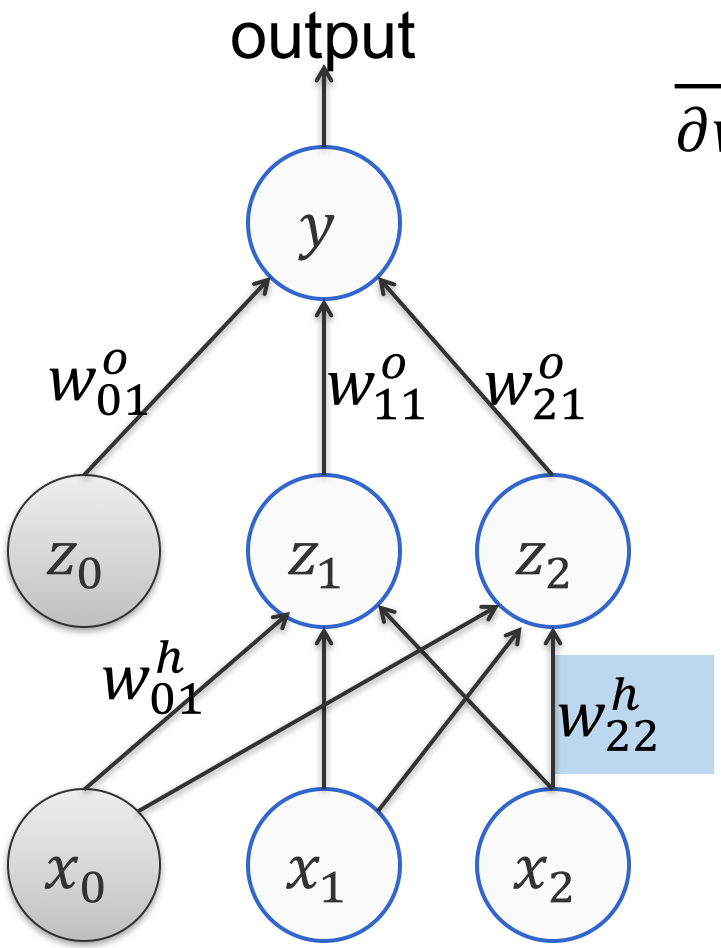


$$\frac{\partial L}{\partial w_{22}^{h}} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^{h}}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^{h}}\left(w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2\right)$$

$$y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$$

Hidden layer



$$\frac{\partial L}{\partial w_{22}^{h}} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^{h}}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^{h}}(w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2)$$

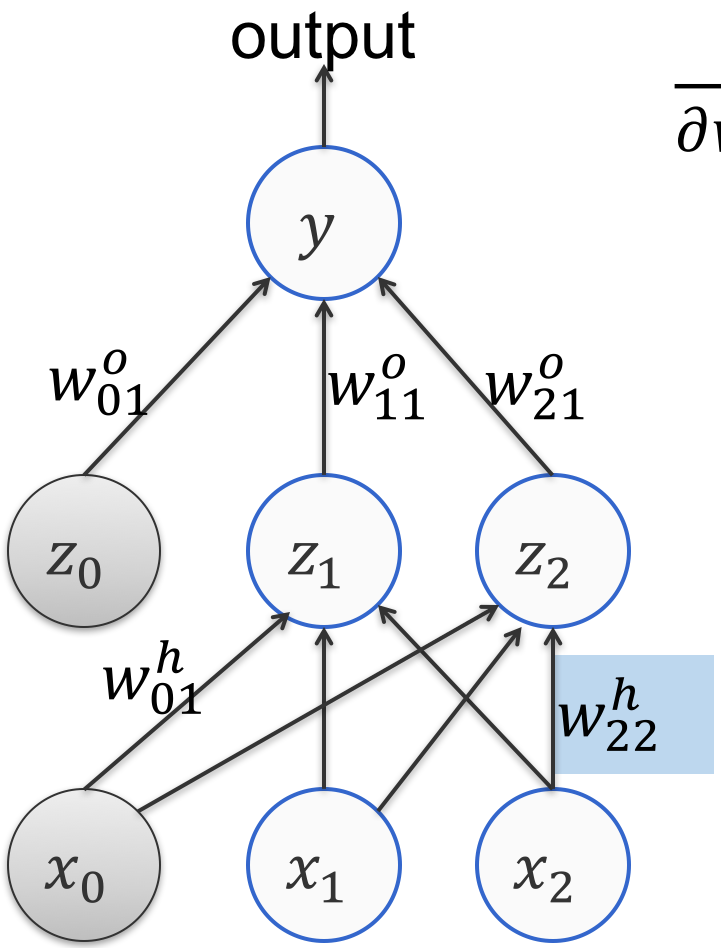
$$= \frac{\partial L}{\partial y}(w_{11}^{o}\frac{\partial}{\partial w_{22}^{h}} z_1 + w_{21}^{o}\frac{\partial}{\partial w_{22}^{h}} z_2)$$

$\frac{\partial}{\partial w_{22}^{h}} z_1 \rightarrow 0$

z_1 is not a function of w_{22}^{h}

$$y = w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2$$

Hidden layer



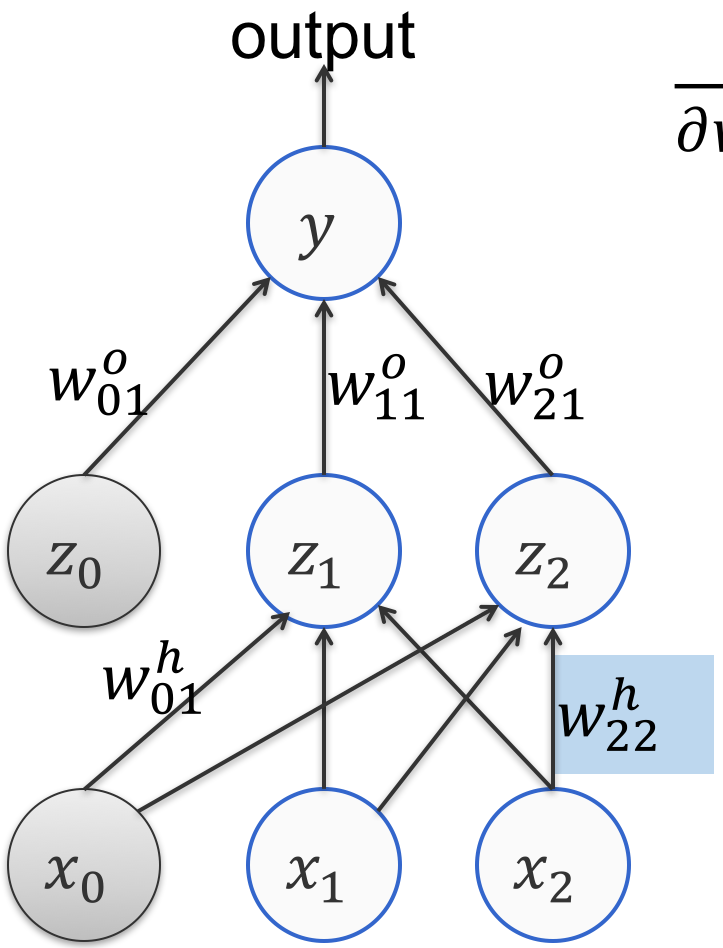
$$\frac{\partial L}{\partial w_{22}^{h}} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^{h}}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^{h}}\left(w_{01}^{o} + w_{11}^{o} z_1 + w_{21}^{o} z_2\right)$$

$$= \frac{\partial L}{\partial y} w_{21}^{o} \frac{\partial z_2}{\partial w_{22}^{h}}$$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

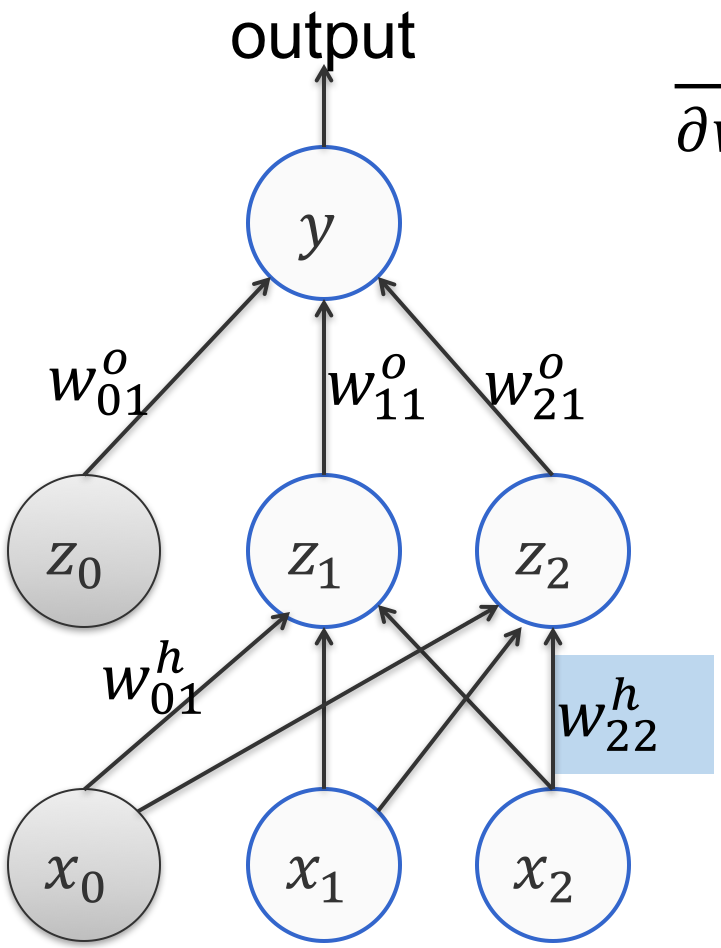
$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

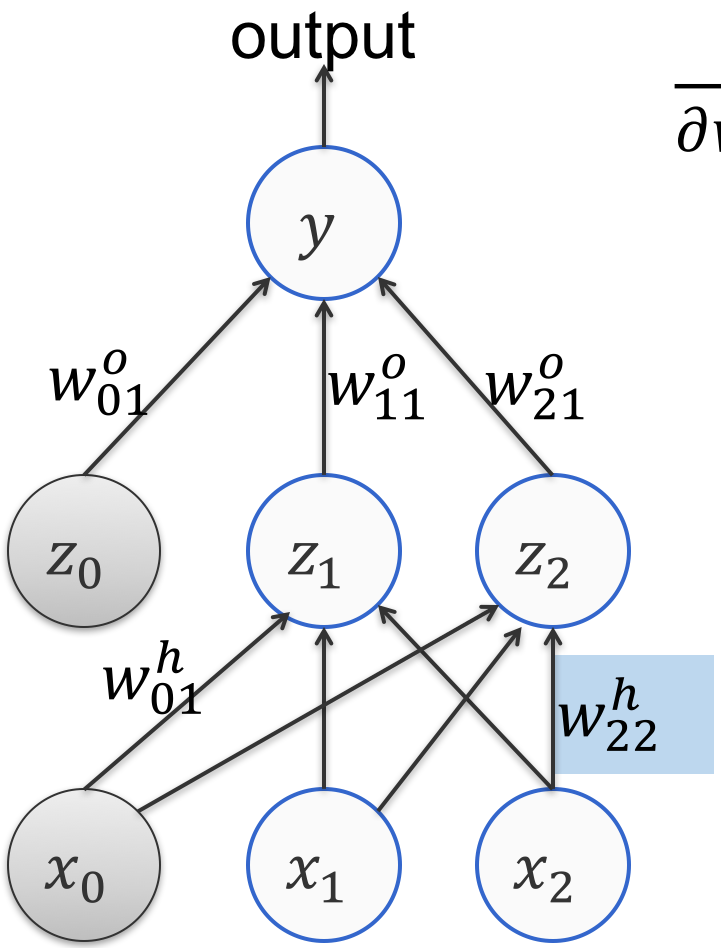
$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y}\frac{\partial y}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y}\frac{\partial}{\partial w_{22}^h}(w_{01}^o + w_{11}^o z_1 + w_{21}^o z_2)$$

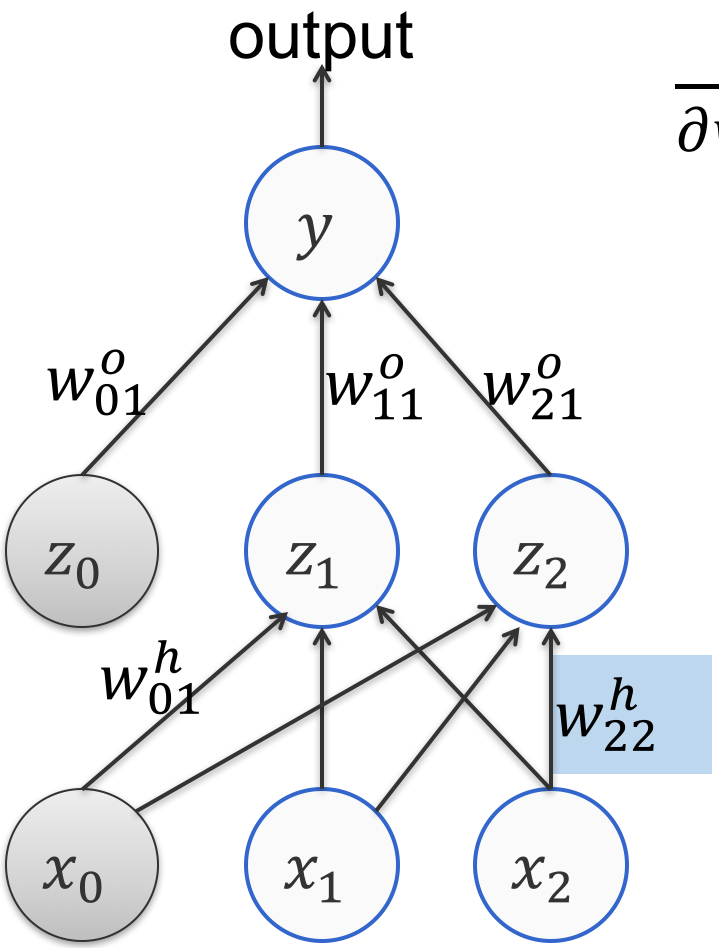
$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial w_{22}^h}$$

$$= \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s}\frac{\partial s}{\partial w_{22}^h}$$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer

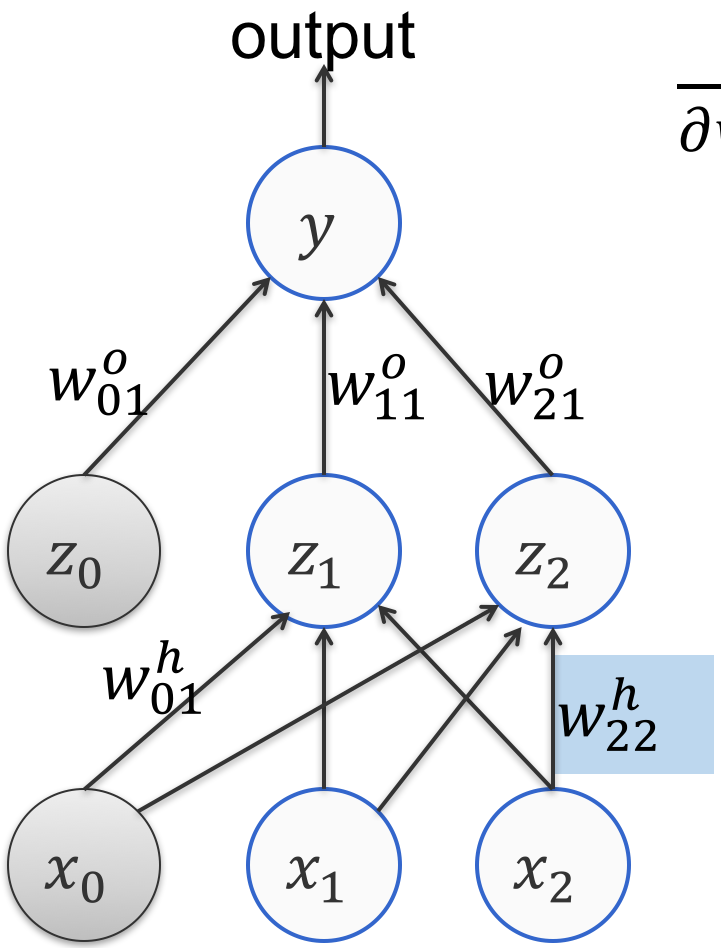


$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$ (From previous slide)

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



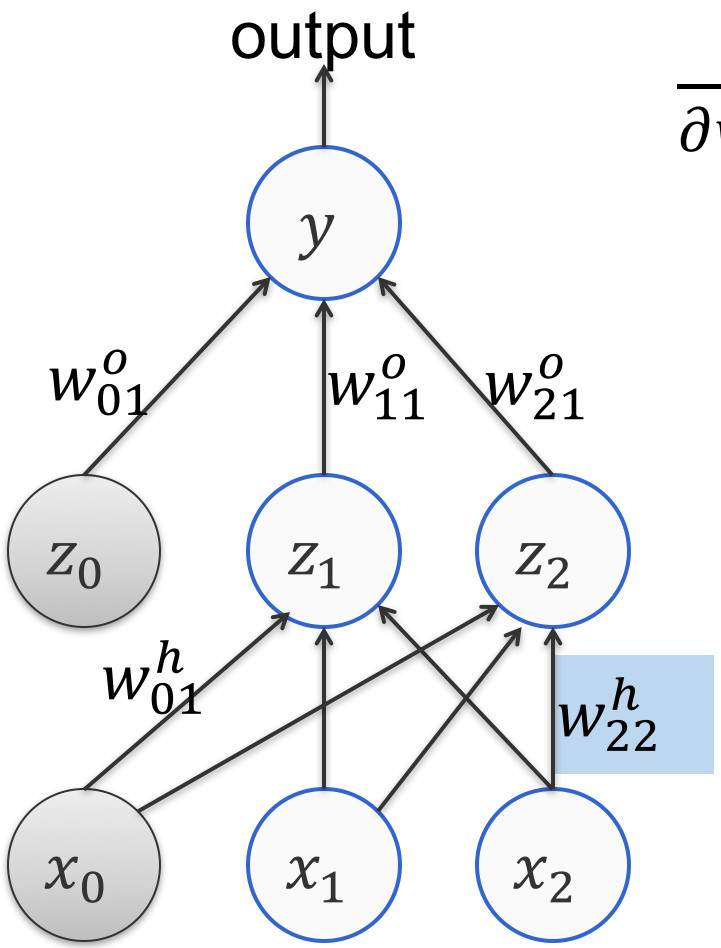
$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

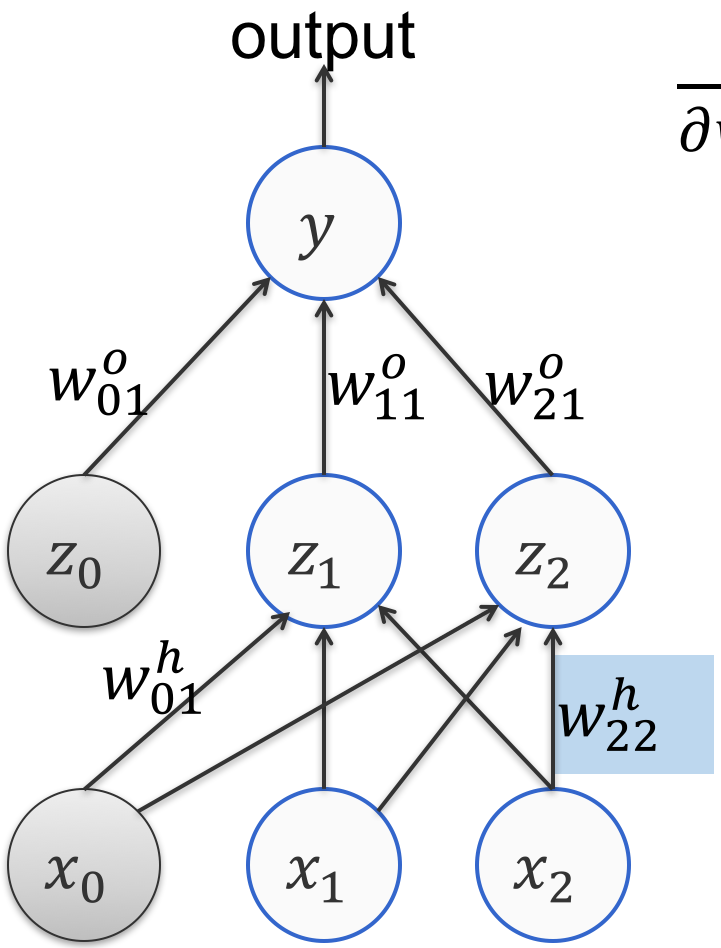
Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

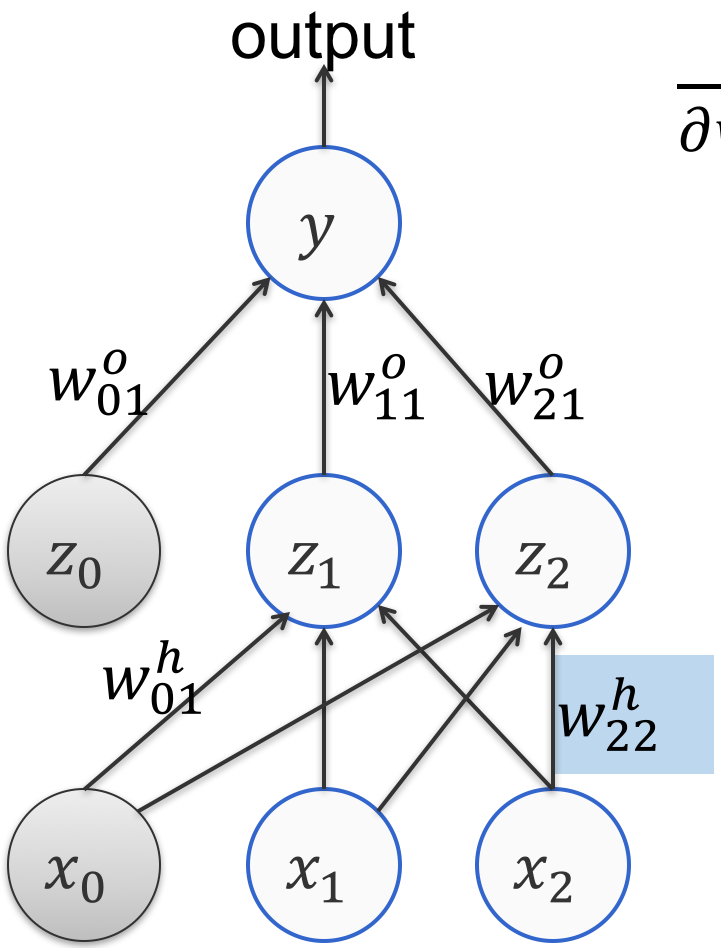
$$\frac{\partial z_2}{\partial s} = z_2(1 - z_2)$$

Why? Because $z_2(s)$ is the logistic function we have already seen

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

$$\frac{\partial L}{\partial y} = y - y^*$$

$$\frac{\partial z_2}{\partial s} = z_2(1 - z_2)$$

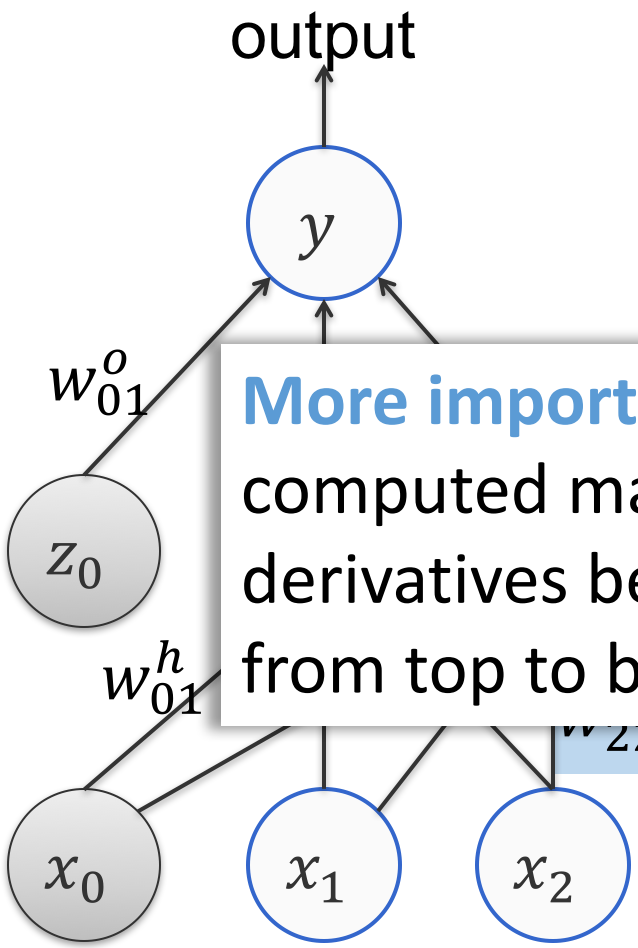
$$\frac{\partial s}{\partial w_{22}^h} = x_2$$

Why? Because $z_2(s)$ is the logistic function we have already seen

$$z_2 = \sigma(w_{02}^h + w_{12}^h x_1 + w_{22}^h x_2)$$

Call this s

Hidden layer



$$\frac{\partial L}{\partial w_{22}^h} = \frac{\partial L}{\partial y} w_{21}^o \frac{\partial z_2}{\partial s} \frac{\partial s}{\partial w_{22}^h}$$

Each of these partial derivatives is easy

More important: We have already computed many of these partial derivatives because we are proceeding from top to bottom (i.e. backwards)

cause $z_2(s)$
istic
we have
een

$$\frac{\partial s}{\partial w_{22}^h} = x_2$$

The Backpropagation Algorithm

The same algorithm works for multiple layers

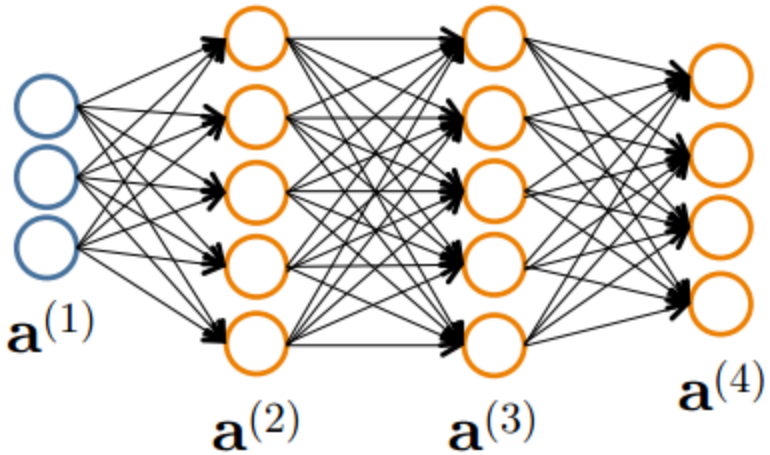
Repeated application of the chain rule for partial derivatives

- First perform forward pass from inputs to the output
- Compute loss

- From the loss, proceed backwards to compute partial derivatives using the chain rule
- Cache partial derivatives as you compute them
  - Will be used for lower layers

Forward Propagation

- Given one labeled training instance $(\mathbf{x}, y)$:

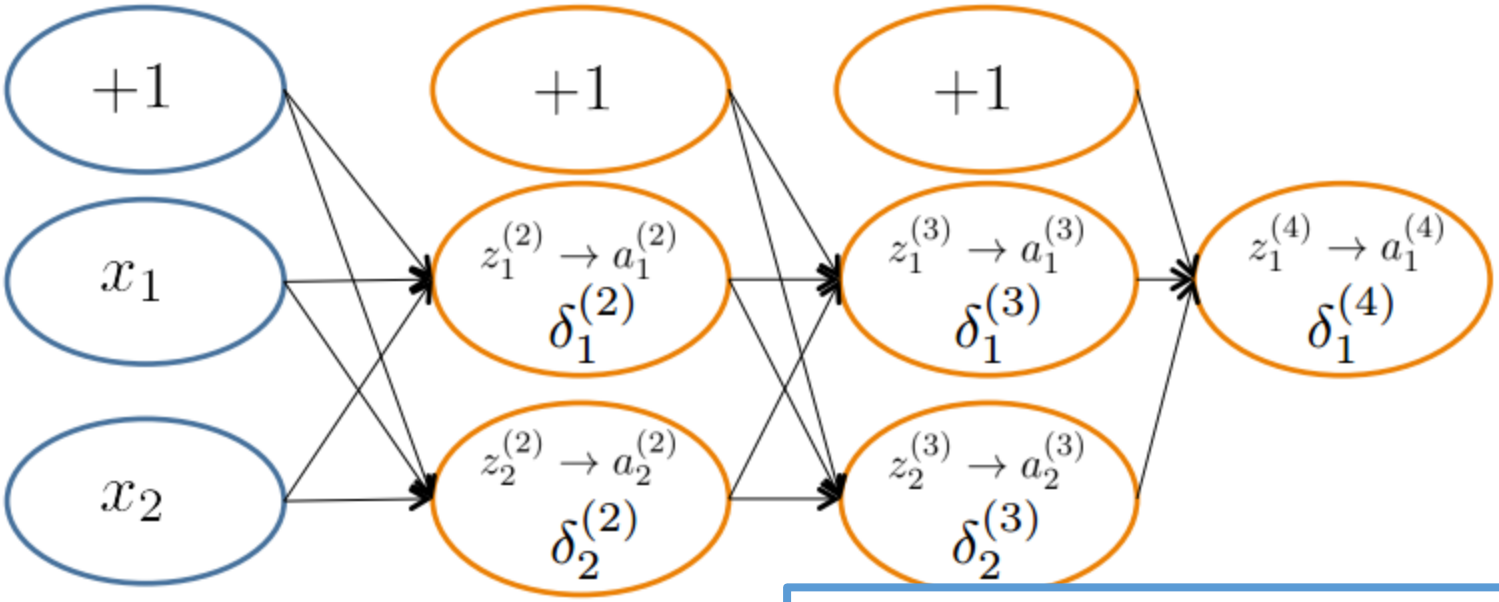


Forward Propagation

- $\mathbf{a}^{(1)} = \mathbf{x}$
- $\mathbf{z}^{(2)} = \Theta^{(1)}\mathbf{a}^{(1)}$
- $\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$ [add $a_0^{(2)}$]
- $\mathbf{z}^{(3)} = \Theta^{(2)}\mathbf{a}^{(2)}$
- $\mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$ [add $a_0^{(3)}$]
- $\mathbf{z}^{(4)} = \Theta^{(3)}\mathbf{a}^{(3)}$
- $\mathbf{a}^{(4)} = h_\Theta(\mathbf{x}) = g(\mathbf{z}^{(4)})$

Based on slide by Andrew Ng

Backpropagation: Compute Gradient



$$\frac{d}{dt} f(g(t)) = f'(g(t))g'(t) = \frac{df}{dg} \cdot \frac{dg}{dt}$$

$\delta_j^{(l)}$ = "error" of node j in layer l

Formally, $\delta_j^{(l)} = \dfrac{\partial}{\partial z_j^{(l)}} \text{cost}(\mathbf{x}_i)$

where $\text{cost}(\mathbf{x}_i) = y_i \log h_\Theta(\mathbf{x}_i) + (1 - y_i) \log(1 - h_\Theta(\mathbf{x}_i))$

Based on slide by Andrew Ng

Mechanizing learning

- Backpropagation gives you the gradient that will be used for gradient descent
  - SGD gives us a generic learning algorithm
  - Backpropagation is a generic method for computing partial derivatives

- A recursive algorithm that proceeds from the top of the network to the bottom

- Modern neural network libraries implement automatic differentiation using backpropagation
  - Allows easy exploration of network architectures
  - Don’t have to keep deriving the gradients by hand each time

Stochastic gradient descent

$$\min_{w} \sum_{i} L(NN(x_i, w), y_i)$$

Given a training set S = $\{(\mathbf{x}_i, y_i)\}$

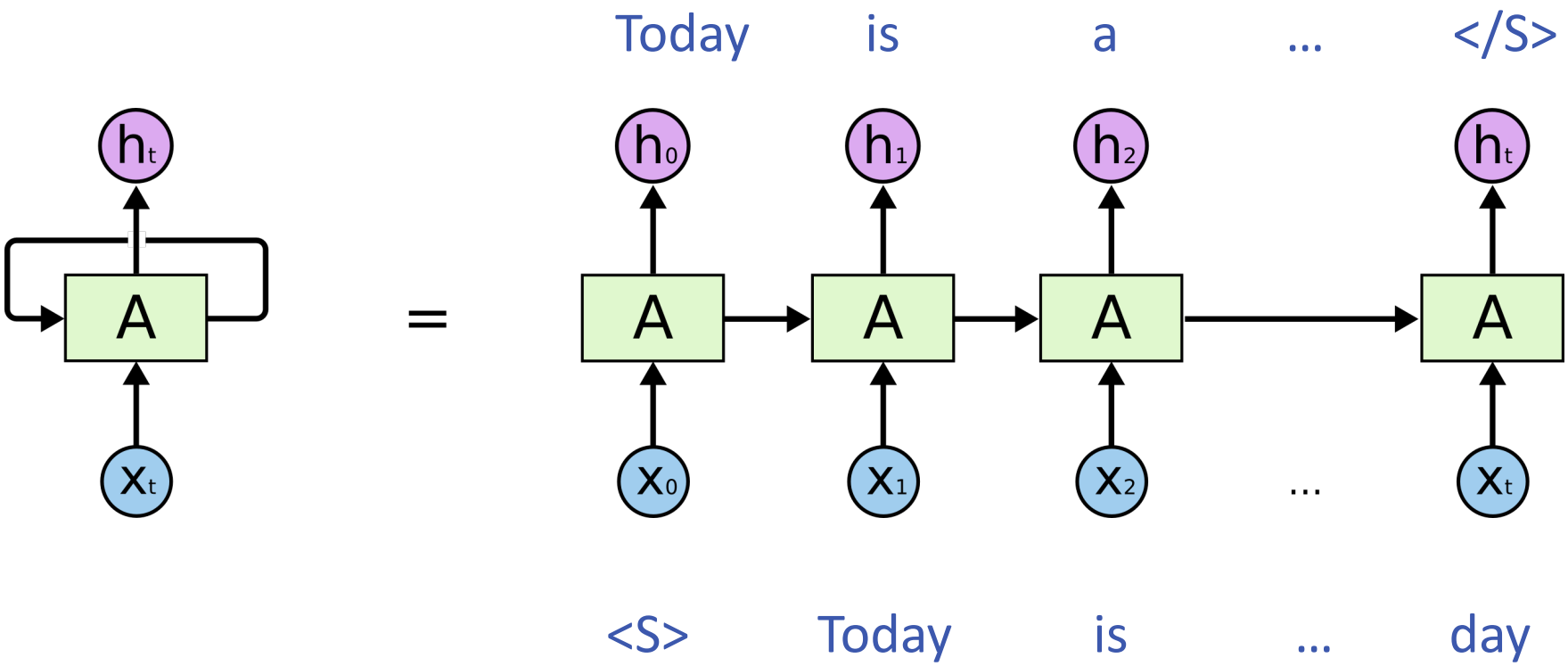
1. Initialize parameters w
2. For epoch = 1 … T:
   1. Shuffle the training set
   2. For each training example $(\mathbf{x}_i, y_i)2$ S:
      - Treat this example as the entire dataset
      - Compute the gradient of the loss $\nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i)$ using backpropagation
      - Update: $\boldsymbol{w} \leftarrow \boldsymbol{w} - \gamma_t \nabla L(NN(\boldsymbol{x}_i, \boldsymbol{w}), y_i))$
3. Return w

This lecture

- Neural Network
- Recurrent NN

How to deal with input with variant size?

- Use same parameters

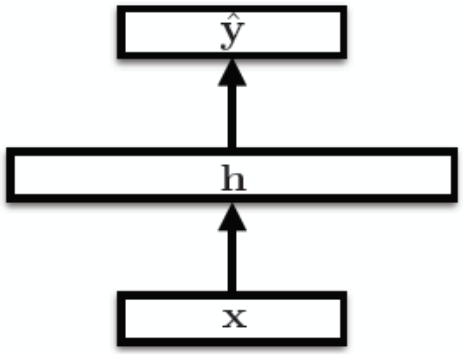


Recurrent Neural Networks

Feed-forward NN

$$\mathbf{h} = g(\mathbf{V}\mathbf{x} + \mathbf{c})$$

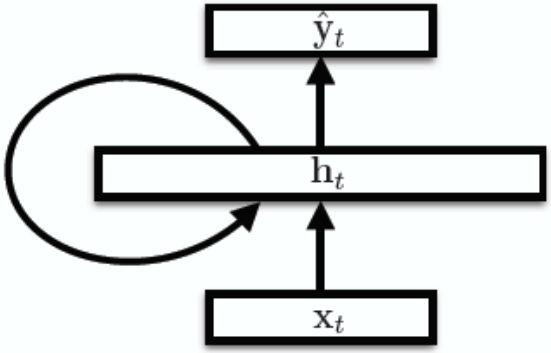
$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h} + \mathbf{b}$$



Recurrent NN

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

$$\hat{\mathbf{y}}_t = \mathbf{W}\mathbf{h}_t + \mathbf{b}$$

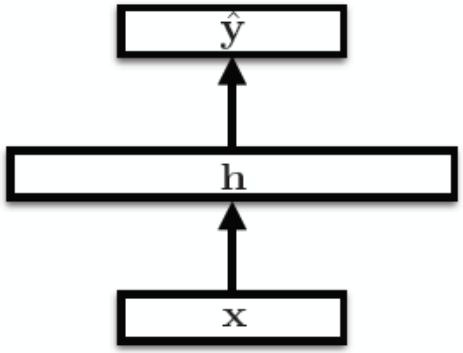


Recurrent Neural Networks

Feed-forward NN

$$\mathbf{h} = g(\mathbf{V}\mathbf{x} + \mathbf{c})$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h} + \mathbf{b}$$

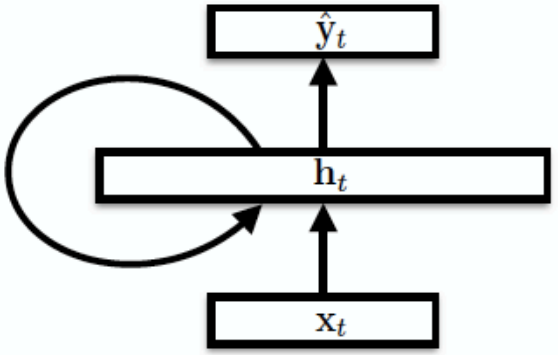


Recurrent NN

~~$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$~~

$$\mathbf{h}_t = g(\mathbf{V}[\mathbf{x}_t; \mathbf{h}_{t-1}] + \mathbf{c})$$

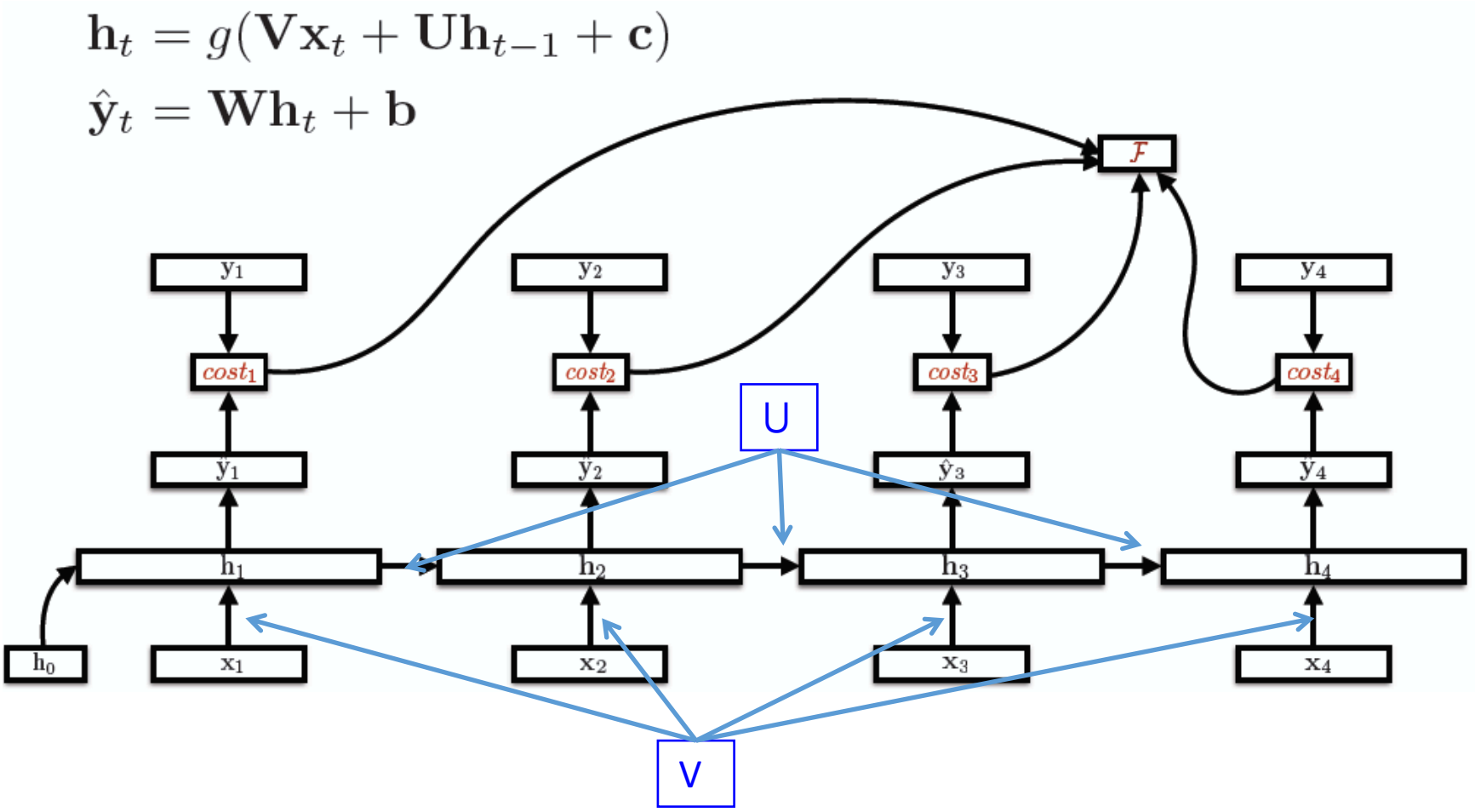
$$\hat{\mathbf{y}}_t = \mathbf{W}\mathbf{h}_t + \mathbf{b}$$



Unroll RNNs

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$

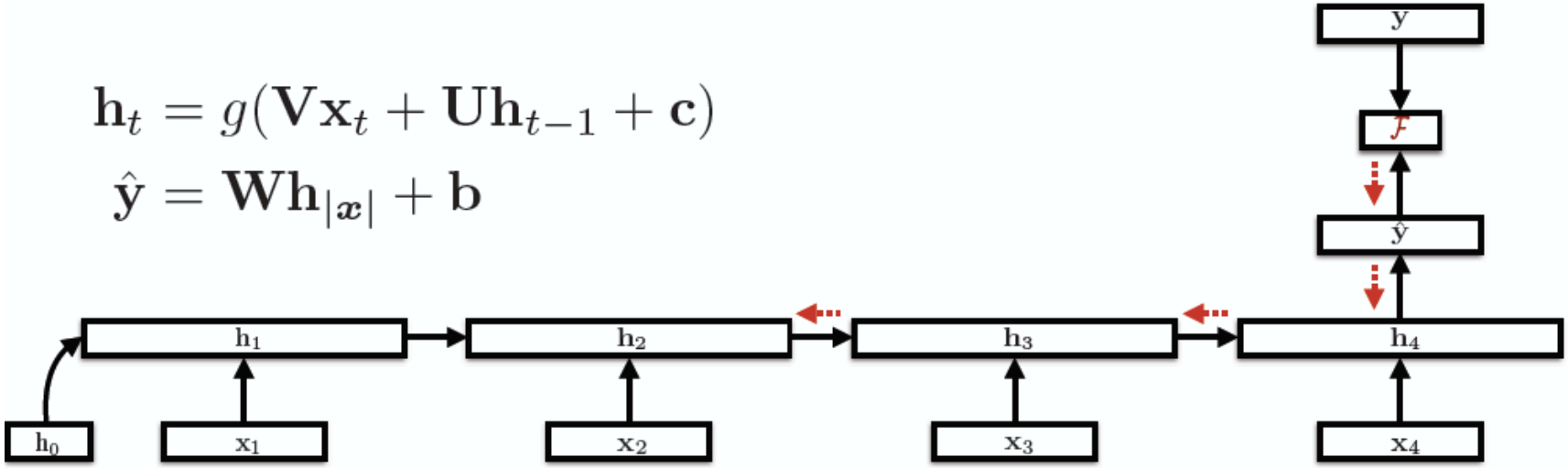
$$\hat{\mathbf{y}}_t = \mathbf{W}\mathbf{h}_t + \mathbf{b}$$



RNN training

- Back-propagation over time

$$\mathbf{h}_t = g(\mathbf{V}\mathbf{x}_t + \mathbf{U}\mathbf{h}_{t-1} + \mathbf{c})$$
$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{h}_{|\boldsymbol{x}|} + \mathbf{b}$$



What happens to gradients as you go back in time?

$$\frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}\frac{\partial \mathbf{h}_4}{\partial \mathbf{h}_3}\frac{\partial \hat{\mathbf{y}}}{\partial \mathbf{h}_4}\frac{\partial \mathcal{F}}{\partial \hat{\mathbf{y}}}\frac{\partial \mathcal{F}}{\partial \mathcal{F}}$$

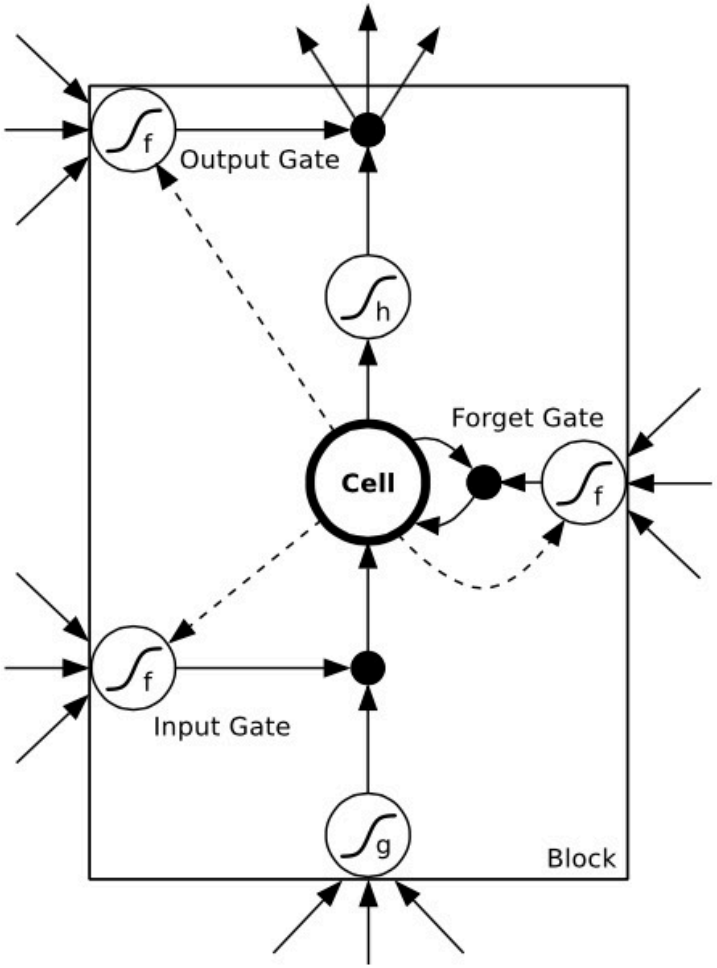
Vanishing Gradients

- For the traditional activation functions, each gradient term has the value in range (-1, 1).
- Multiplying *n* of these small numbers to compute gradients
- The longer the sequence is, the more severe the problems are.

RNNs characteristics

- Model hidden states (input) dependencies
- Errors “back propagation over time”
- Feature learning methods
- Vanishing gradient problem:
  cannot model long-distant dependencies of the hidden states.

Long-Short Term Memory Networks (LSTMs)



$$\begin{pmatrix} i_t \\ f_t \\ o_t \\ g_t \end{pmatrix} = \begin{pmatrix} \sigma(W_i[x_t, h_t] + b_i) \\ \sigma(W_f[x_t, h_t] + b_f) \\ \sigma(W_o[x_t, h_t] + b_o) \\ f(W_g[x_t, h_t] + b_g) \end{pmatrix}$$

$$c_t = f_t * c_{t-1} + i_t * g_t$$

$$h_t = o_t * f(c_t)$$

Use gates to control the information to be added from the input, forgot from the previous memories, and outputted.
σ and f are *sigmoid* and *tanh* function respectively, to map the value to [-1, 1]