Lecture 9:
Deep Learning
Learning Theory
Fall 2022

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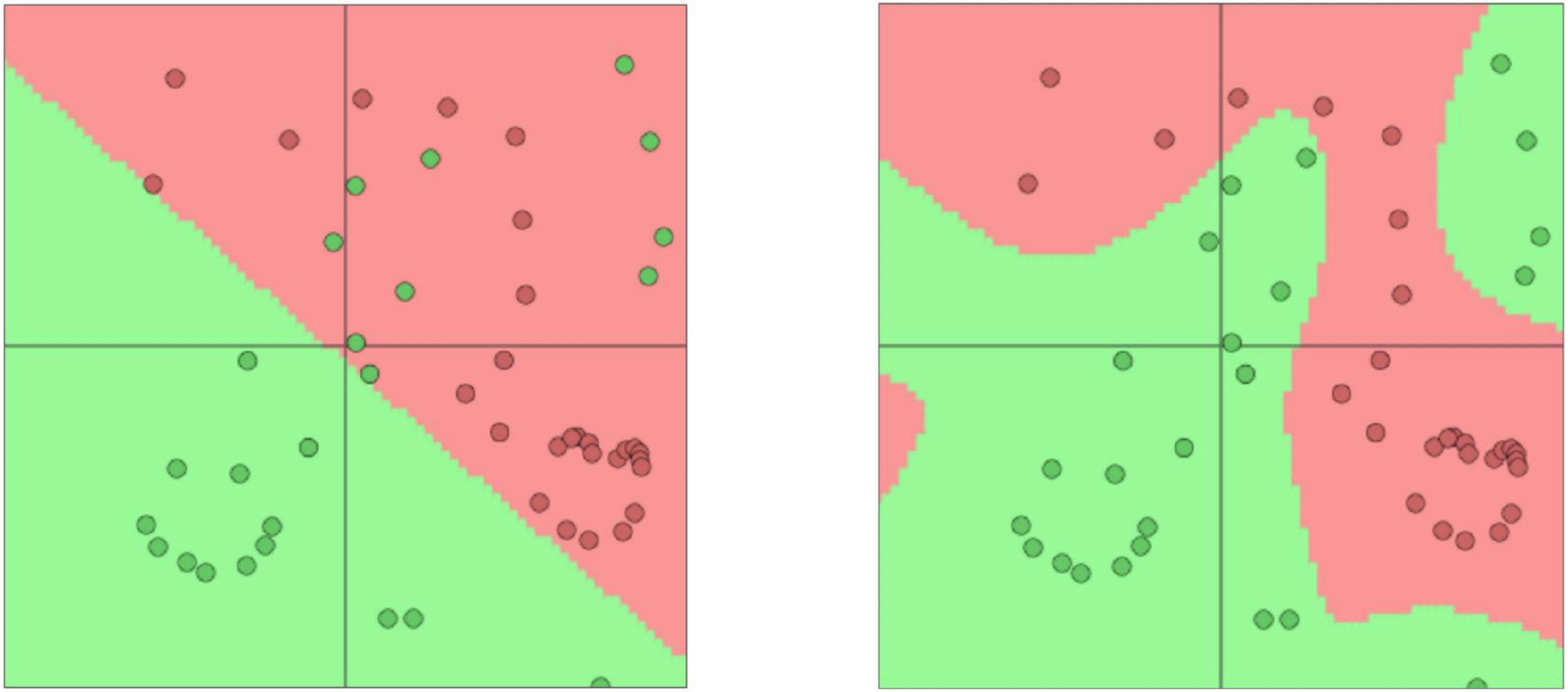
Announcements

- Midterm postpones to 11/3
  - The practice exam is posted
- Hw1 is due next Tue!
- Hw 2 & Quiz 3 will be released tomorrow

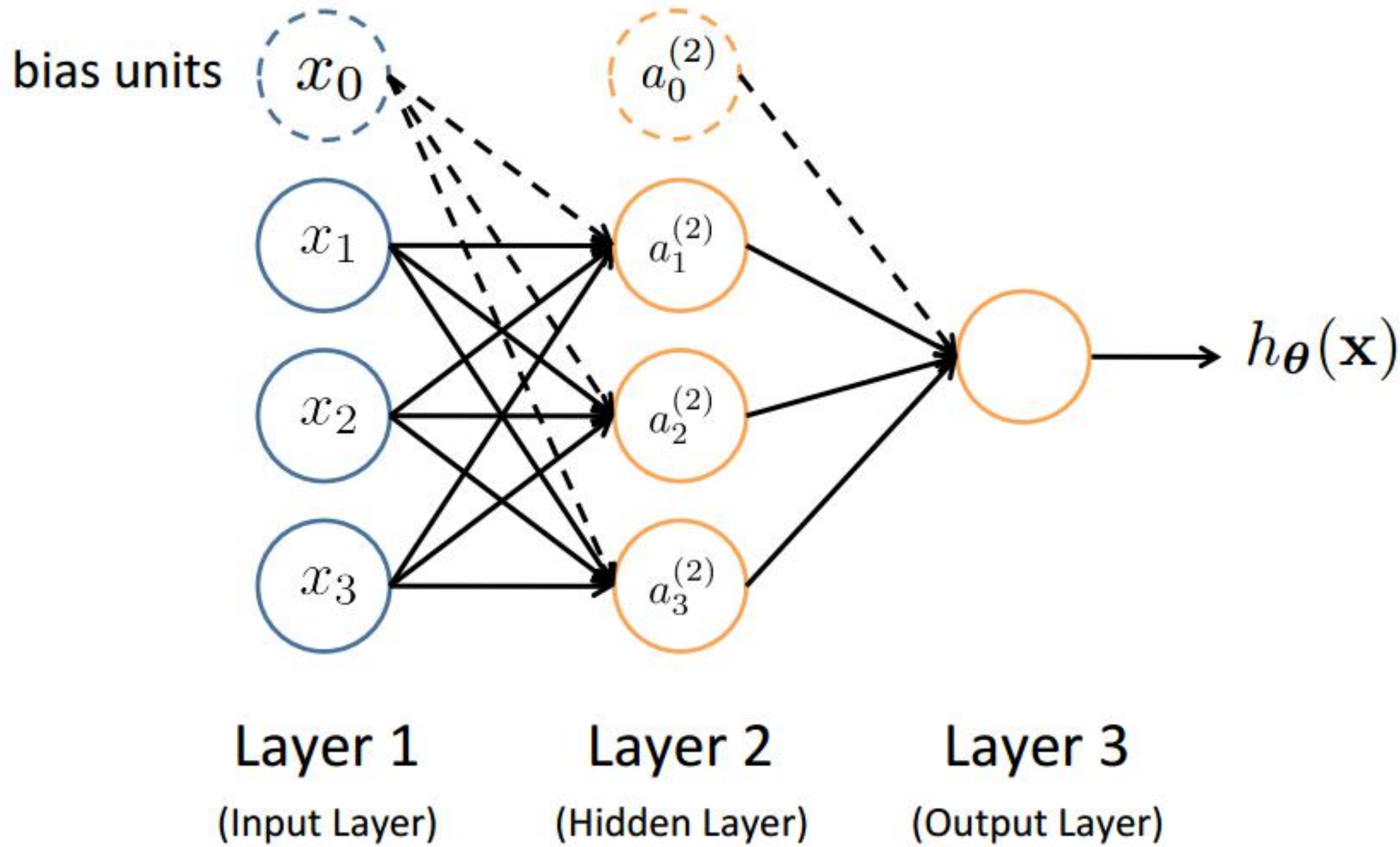
What you will learn today

- Neural network / Deep learning
  - Non-linear classifier
  - Feed-forward neural network
  - Back Propagation
  - Deep learning architecture

Non-Linear Decision Boundary

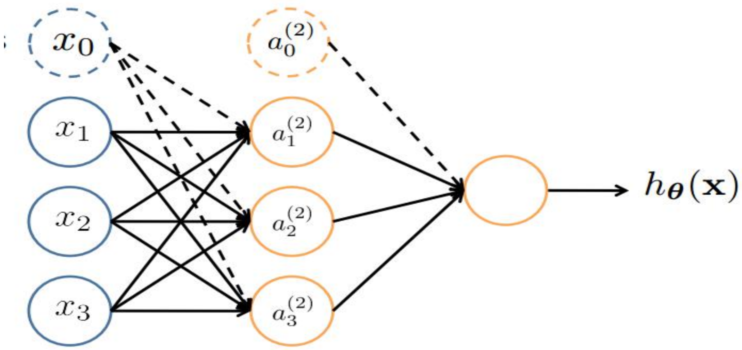


Neural Network



Slide by Andrew Ng

Neural Network



$a_i^{(j)}$ = "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 $s_{j+1} \times (s_j+1)$.

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

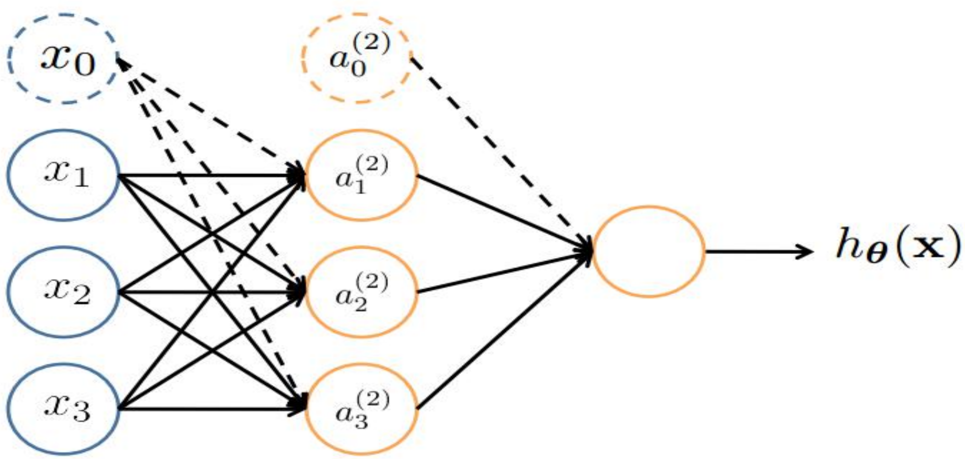
Vectorization

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

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

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

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



Feed-Forward Steps:

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

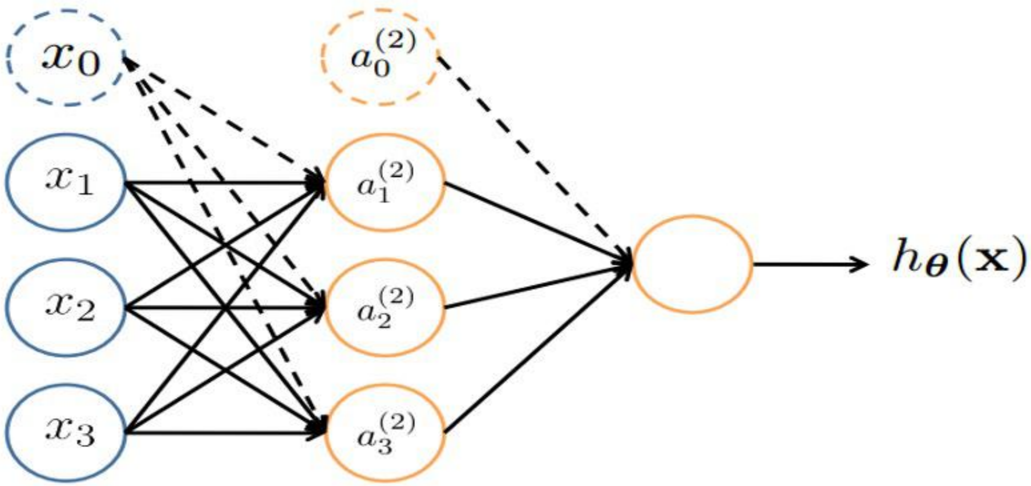
$$\mathbf{a}^{(2)} = g(\mathbf{z}^{(2)})$$

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

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

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

Example



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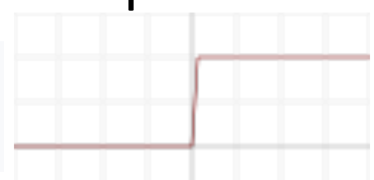
$$h_\Theta(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

Let $\Theta^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 2 & 0 & 1 & 1 \end{bmatrix}$

$\Theta^{(2)} = \begin{bmatrix} 0 & 1 & 1 & 0 \end{bmatrix}$

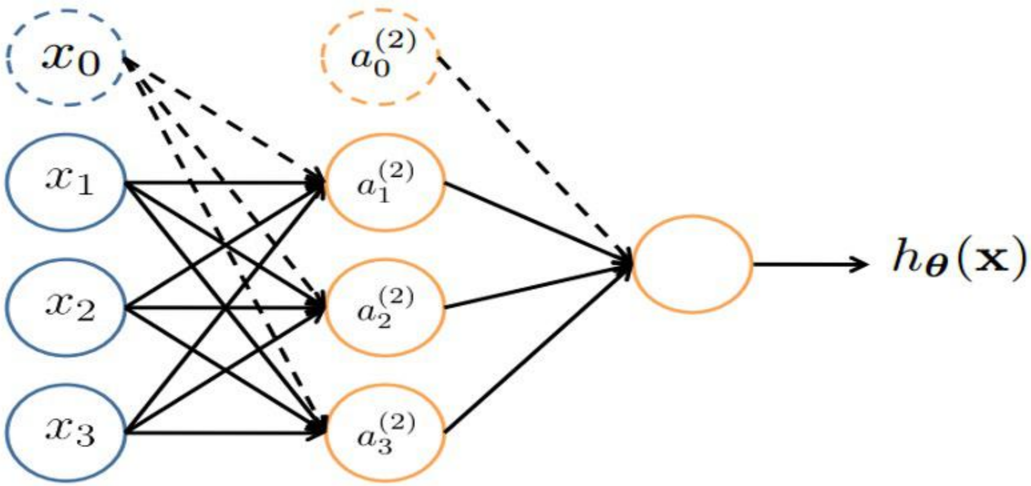
$g(z)$ is a step function

$$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$$



What is the output of $x = \begin{bmatrix} 1 \\ 0 \\ 2 \\ 1 \end{bmatrix}$?

Example



Feed-Forward Steps:

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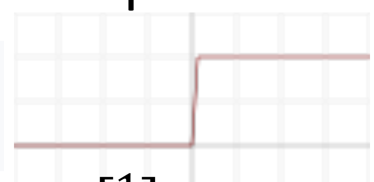


What is the output of $x = \begin{bmatrix} 1 \\ 0 \\ 2 \\ 1 \end{bmatrix}$?

$z^{(2)} = \begin{bmatrix} 2 \\ 2 \\ 5 \end{bmatrix}$ $a^{(2)} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ $z^{(3)} = 2$ $h_\Theta(x) = 1$

Exercise

- Why do we need non-linear activation functions?
  - What happen if $g(z) = z$

Feed-Forward Steps:

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

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

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

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

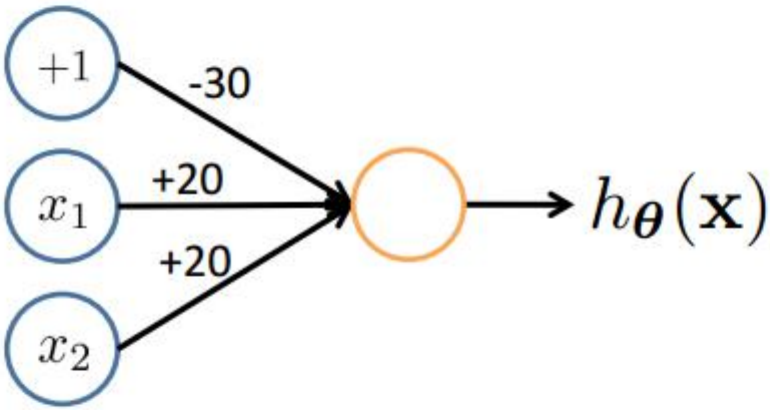
$$h_\Theta(\mathbf{x}) = \mathbf{a}^{(3)} = g(\mathbf{z}^{(3)})$$

Non-Linear Representations

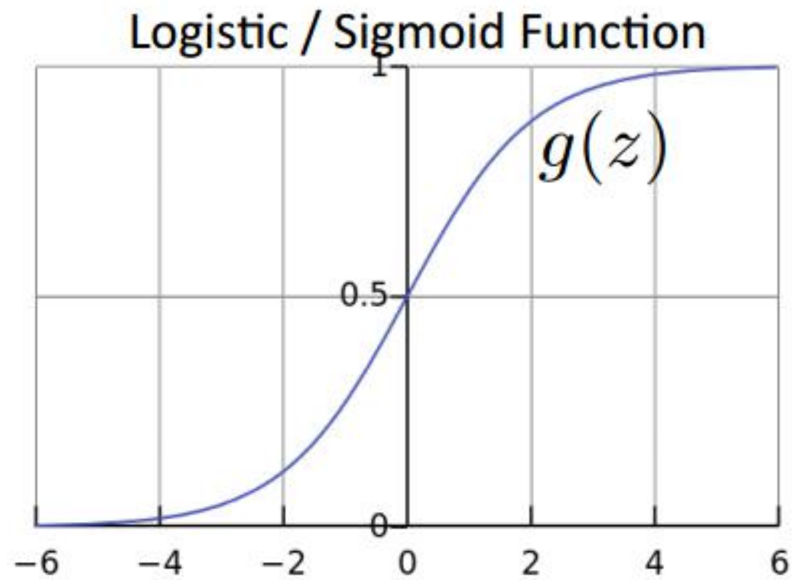
Simple example: AND

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

$y = x_1 \text{ AND } x_2$

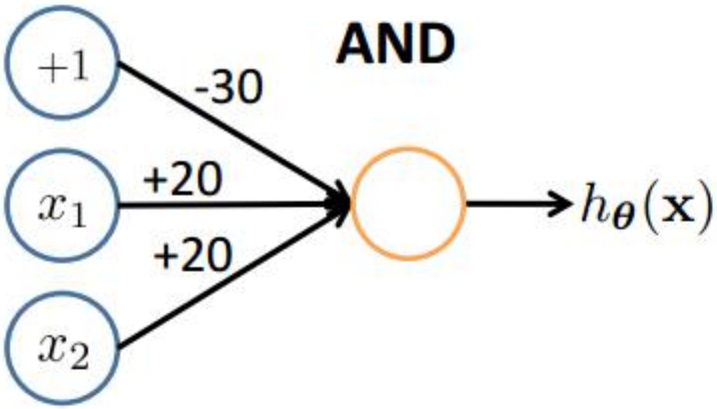


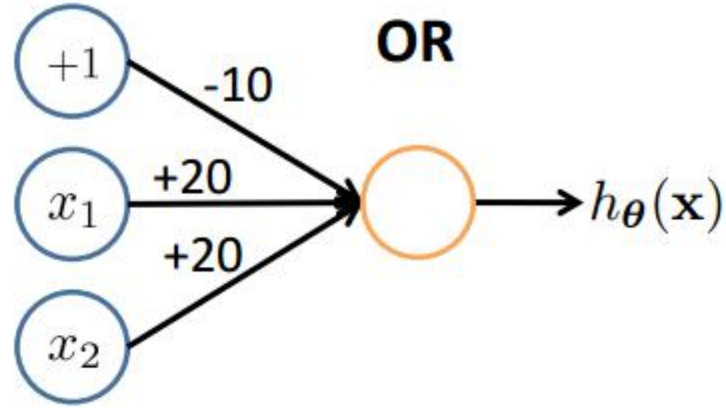
$$h_{\Theta}(\mathbf{x}) = g(-30 + 20x_1 + 20x_2)$$

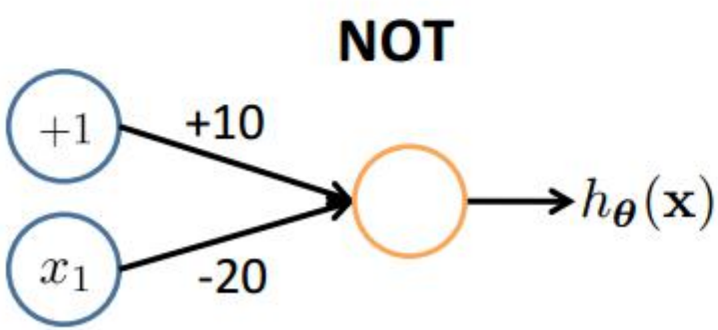


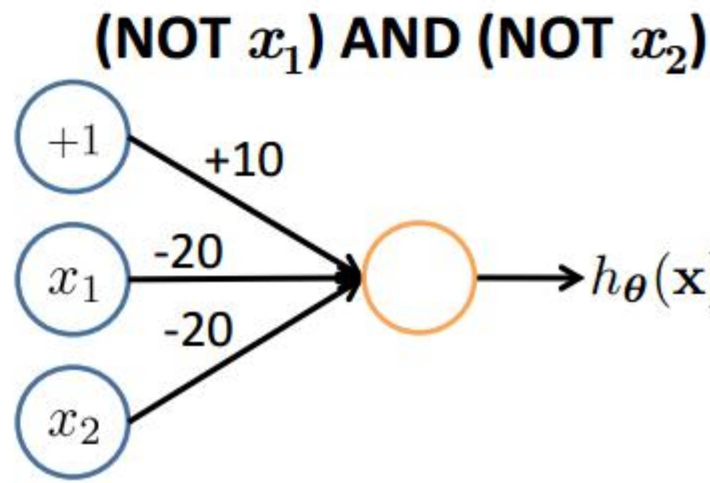
x_1	x_2	$h_{\Theta}(\mathbf{x})$
0	0	$g(-30) \approx 0$
0	1	$g(-10) \approx 0$
1	0	$g(-10) \approx 0$
1	1	$g(10) \approx 1$

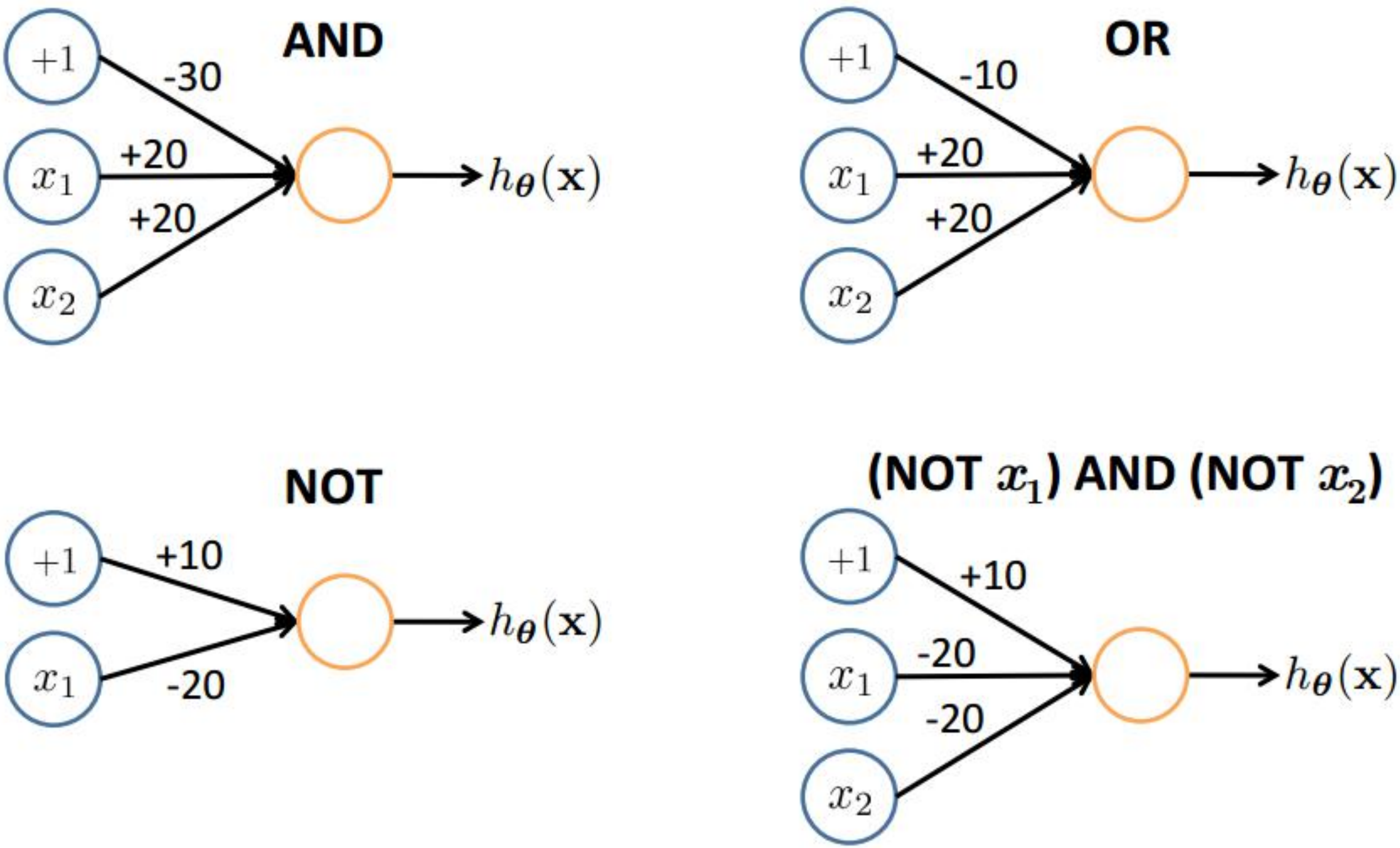
Based on slide and example by Andrew Ng


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

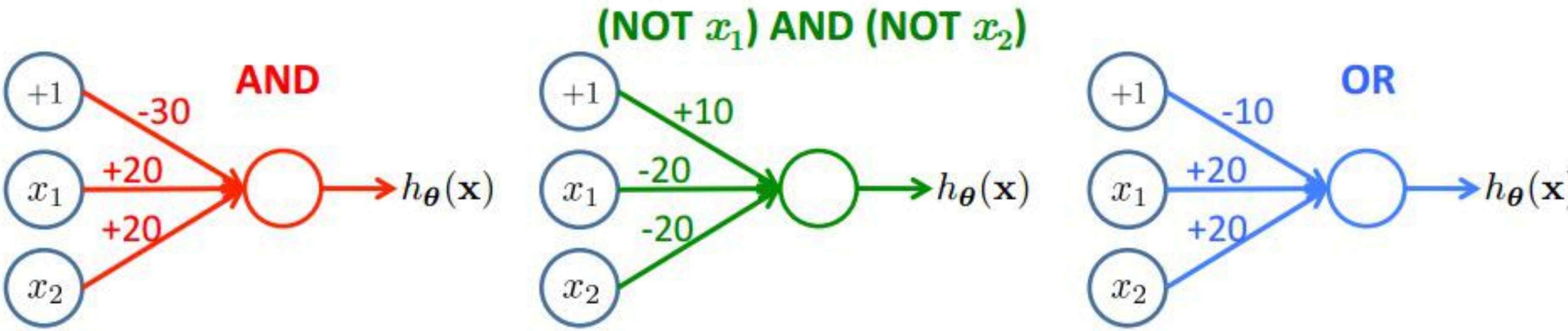

OR
$+1$
-10
x_1
+20
x_2
+20
$h_{\theta}(\mathbf{x})$


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

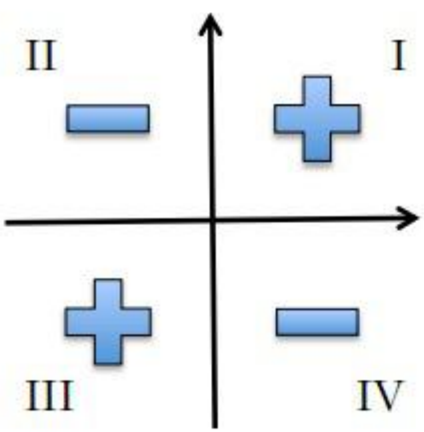

(NOT x_1) AND (NOT x_2)
$+1$
+10
x_1
-20
x_2
-20
$h_{\theta}(\mathbf{x})$


AND
+1
-30
x1
+20
+20
x2
hθ(x)
OR
+1
-10
x1
+20
+20
x2
hθ(x)
NOT
+1
+10
x1
-20
hθ(x)
(NOT x1) AND (NOT x2)
+1
+10
x1
-20
-20
x2
hθ(x)

Combining Representations to Create Non-Linear Functions



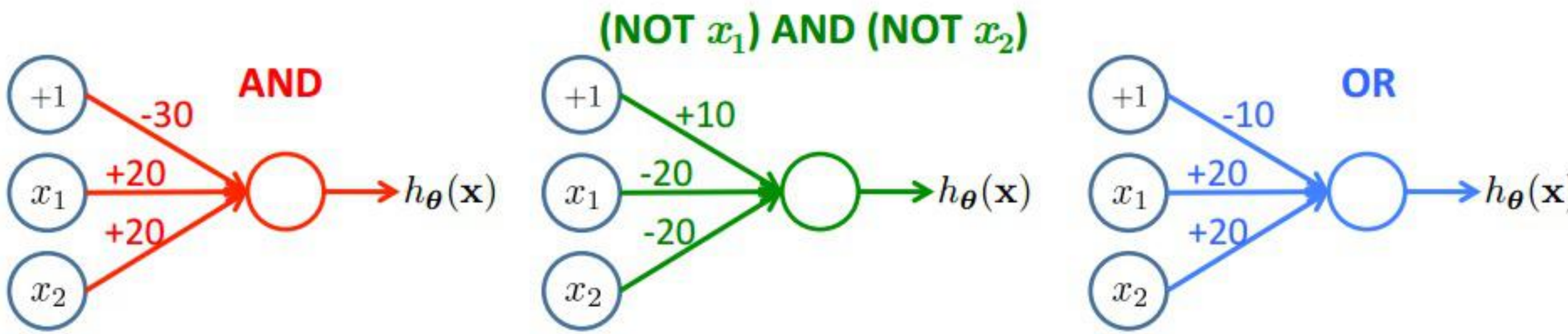
XNOR



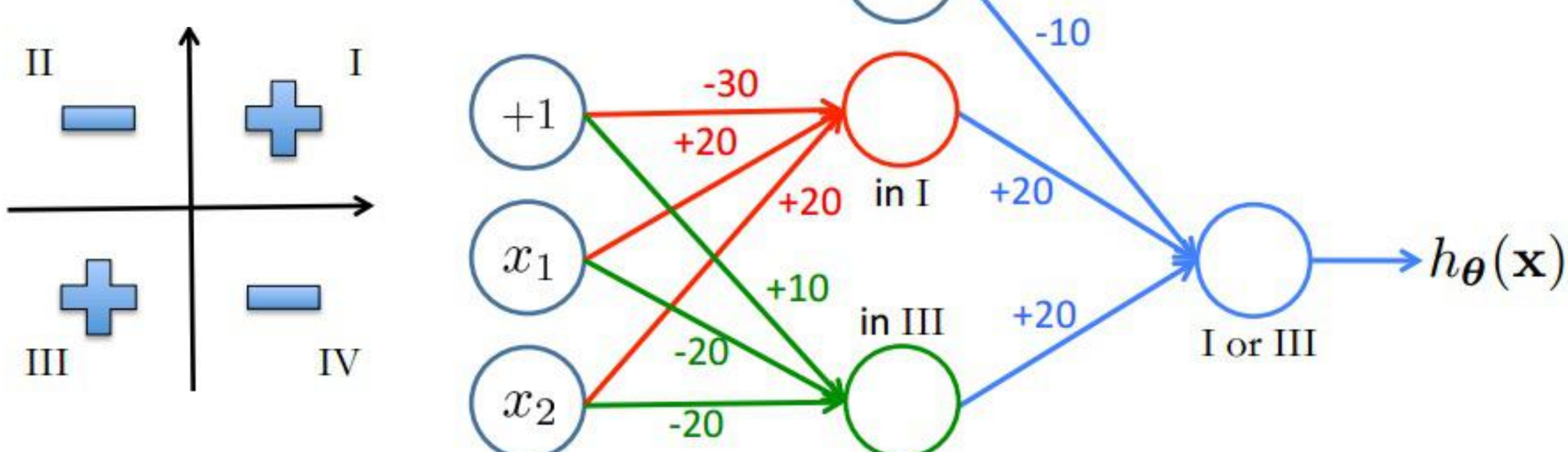
XNOR

Based on example by Andrew Ng

Combining Representations to Create Non-Linear Functions

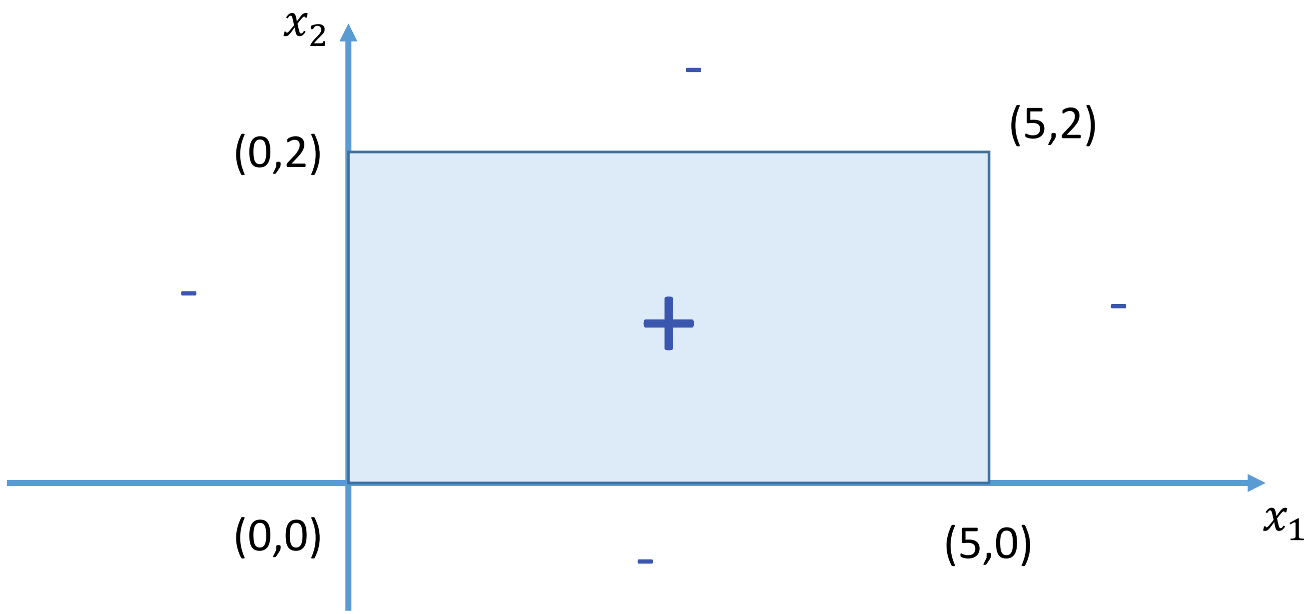


XNOR



Based on example by Andrew Ng

Exercise



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

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

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

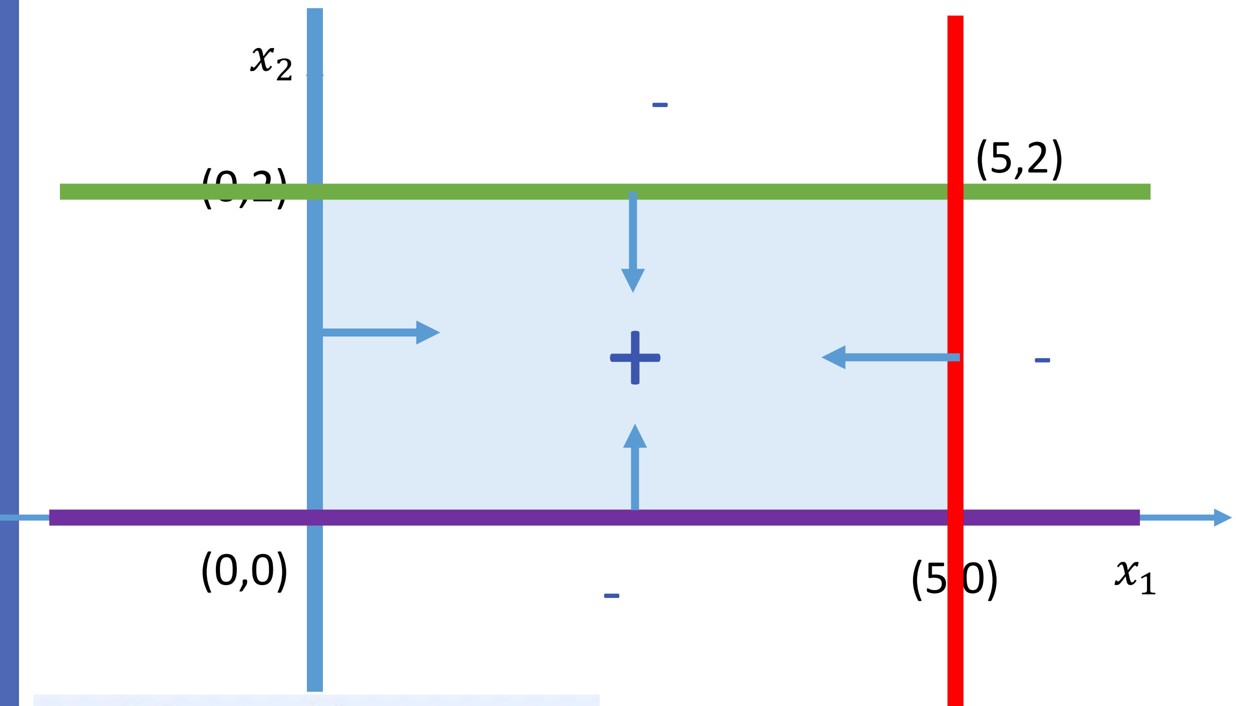
If all the samples inside the rectangle are positive; otherwise are negative

Show a feedforward NN can classify all the samples correctly

For simplicity, we assume g(z) is a step function.

What are $\Theta^{(1)}$ and $\Theta^{(2)}$

Exercise



$$\begin{cases} x_1 > 0 \\ 5 - x_1 > 0 \\ x_2 > 0 \\ 2 - x_2 > 0 \end{cases}$$

$$\Rightarrow \ \Theta^{(1)} = \begin{bmatrix} 0 & 1 & 0 \\ 5 & -1 & 0 \\ 0 & 0 & 1 \\ 2 & 0 & -1 \end{bmatrix}$$

$$\Theta_0^{(1)} \ \Theta_1^{(1)} \ \Theta_2^{(1)}$$

$$-3.5 + a_1 + a_2 + a_3 + a_4 > 0$$

$$\Theta^{(2)} = [-3.5 \quad 1 \quad 1 \quad 1 \quad 1]$$

$$\Theta_0^{(2)} \ \Theta_1^{(2)} \ \Theta_2^{(2)} \Theta_3^{(2)} \ \Theta_4^{(2)}$$

Feed-Forward Steps:

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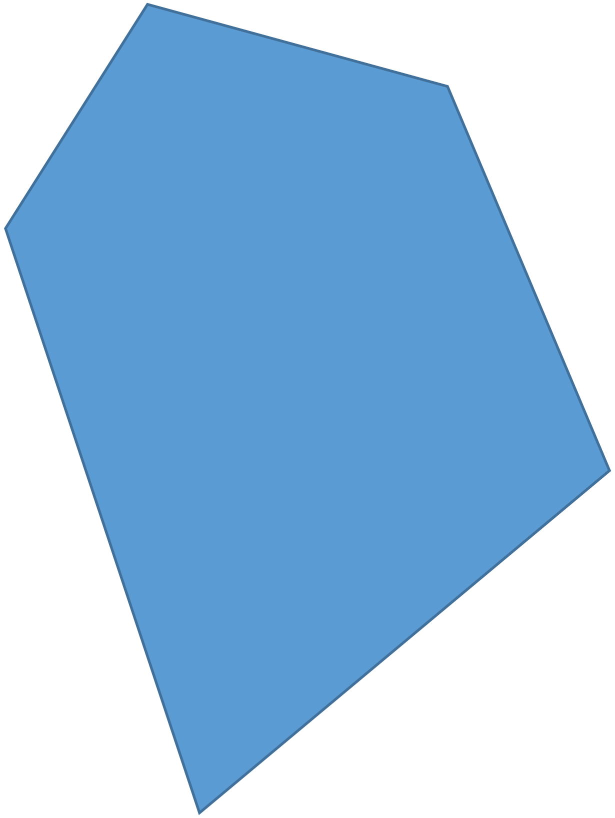
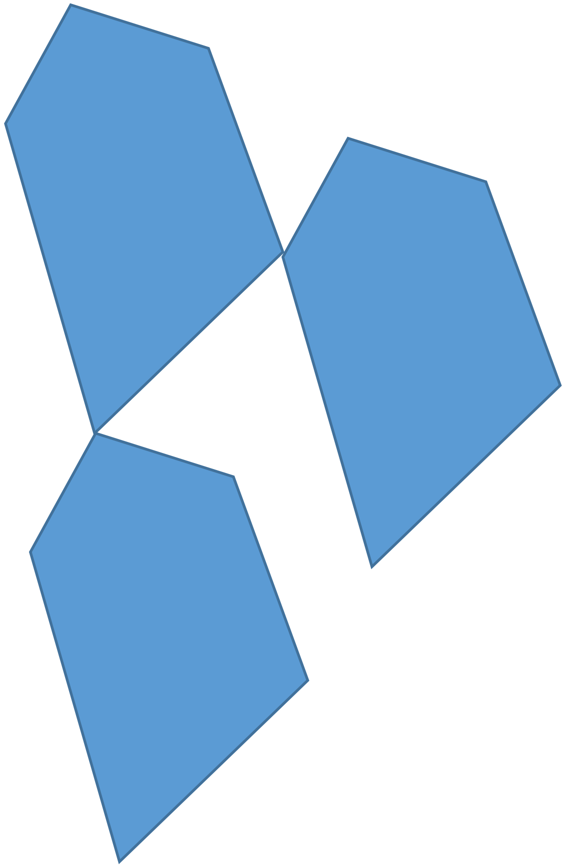
If all the samples inside the rectangle are positive;
otherwise are negative
Show a feedforward NN can classify all the samples correctly
For simplicity, we assume g(z) is a step function.
What are $\Theta^{(1)}$ and $\Theta^{(2)}$

Arbitrary Decision Boundary

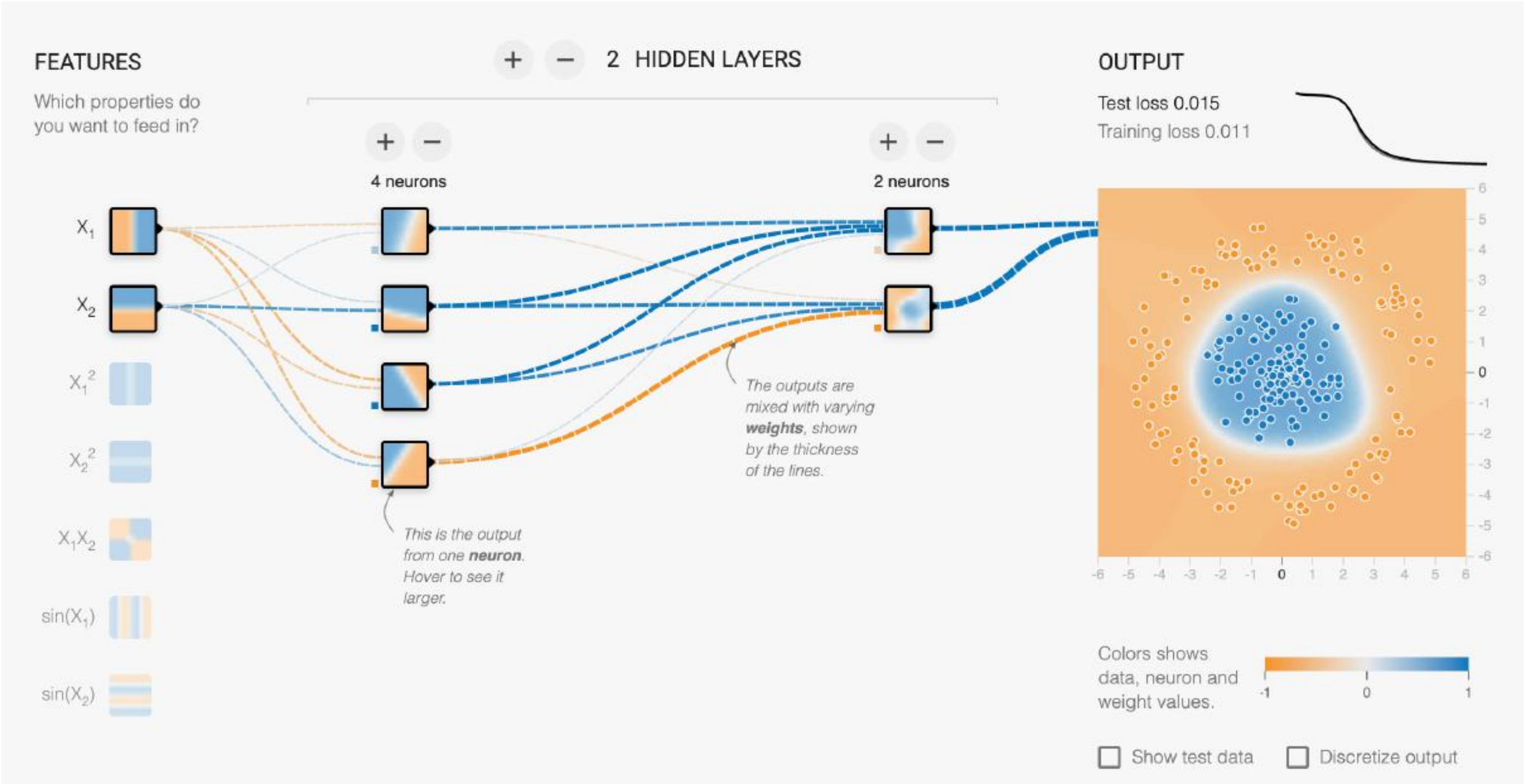


Arbitrary Decision Boundary



Neural Network Training Animation

- https://playground.tensorflow.org/



Neural Network Learning

Maximum Likelihood

- Training data: $S = \{(x_i, y_i)\}$, m examples
  $y_i = \{0,1\}$
- Consider a NN $h_\Theta(x) \in [0,1]$ modeling $P(y=1|x)$

$$a_1^{(2)} = g\left(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3\right) = g\left(z_1^{(2)}\right)$$
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$$h_\Theta(\mathbf{x}) = \underbrace{g\left(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)}\right)} = g\left(z_1^{(3)}\right)$$

Remember in logistic regression, $h_{w,b}(x) = \sigma(w^T x + b)$
If we choose the activation function g as a sigmoid function,
this part is equivalent to a logistic regression with input a

Based on slide by Andrew Ng

Maximum Likelihood

- Training data: $S = \{(x_i, y_i)\}$, m examples
  $y_i = \{0,1\}$
- Consider a NN $h_\Theta(x) \in [0,1]$ modeling $P(y = 1|x)$
- Maximum Likelihood estimator $\Theta^* = \arg\max_\Theta L(\Theta; S)$
  $L(\Theta; S) = \prod_{i=1}^{m} P_\Theta(y_i|x_i)$
  $$P_\Theta(y_i|x_i) = \begin{cases} h_\Theta(x_i), & y_i = 1 \\ 1 - h_\Theta(x_i), & y_i = -1 \end{cases}$$
- We can rewrite $L(\Theta; S)$ as
  $$L(\Theta; S) = \prod_{i=1}^{m} h_\Theta(x_i)^{y_i} (1 - h_\Theta(x_i))^{1-y_i}$$

Based on slide by Andrew Ng

Minimum Negative Log-Likelihood & Cross-Entropy Loss

- Training data: $S = \{(x_i, y_i)\}$, m examples
  $y_i = \{0,1\}$
- Consider a NN $h_\Theta(x) \in [0,1]$ modeling $P(y = 1|x)$
- Likelihood $L(\Theta; S)$ is
  $$L(\Theta; S) = \prod_{i=1}^{m} h_\Theta(x_i)^{y_i} (1 - h_\Theta(x_i))^{1-y_i}$$
- Log-Likelihood:
  $$\log L(\Theta; S) = \sum_i^m [y_i \log h_\Theta(x_i) + (1 - y_i) \log\big(1 - h_\Theta(x_i)\big)]$$
- Optimal Θ can be obtained by solving $\arg\min_\Theta J(\Theta)$
  $$\mathrm{J}(\Theta) = -\sum_i^m \underbrace{[y_i \log h_\Theta(x_i) + (1 - y_i) \log\big(1 - h_\Theta(x_i)\big)]}_{\text{Cross-entropy between prediction } h_\Theta(x) \text{ and true label } y_i}$$

Based on slide by Andrew Ng

Stochastic gradient Descent

Given a training set $\mathcal{D} = \{(\boldsymbol{x}, y)\}$

1. Initialize $\Theta \leftarrow \mathbf{0} \in \mathbb{R}^n$
2. For epoch $1 \ldots T$:
3. For $(\boldsymbol{x}, y)$ in $\mathcal{D}$:
4. Update $w \leftarrow w - \eta \boxed{\nabla J(\Theta)}$
5. Return Θ

(Similar to logistic regression)

$$J(\Theta) = -\sum_i^m [y_i \log h_\Theta(x_i) + (1 - y_i) \log\big(1 - h_\Theta(x_i)\big)]$$

Optimizing the Neural Network

$$\mathrm{J}(\Theta) = -\sum_i^m [y_i \log h_\Theta(x_i) \ + (1 - y_i) \log\big(1 - h_\Theta(x_i)\big)]$$

- Need to compute $\nabla J(\Theta)$

Based on slide by Andrew Ng

Chain Rule

- Given a function

$$f(x) = A(B(C(x)))$$

- The derivative is

$$f'(x) = A'(B) \cdot B'(C) \cdot C'(x)$$

Backpropagation through Computation Graphs

Computation Graphs and Backpropagation

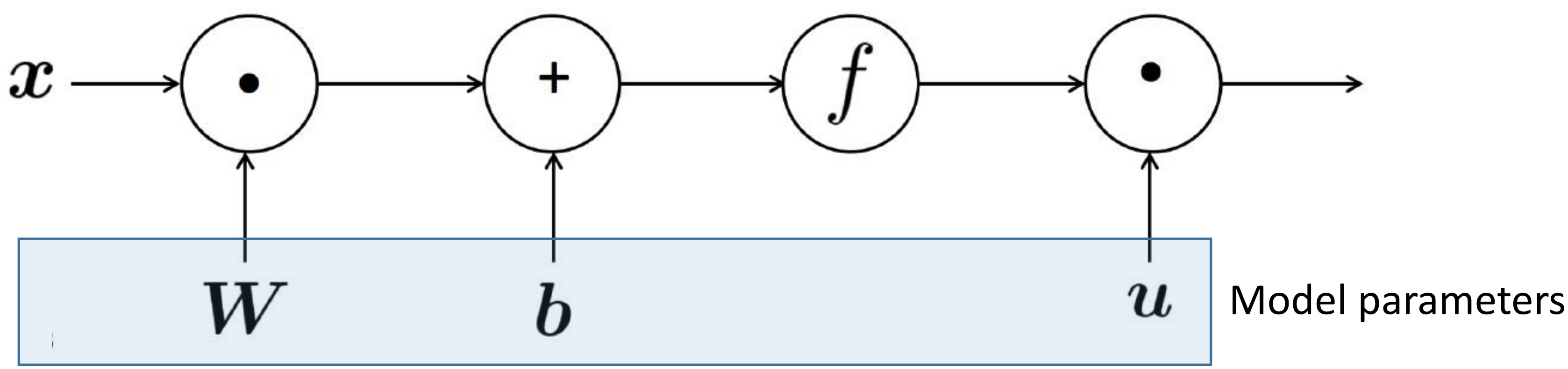
- Consider the NN on the right
- We represent NN as a graph

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

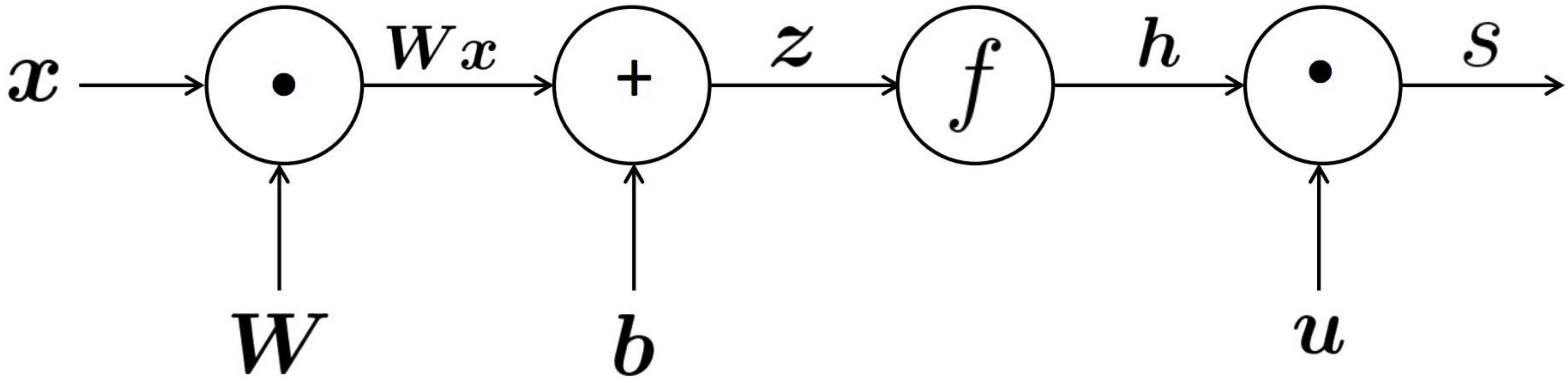
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$



Forward Propagation

- Edges pass along result of the operation



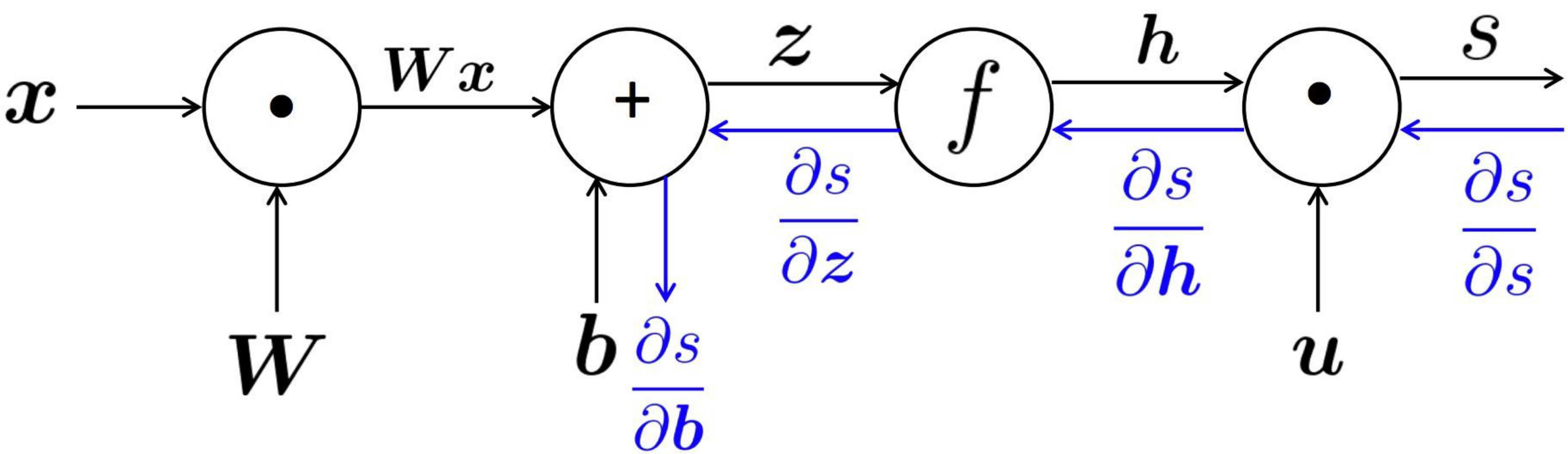
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

Back Propagation

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

- Compute $\frac{\partial s}{\partial \boldsymbol{b}}$

Chain Rule: $\frac{\partial s}{\partial b} = \frac{\partial s}{\partial z}\frac{\partial z}{\partial b} = \cdots$

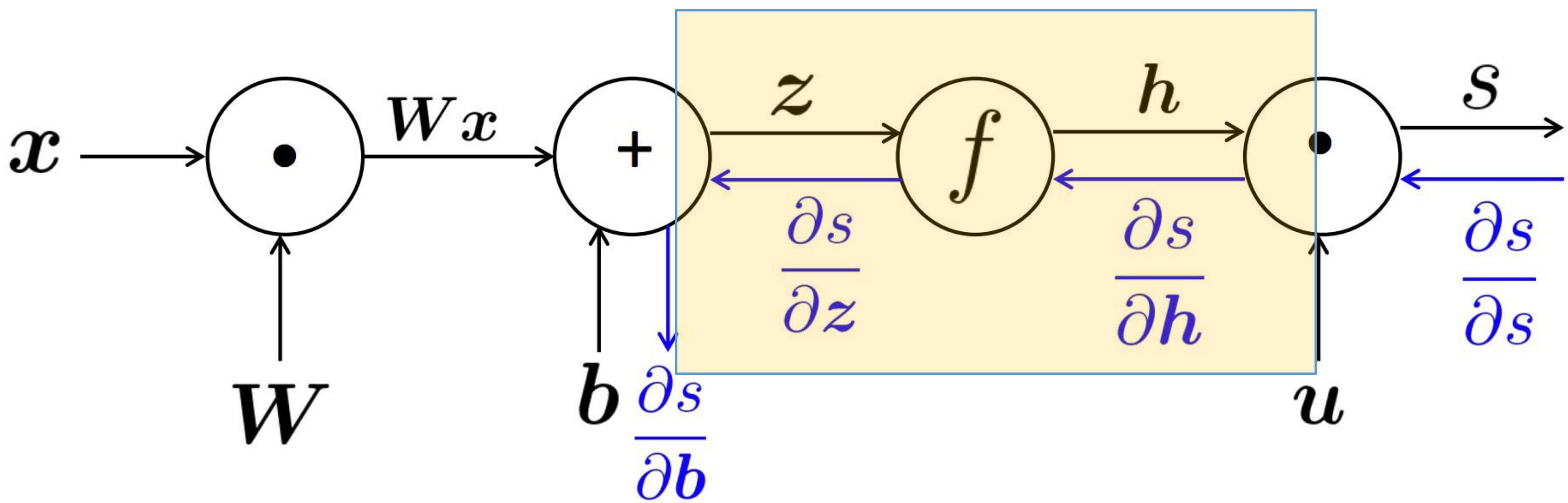


Back Propagation

- Compute $\frac{\partial s}{\partial \boldsymbol{b}}$

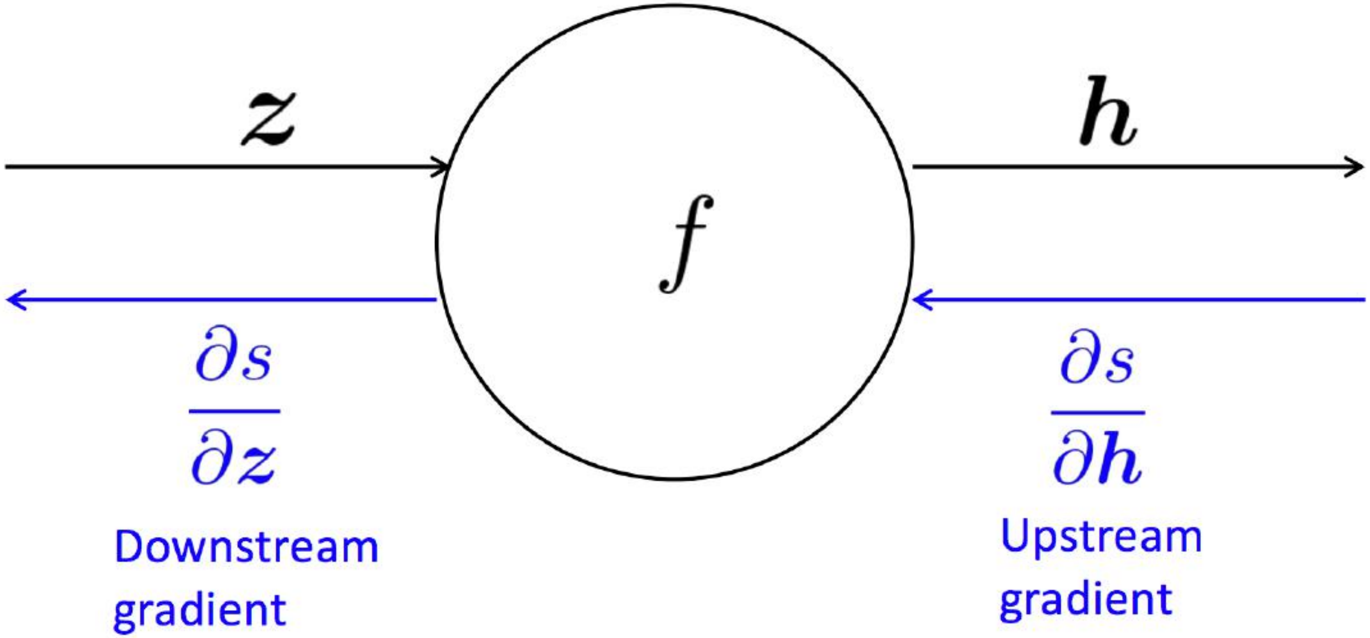
$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

Chain Rule: $\frac{\partial s}{\partial b} = \frac{\partial s}{\partial z}\frac{\partial z}{\partial b} = \frac{\partial s}{\partial h}\frac{\partial h}{\partial z}\frac{\partial z}{\partial b}$



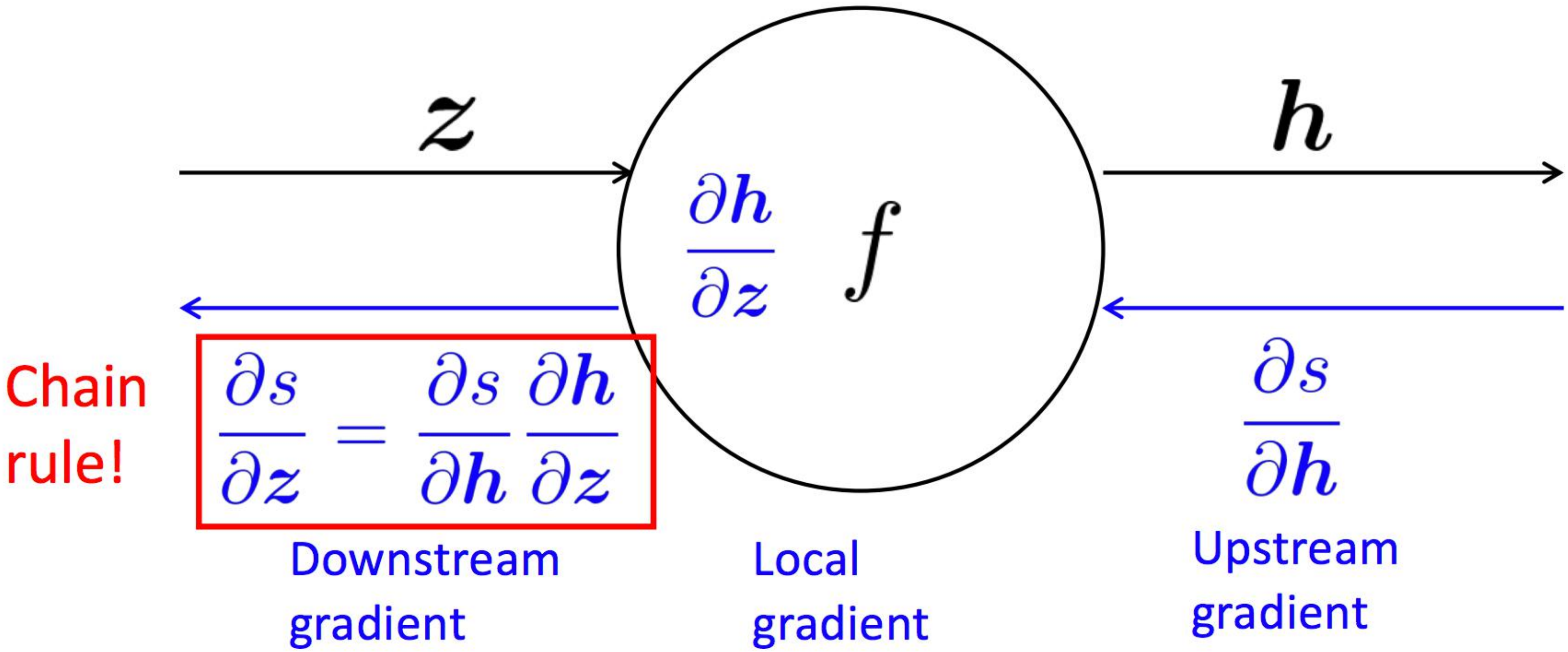
Backpropagation: Single Node

$$\boxed{\boldsymbol{h} = f(\boldsymbol{z})}$$



Chain Rule

$$\boxed{\boldsymbol{h} = f(\boldsymbol{z})}$$



Back Propagation

$$s = \boldsymbol{u}^T \boldsymbol{h}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\boldsymbol{x} \quad \text{(input)}$$

- Compute $\frac{\partial s}{\partial \boldsymbol{b}}$

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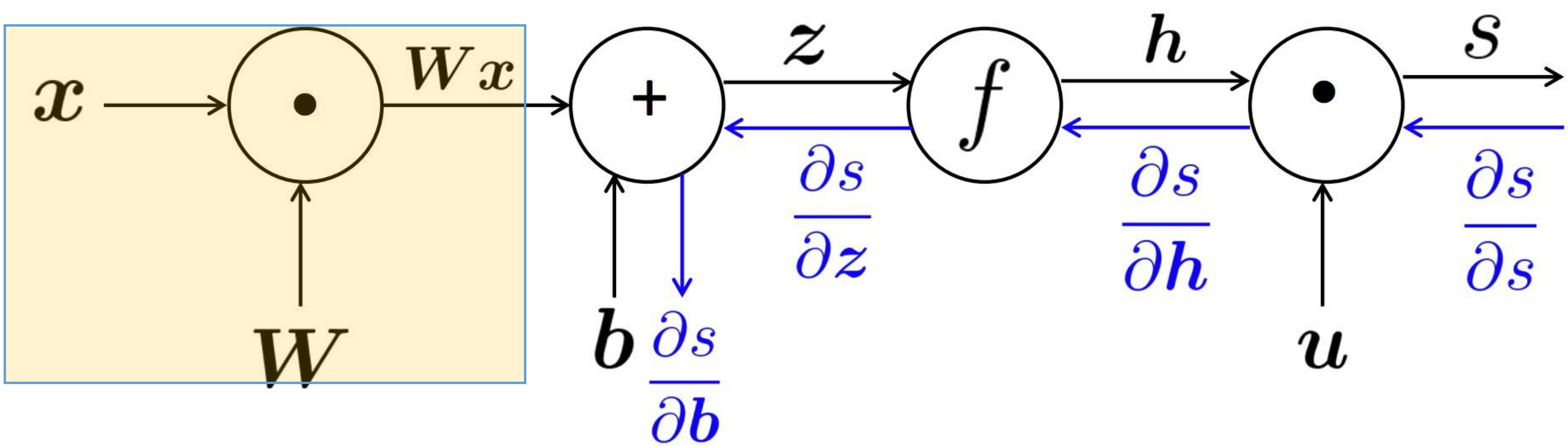
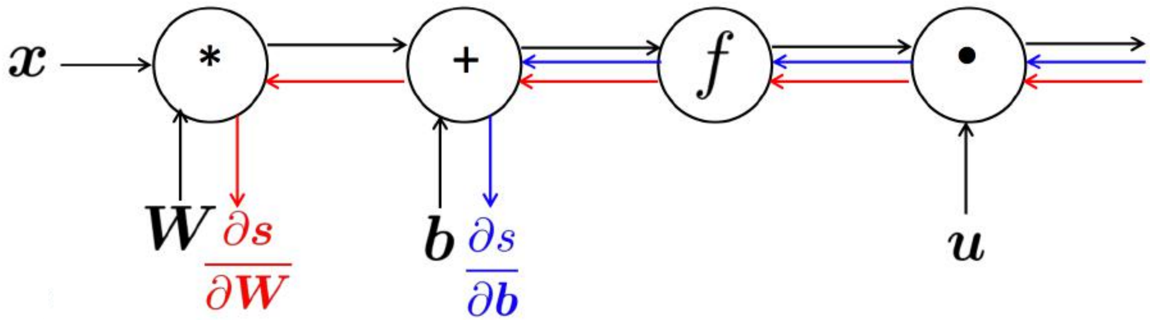


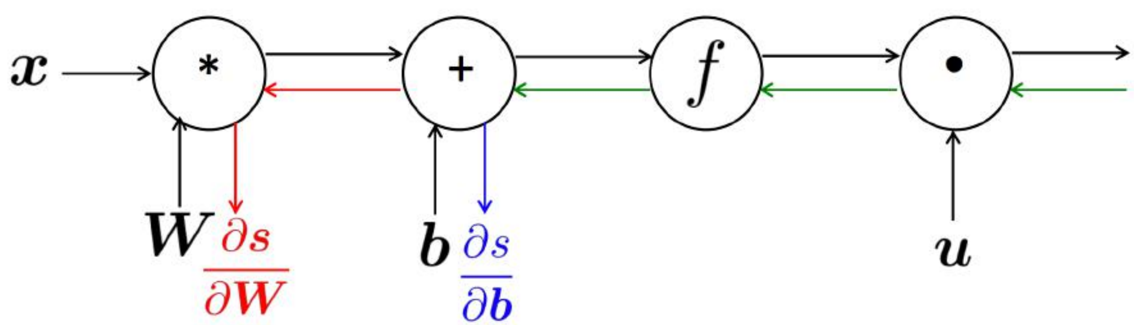
Compute all gradients at once



Naïve way to compute gradients:

Compute each component separately

⇒ Redundant computation



Example

$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Draw the computation graph and calculate $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Example

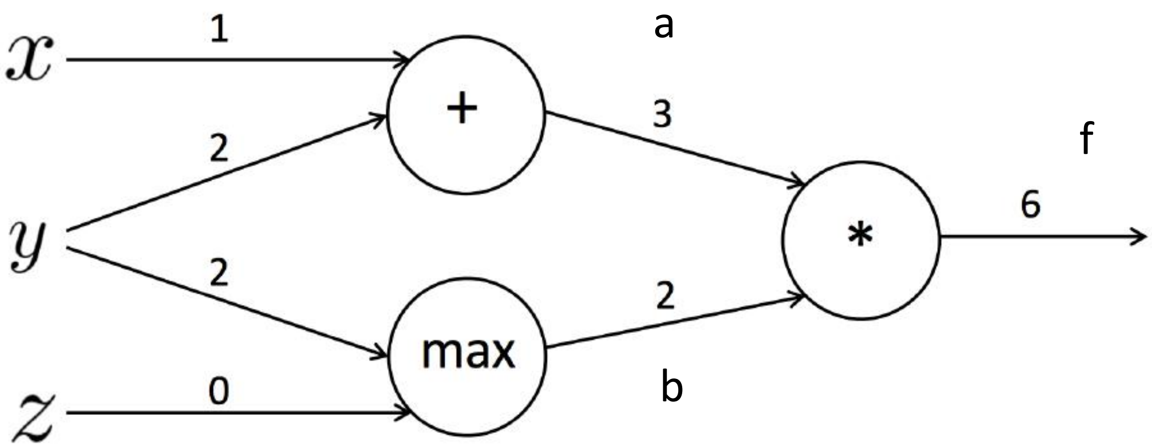
$$f(x, y, z) = (x + y)\max(y, z)$$
$$x = 1, y = 2, z = 0$$

Forward prop steps

$$a = x + y$$

$$b = \max(y, z)$$

$$f = ab$$



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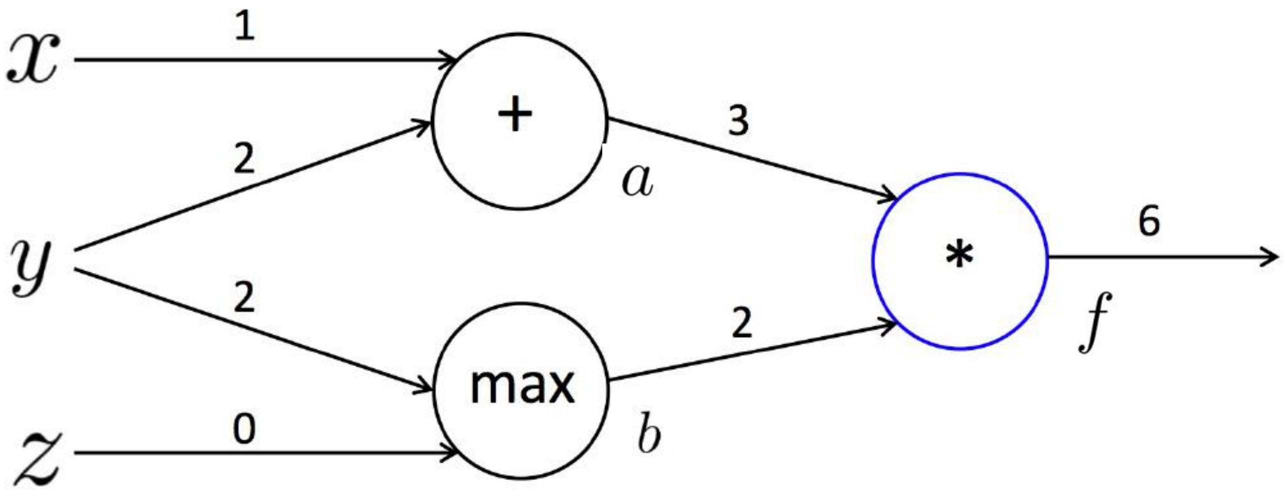
Local gradients

$$\frac{\partial a}{\partial x} = 1 \quad \frac{\partial a}{\partial y} = 1$$
$$\frac{\partial b}{\partial y} = \mathbf{1}(y > z) = 1 \quad \frac{\partial b}{\partial z} = \mathbf{1}(z > y) = 0$$
$$\frac{\partial f}{\partial a} = b = 2 \quad \frac{\partial f}{\partial b} = a = 3$$



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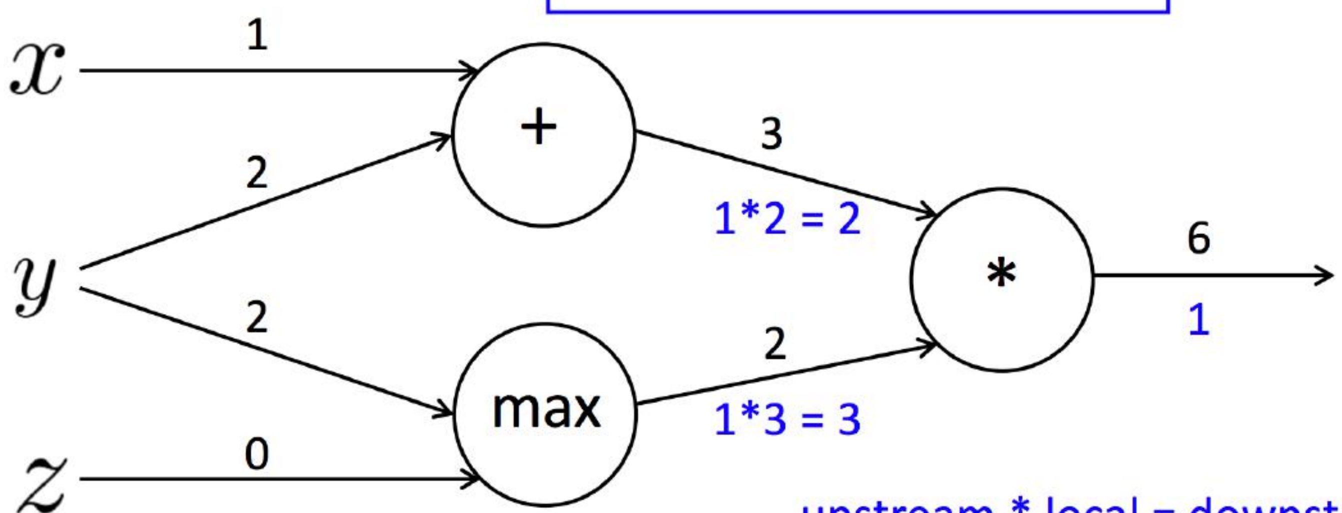

upstream * local = downstream

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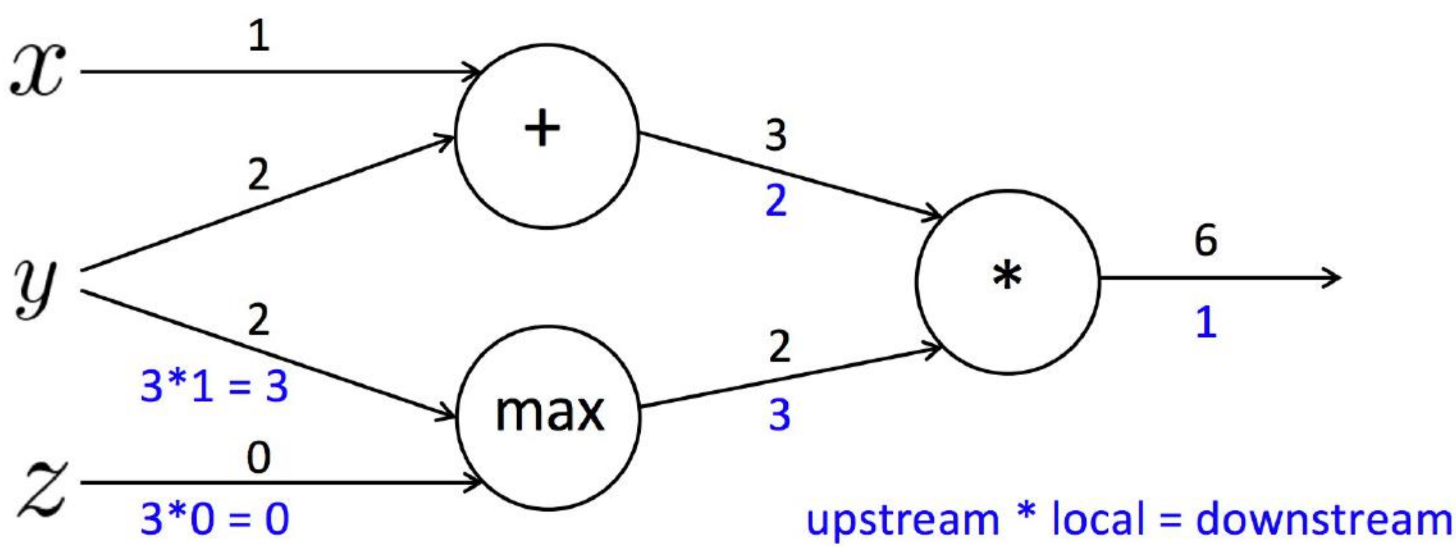

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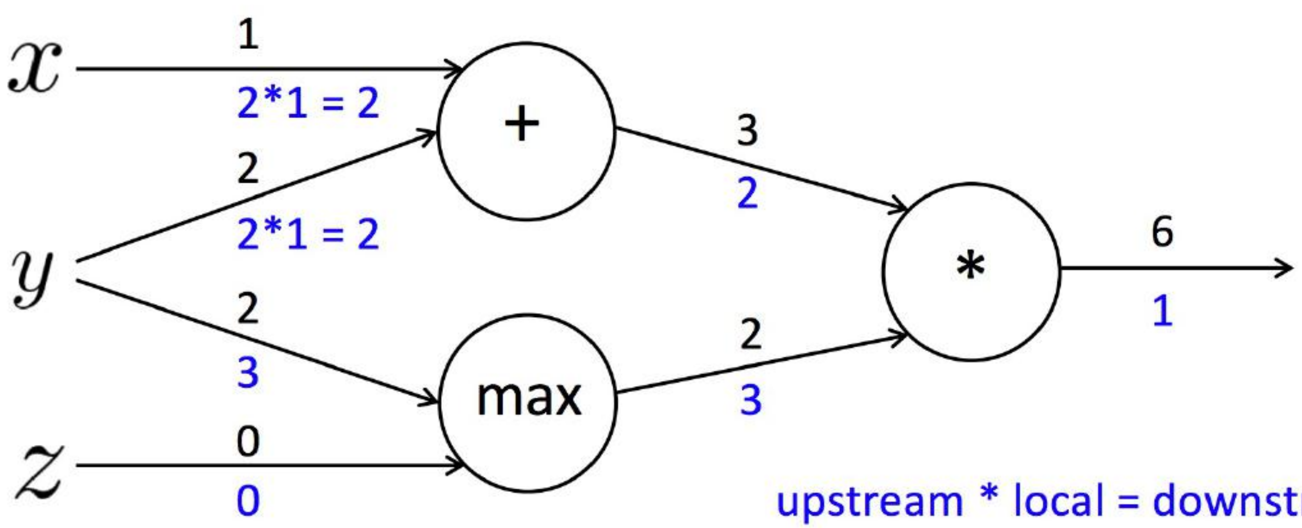

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Example

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$$x = 1, y = 2, z = 0$$

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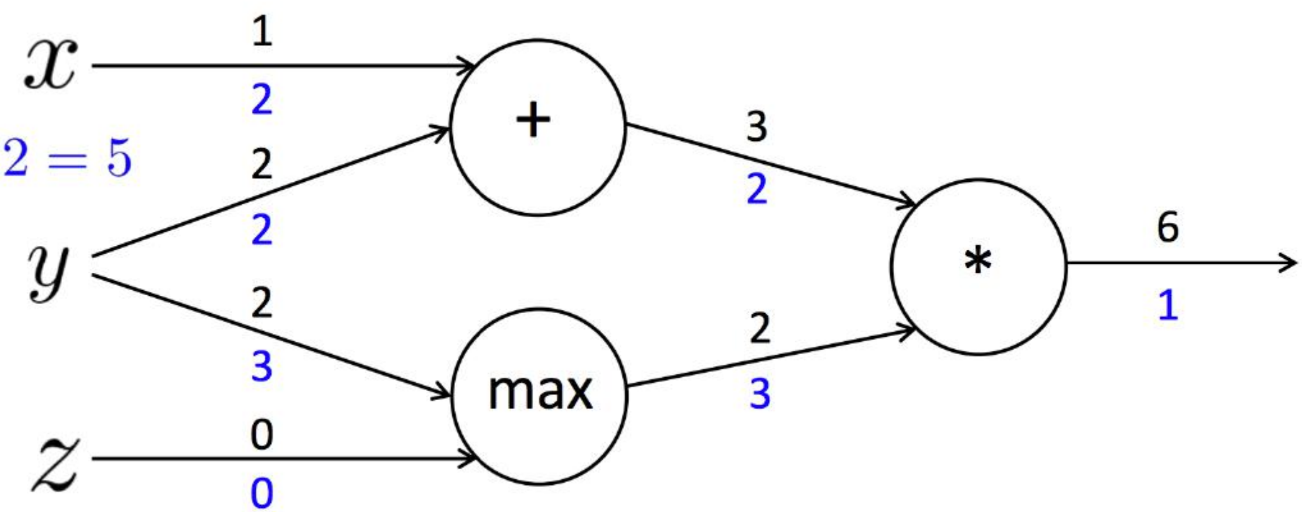
$$\frac{\partial f}{\partial x} = 2$$
$$\frac{\partial f}{\partial y} = 3 + 2 = 5$$
$$\frac{\partial f}{\partial z} = 0$$

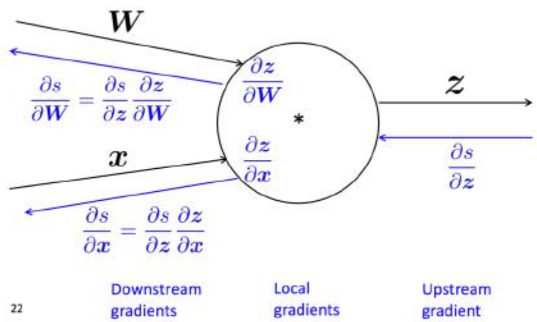


Why you should understand Backprop

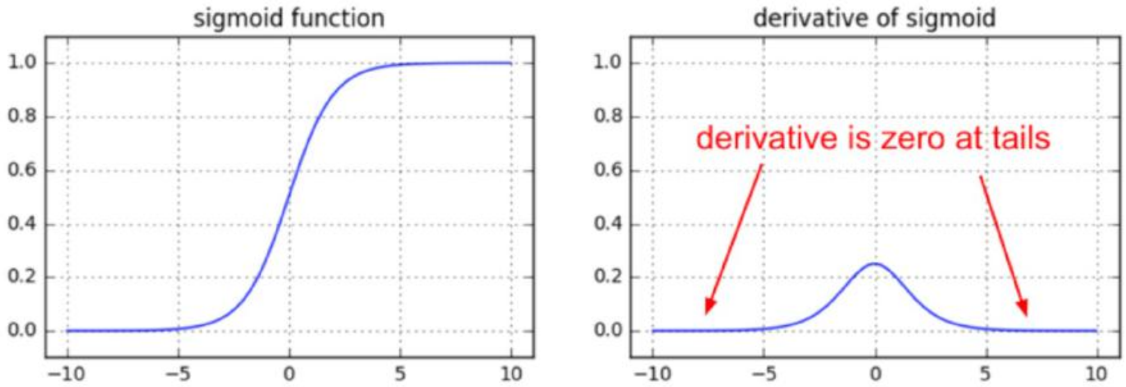
- Modern deep learning library implements backprop as a black-box for you
  - You can take a plane without knowing why it flies
  - but you're designing aircraft…
- Backpropagation doesn't always work perfectly.
  - Understanding why is crucial for debugging and improving models

https://medium.com/@karpathy/yes-you-should-understand-backprop-e2f06eab496b

Example: Gradient of sigmoid




```
z = 1/(1 + np.exp(-np.dot(W, x))) # forward pass
dx = np.dot(W.T, z*(1-z)) # backward pass: local gradient for x
dW = np.outer(z*(1-z), x) # backward pass: local gradient for W
```



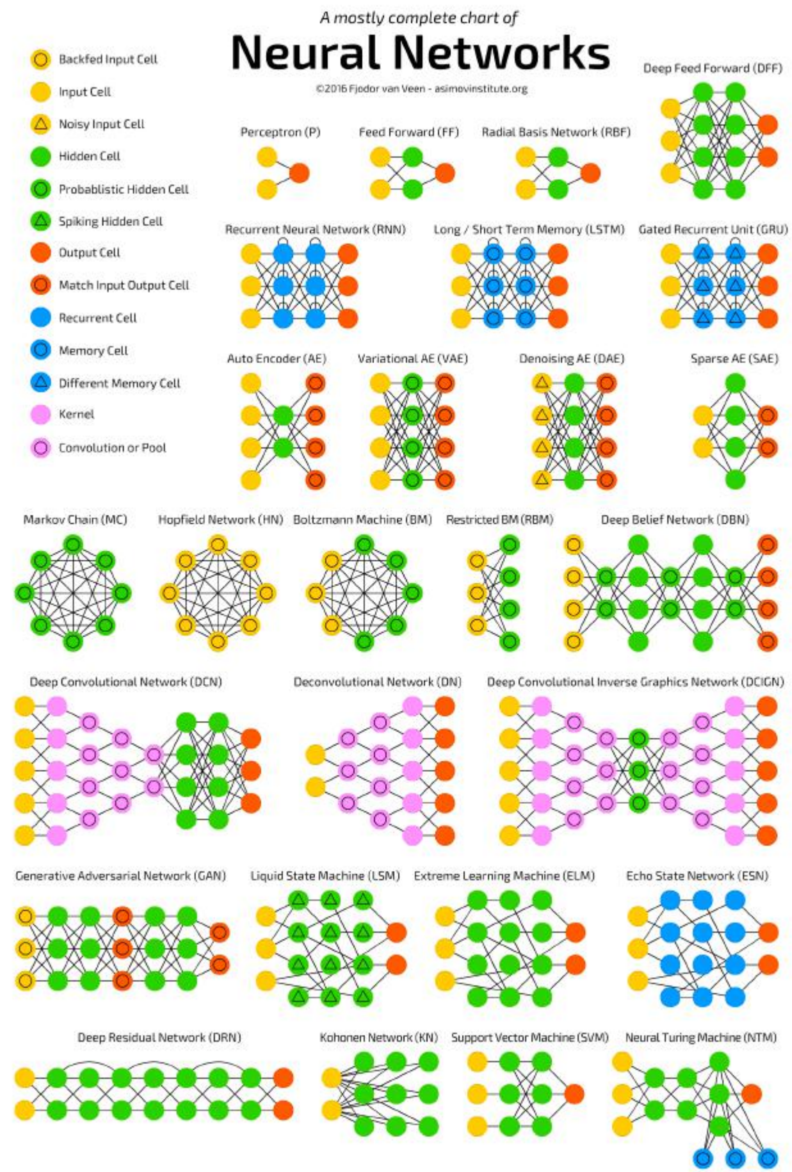
vanish gradient issue

More Details

- Parameter Initialization
  - Normally initialize weights to small random values; various designs
- Optimizer
  - Usually SGD works
  - Several SGD variants (e.g,. ADAM) automatically adjust learning rate based on an accumulated gradient

A neural network zoo

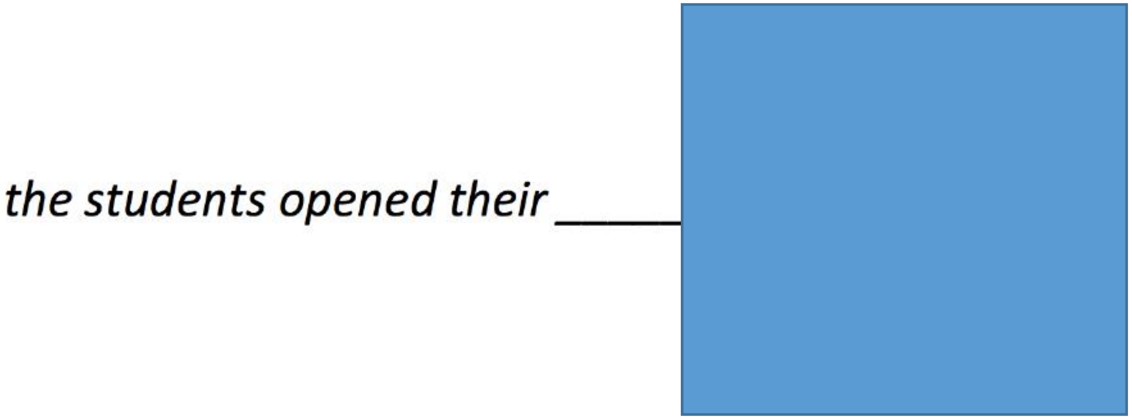
- The flexibility of NN allows us to try out different ideas
- However,
  there is no magic



Modeling with Neural Networks
(Advanced Topic/Not Included in Final)

Example – Language Model

- Predict next word



Idea 1:
A fixed-window neural Language Model

output distribution

$$\hat{\boldsymbol{y}} = \mathrm{softmax}(\boldsymbol{U}\boldsymbol{h} + \boldsymbol{b}_2) \in \mathbb{R}^{|V|}$$

hidden layer

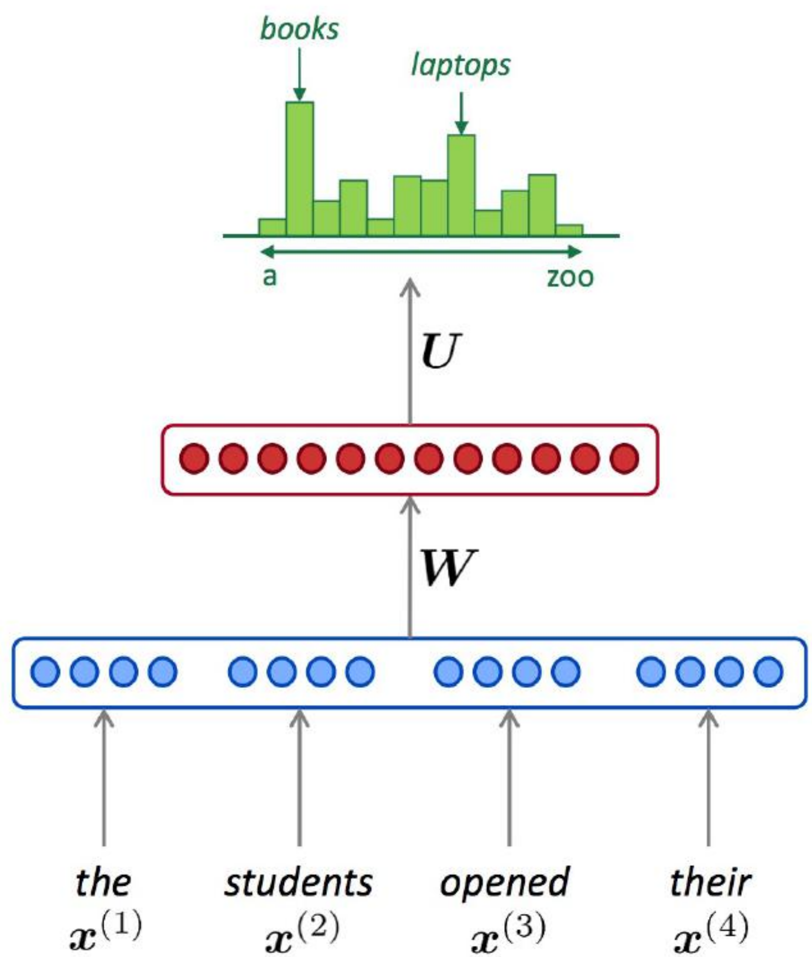
$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{e} + \boldsymbol{b}_1)$$

concatenated word embeddings

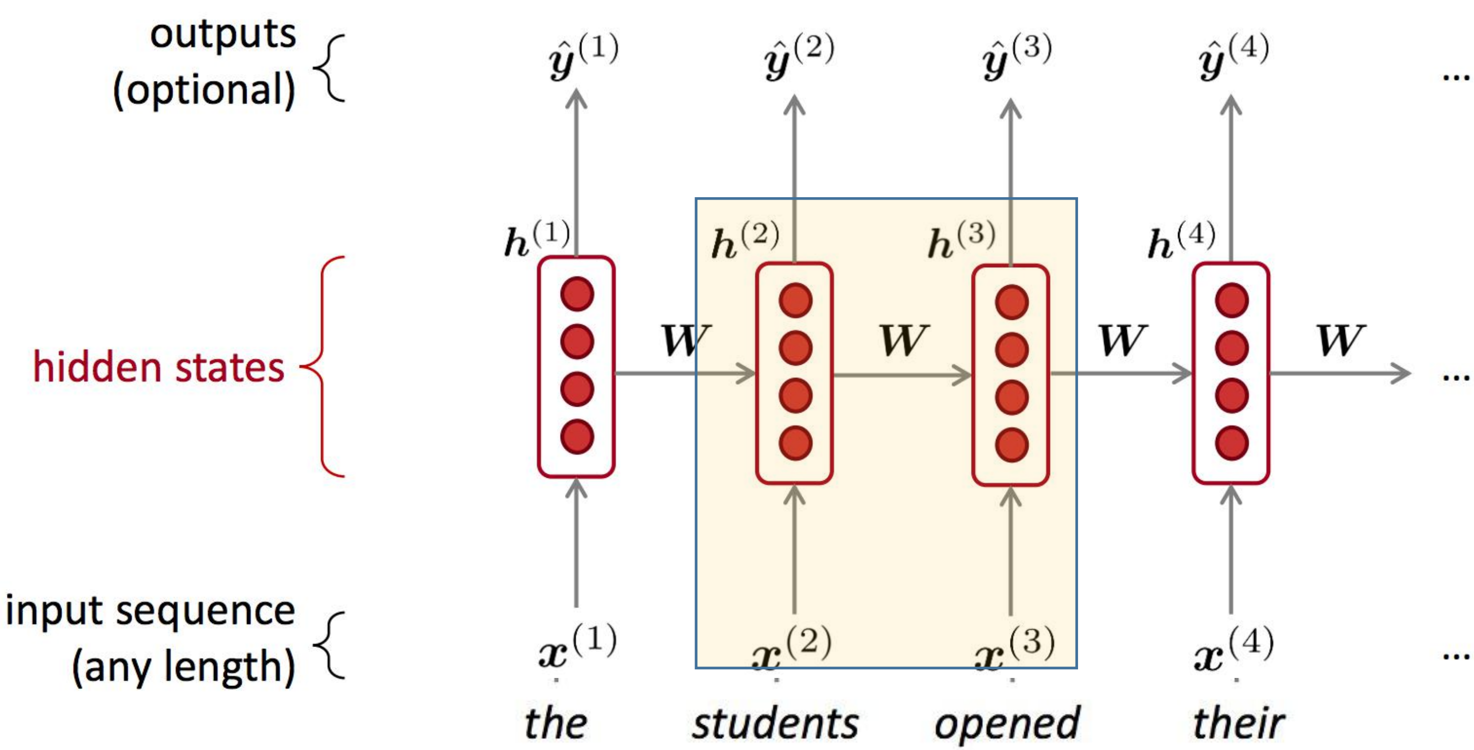
$$\boldsymbol{e} = [\boldsymbol{e}^{(1)}; \boldsymbol{e}^{(2)}; \boldsymbol{e}^{(3)}; \boldsymbol{e}^{(4)}]$$

words / one-hot vectors

$$\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \boldsymbol{x}^{(3)}, \boldsymbol{x}^{(4)}$$

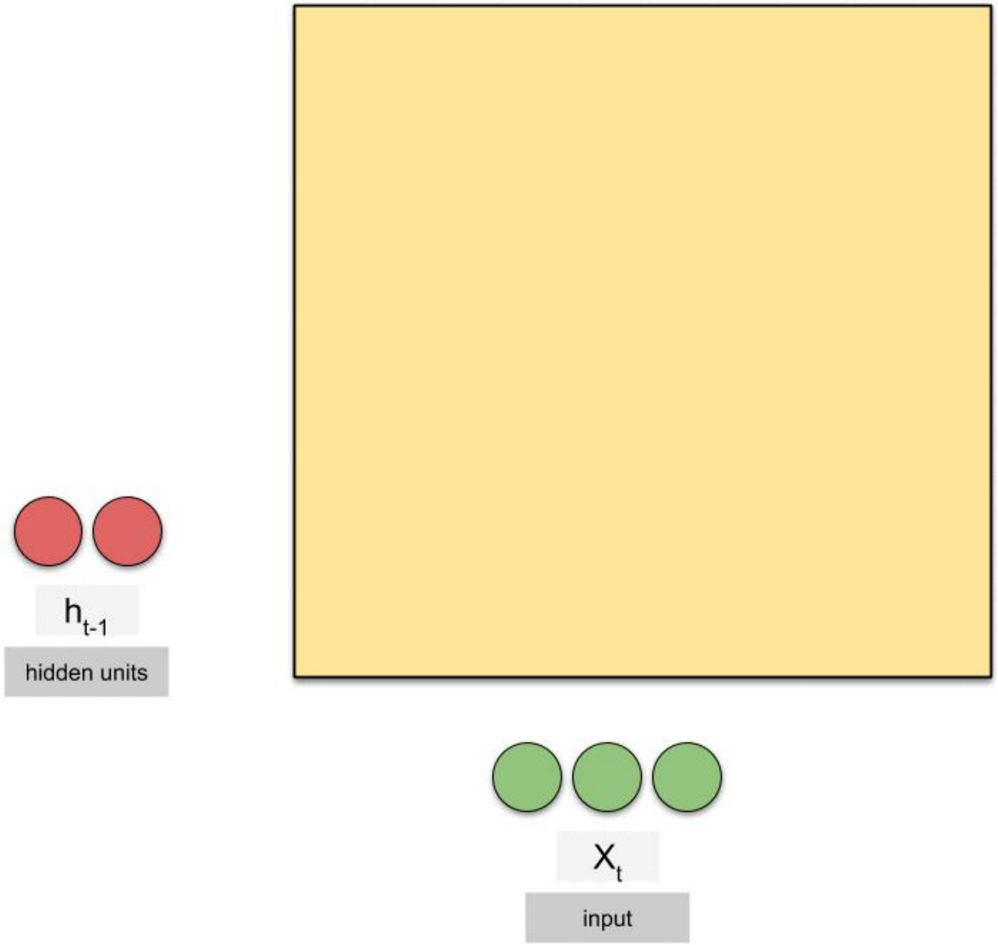


Idea 2: Recurrent Neural Networks (RNN)



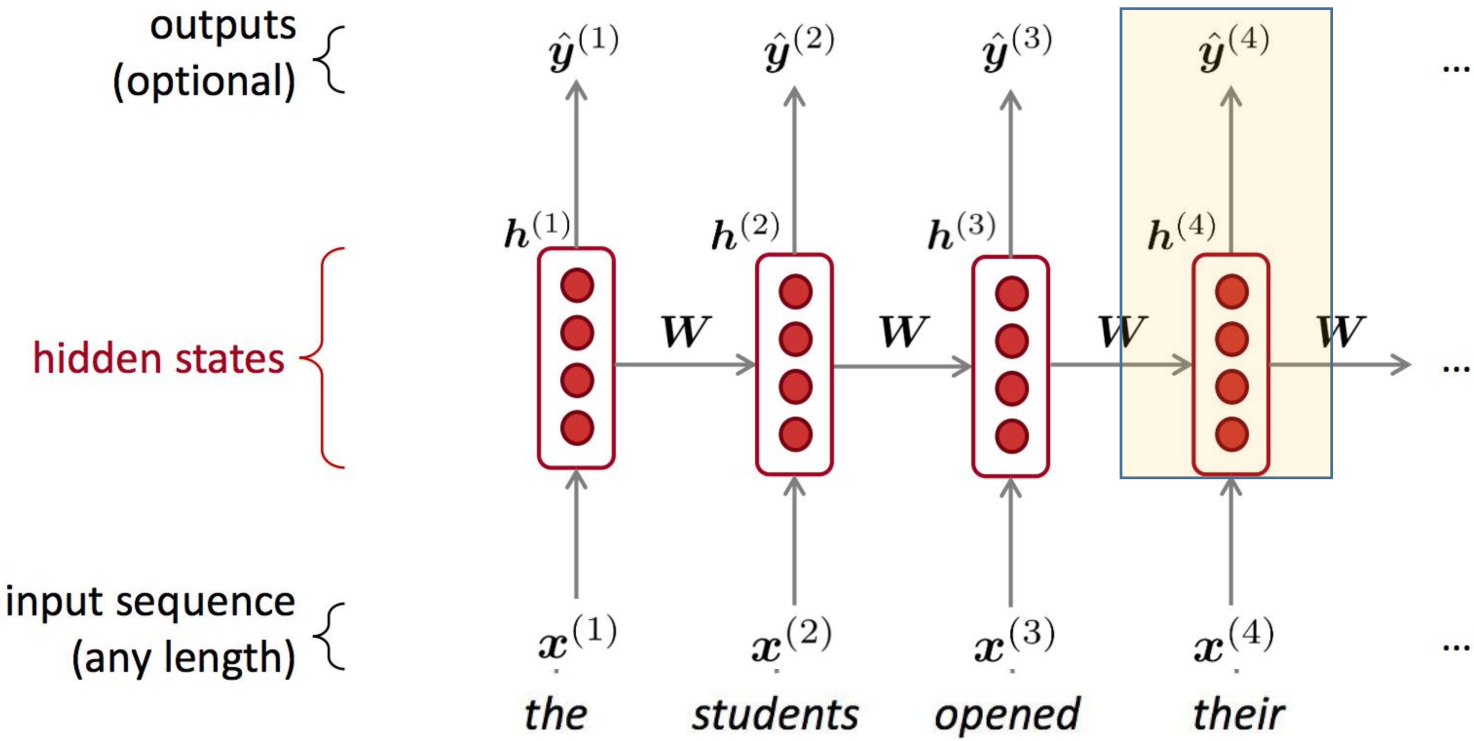
Core idea: Apply the same weights W *repeatedly*

Recurrent Neural Network



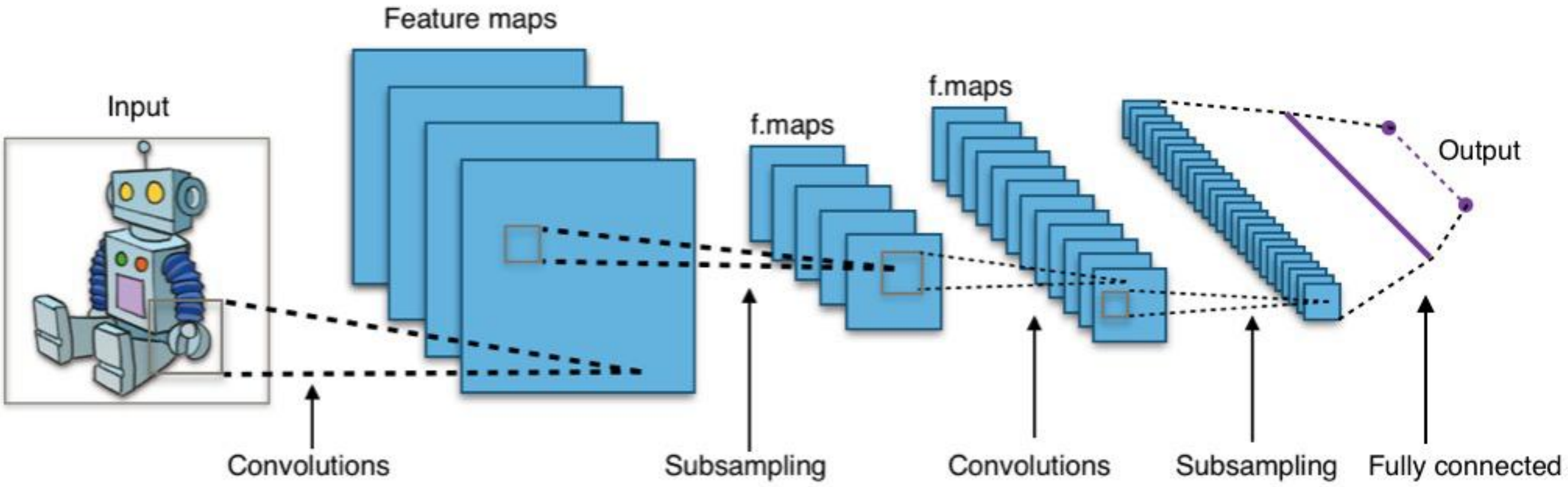
https://towardsdatascience.com/animated-rnn-lstm-and-gru-ef124d06cf45

Prediction using Latent State

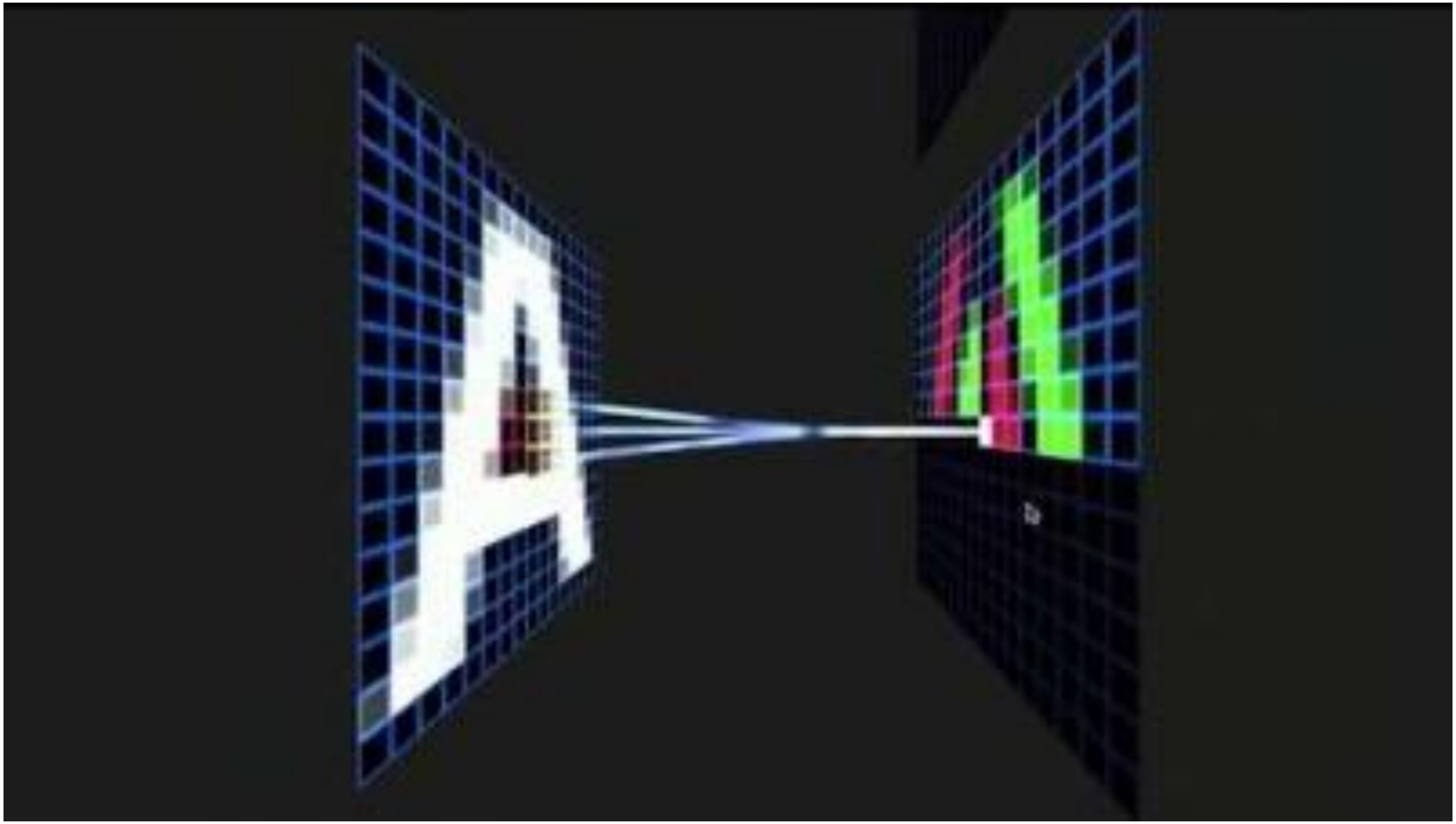


Core idea: Apply the same weights W *repeatedly*

Idea 3: Convolutional NN



Convolutional NN



https://www.youtube.com/watch?v=f0t-OCG79-U