

### 10-601B Introduction to Machine Learning

### **Neural Networks**

#### **Readings:**

Bishop Ch. 5 Murphy Ch. 16.5, Ch. 28 Mitchell Ch. 4 Matt Gormley Lecture 15 October 19, 2016

# Reminders

## Outline

- Logistic Regression (Recap)
- Neural Networks
- Backpropagation

# RECALL: LOGISTIC REGRESSION

# Using gradient ascent for linear classifiers.

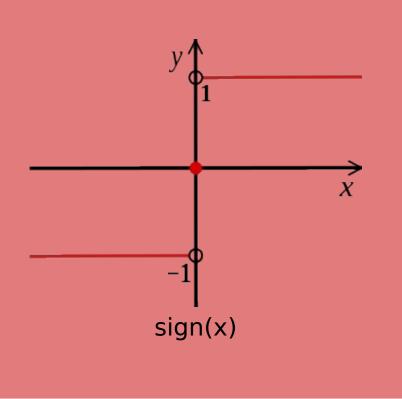
### Key idea behind today's lecture:

- 1. Define a linear classifier (logistic regression)
- 2. Define an objective function (likelihood)
- 3. Optimize it with gradient descent to learn parameters
- 4. Predict the class with highest probability under the model

# Using gradient ascent for linear classifiers

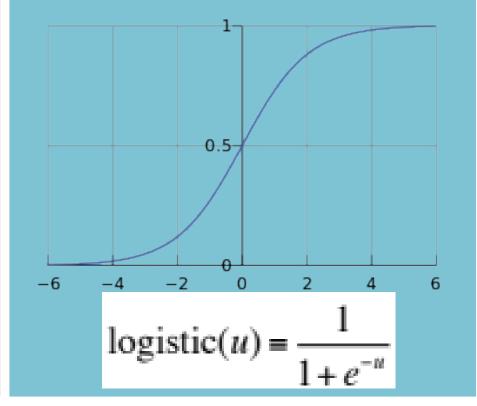
# This decision function isn't differentiable:

$$h(\mathbf{x}) = \mathsf{sign}(oldsymbol{ heta}^T \mathbf{x})$$



# Use a differentiable function instead:

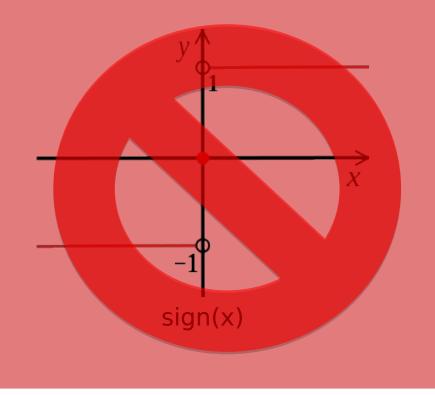
$$p_{\boldsymbol{\theta}}(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})}$$



# Using gradient ascent for linear classifier.

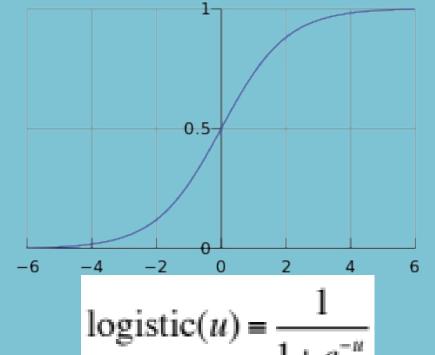
### This decision function isn't differentiable:

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## Use a differentiable function instead:

$$p_{\boldsymbol{\theta}}(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})}$$



$$logistic(u) = \frac{1}{1 + e^{-u}}$$



# Logistic Regression

**Data:** Inputs are continuous vectors of length K. Outputs are discrete.

$$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$$
 where  $\mathbf{x} \in \mathbb{R}^K$  and  $y \in \{0, 1\}$ 

**Model:** Logistic function applied to dot product of parameters vill in a later 1

$$p_{\boldsymbol{\theta}}(y = 1|\mathbf{x}) = \frac{1}{1 + \exp(-\boldsymbol{\theta}^T \mathbf{x})}$$

**Learning:** finds the parameters that minimize some objective fu ${m heta}^* = \mathop{\rm argmin}_{m heta} J({m heta})$ 

Prediction: Output is the most probable class.

$$\hat{y} = \operatorname*{argmax} p_{\theta}(y|\mathbf{x})$$
$$y \in \{0,1\}$$

# **NEURAL NETWORKS**

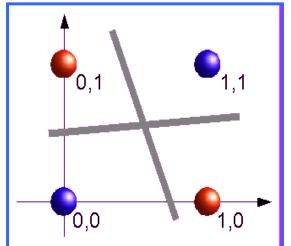
# Learning highly non-linear functions



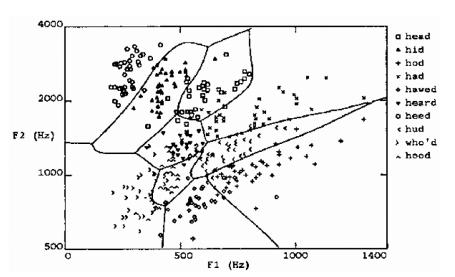
#### f: X € Y

- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

The XOR gate



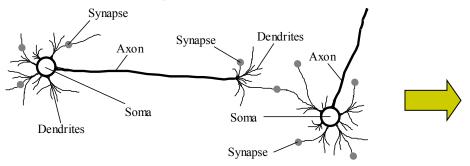
#### Speech recognition

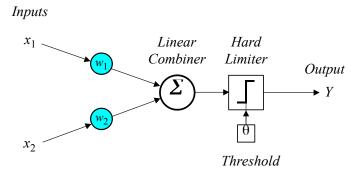


## **Perceptron and Neural Nets**



From biological neuron to artificial neuron (perceptron)



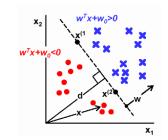


Activation function

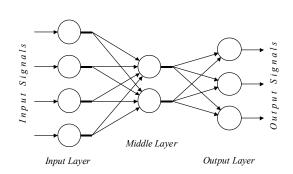
$$X = \sum_{i=1}^{n} x_i w_i$$

$$\mathbf{Y} = \begin{cases} +1, & \text{if } \mathbf{X} \ge \omega_0 \\ -1, & \text{if } \mathbf{X} < \omega_0 \end{cases}$$





- Artificial neuron networks
  - supervised learning
  - gradient descent



#### **Connectionist Models**

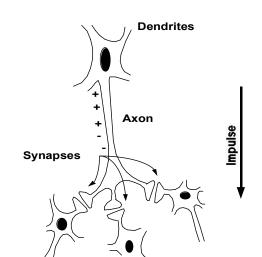


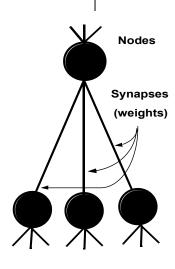
#### Consider humans:

- Neuron switching time
  - ~ 0.001 second
- Number of neurons
  - ~ 1010
- Connections per neuron
  - ~ 104-5
- Scene recognition time
  - ~ 0.1 second
- 100 inference steps doesn't seem like enough
  - much parallel computation



- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed processes





### Motivation

# Why is everyone talking about Deep Learning?

- Because a lot of money is invested in it...
  - DeepMind: Acquired by Google for \$400 million
  - DNNResearch: Three person startup (including Geoff Hinton) acquired by Google for unknown price tag
  - Enlitic, Ersatz, MetaMind, Nervana, Skylab:
     Deep Learning startups commanding
     millions of VC dollars
- Because it made the **front page** of the New York Times



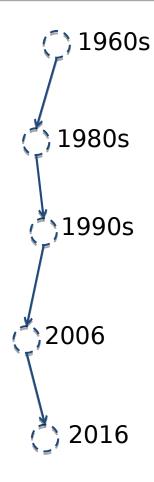






### Motivation

# Why is everyone talking about Deep Learning?



### Deep learning:

- Has won numerous pattern recognition competitions
- Does so with minimal feature engineering

#### This wasn't always the case!

Since 1980s: Form of models hasn't changed much, but lots of new tricks...

- More hidden units
- Better (online) optimization
- New nonlinear functions (ReLUs)
- Faster computers (CPUs and GPUs)

# Background

# A Recipe for Machine Learning

# 1. Given training $\mathsf{data}_{\{\boldsymbol{x}_i,\boldsymbol{y}_i\}_{i=1}^N}$

# 2. Choose each of these:

- Recision function  $\hat{y} = f_{m{ heta}}(x_i)$ 

- Loss function  $\ell(\hat{m{y}},m{y}_i)\in\mathbb{R}$ 

Face Face Not a face

**Examples**: Linear regression, Logistic regression, Neural Network

**Examples**: Mean-squared error, Cross Entropy

# Background

# A Recipe for Machine Learning

# 1. Given training $\mathsf{data}_{\{\boldsymbol{x}_i,\boldsymbol{y}_i\}_{i=1}^N}$

# 3. Define goal:

$$oldsymbol{ heta}^* = rg\min_{oldsymbol{ heta}} \sum_{i=1}^N \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

# 2. Choose each of these:

- Recision function  $\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$
- Loss function  $\ell(\hat{m{y}},m{y}_i)\in\mathbb{R}$

#### 4. Train with SGD:

(take small steps opposite the gradient)

$$oldsymbol{ heta}^{(t+1)} = oldsymbol{ heta}^{(t)} - \eta_t 
abla \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

## Background

#### A Recipe for

## Gradients

1. Given training  $\{oldsymbol{x}_i, oldsymbol{y}_i\}_{i=1}^N$ 

**Backpropagation** can compute this gradient!

And it's a special case of a more general algorithm called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

2. Choose each these:

$$\hat{y} = f_{m{ heta}}(x_i)$$
 function efficiently!

- Loss function  $\ell(\hat{m{y}}, m{y}_i) \in \mathbb{R}$ 

opposite the gradient) 
$$\boldsymbol{\theta}^{(t)} = -\eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

#### A Recipe for

# Goals for Today's Lecture

- 1 1. Explore a **new class of decision functions** (Neural Networks)
  - 2. Consider variants of this recipe for training

# 2. Choose each of these:

 $\hat{m{y}} = f_{m{ heta}}(m{x}_i)$ 

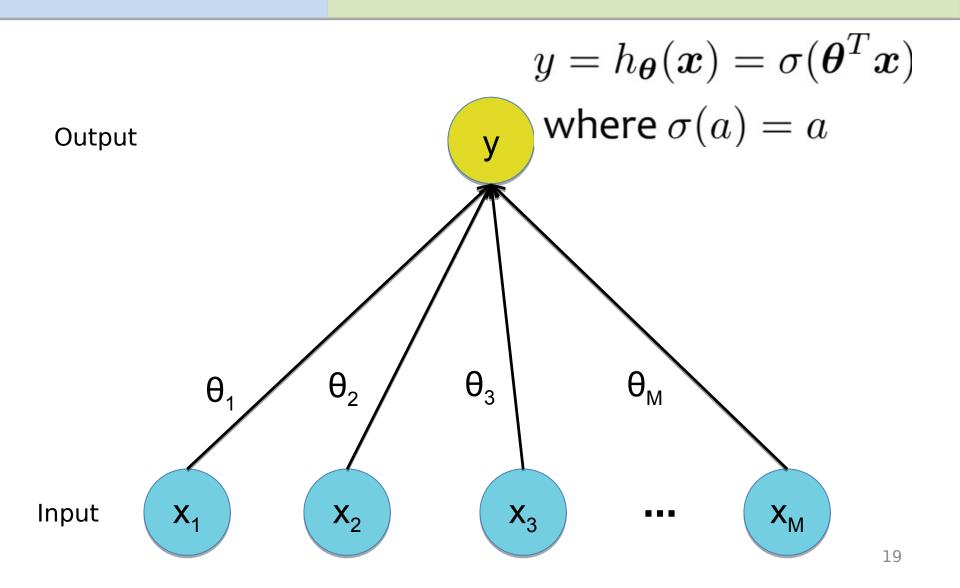
- Loss function  $\ell(\hat{m{y}}, m{y}_i) \in \mathbb{R}$ 

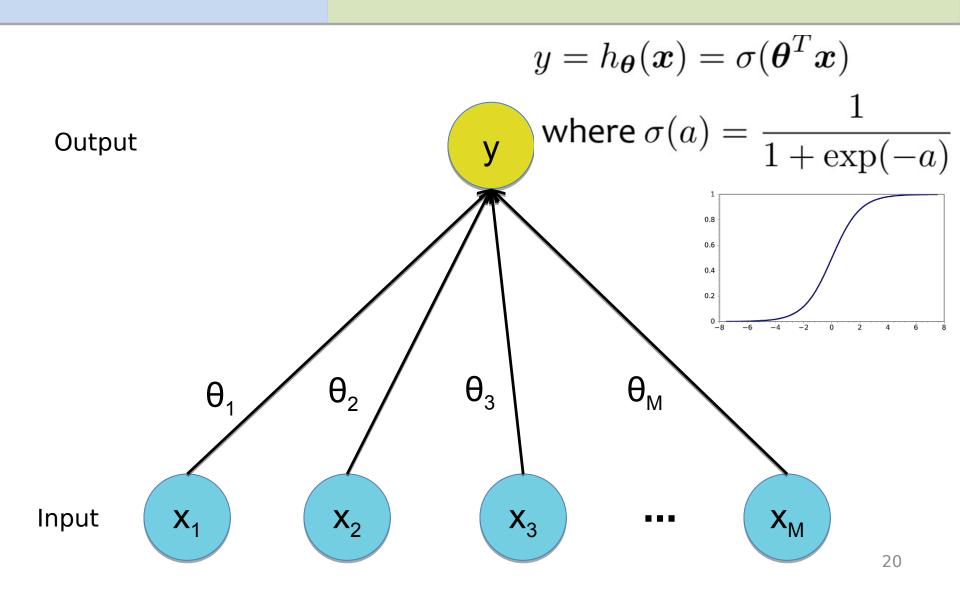
Train with SGD:

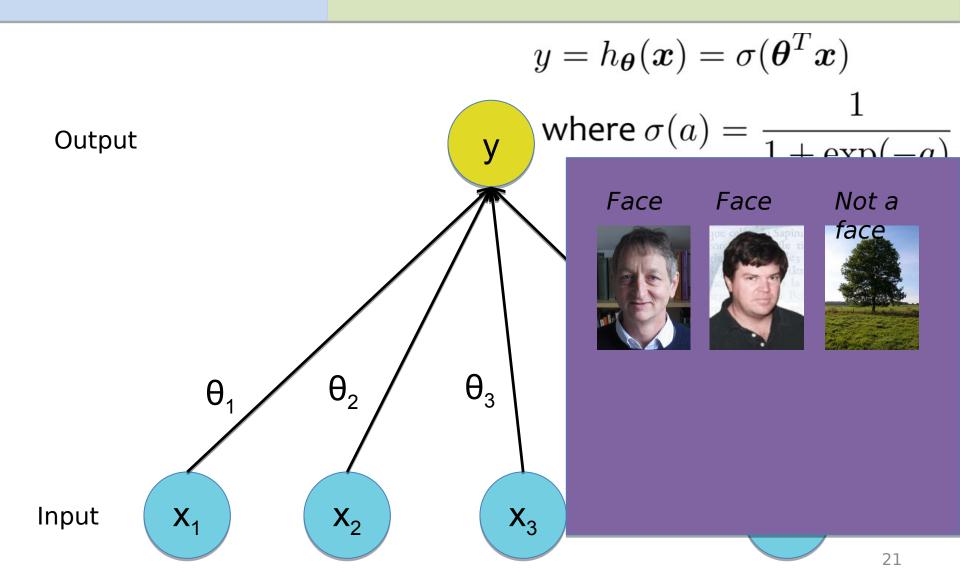
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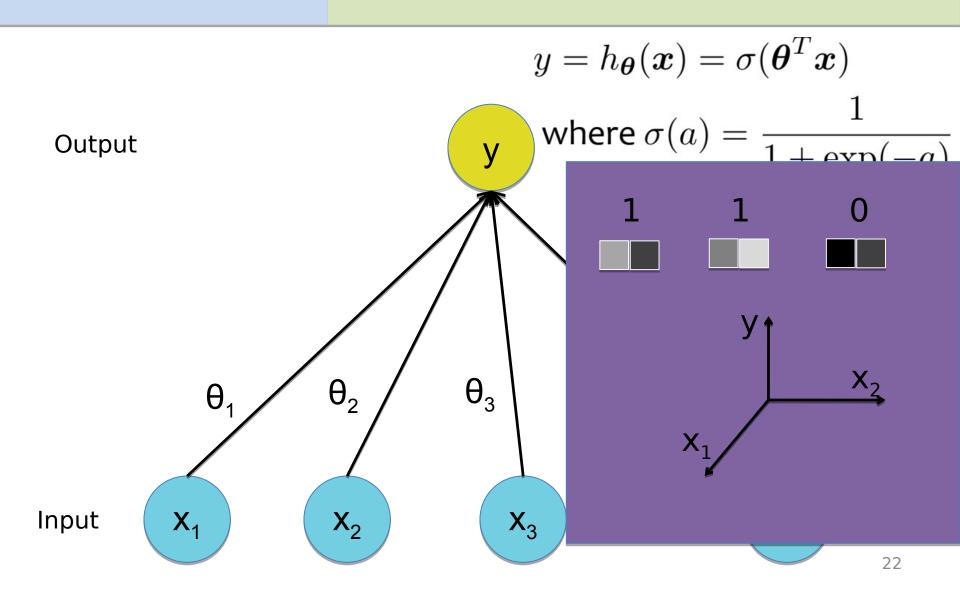
$$oldsymbol{ heta}^{(t+1)} = oldsymbol{ heta}^{(t)} - \eta_t 
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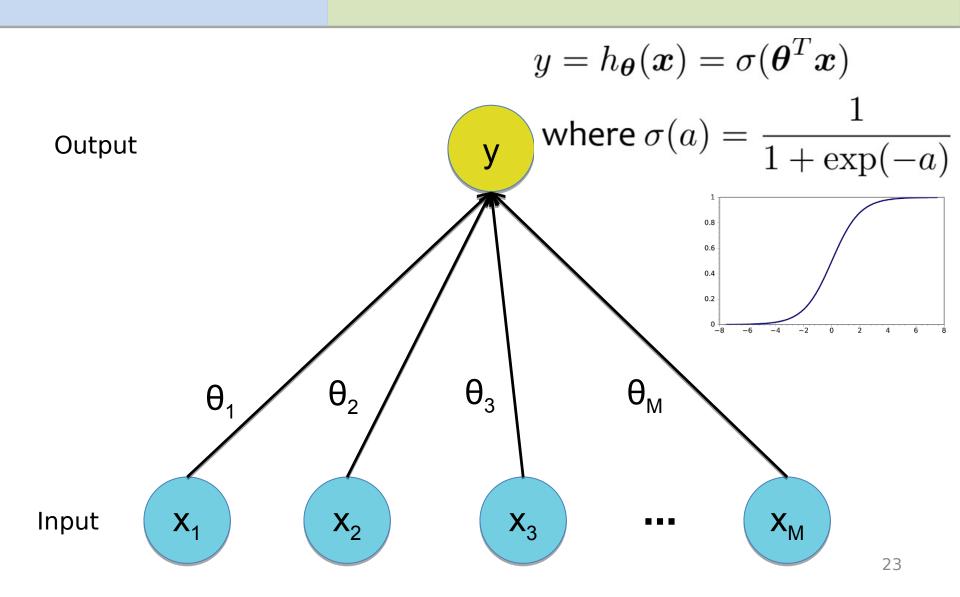
# Linear Regression







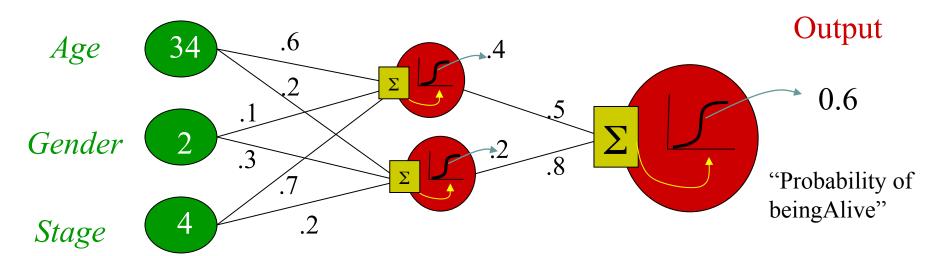




#### **Neural Network Model**







Independent variables

Weights

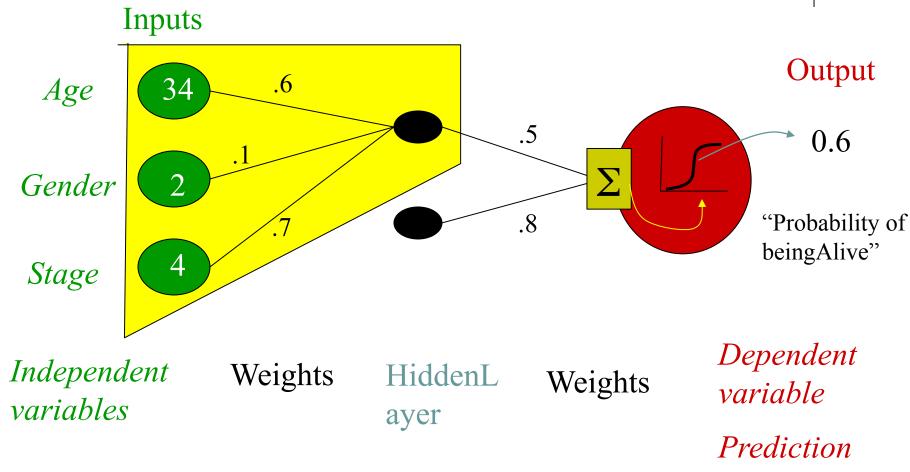
HiddenL ayer

Weights

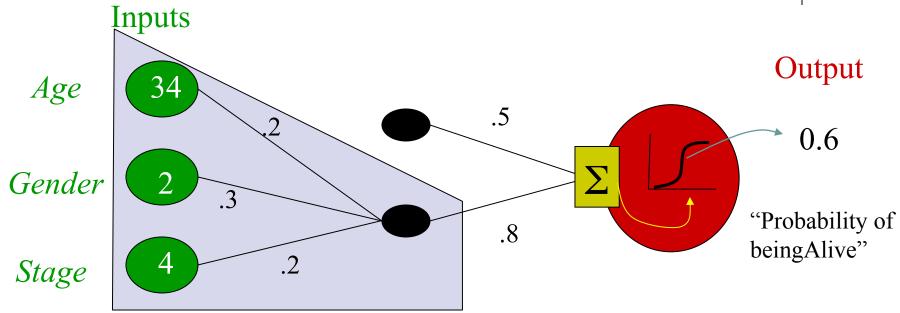
Dependent variable

## "Combined logistic models"









Independent variables

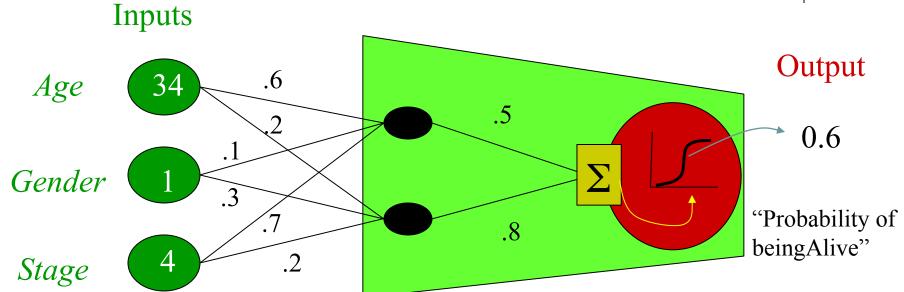
Weights

HiddenL ayer

Weights

Dependent variable





Independent variables

Weights

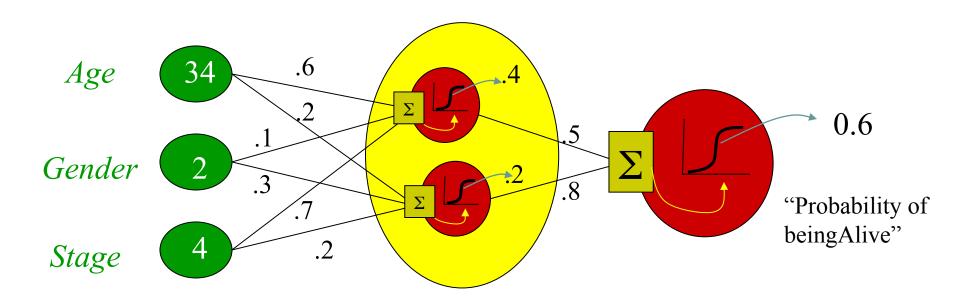
HiddenL ayer

Weights

Dependent variable

# Not really, no target for hidden units...





Independent variables

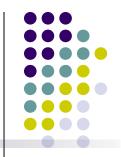
Weights

HiddenL ayer

Weights

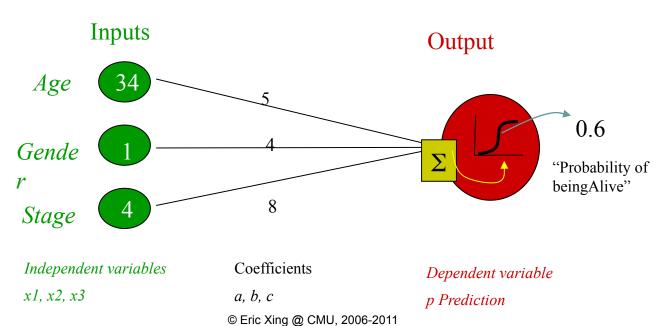
Dependent variable

## Jargon Pseudo-Correspondence

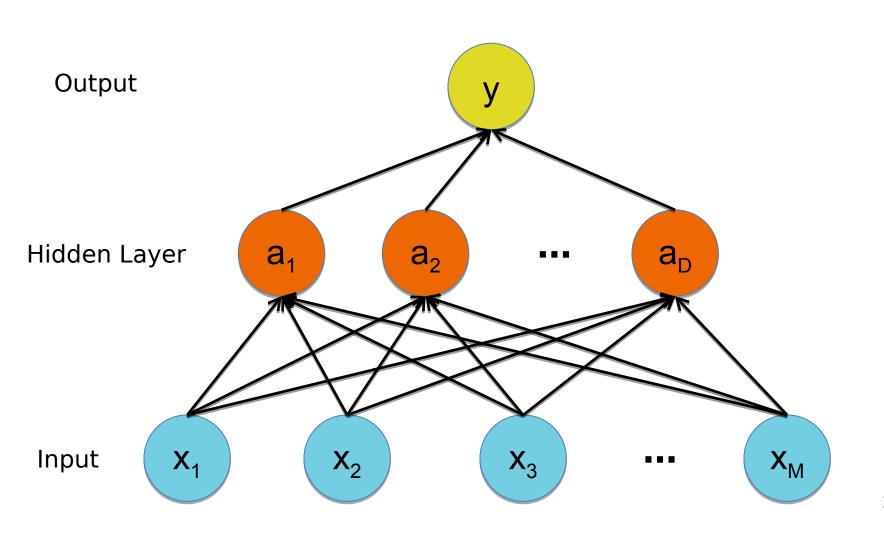


- Independent variable = input variable
- Dependent variable = output variable
- Coefficients = "weights"
- Estimates = "targets"

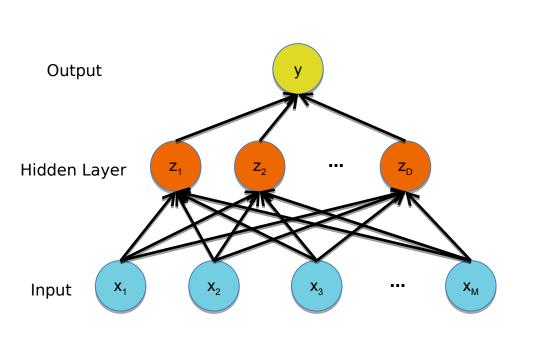
#### Logistic Regression Model (the sigmoid unit)

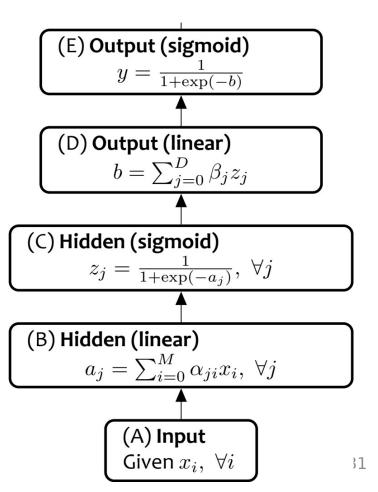


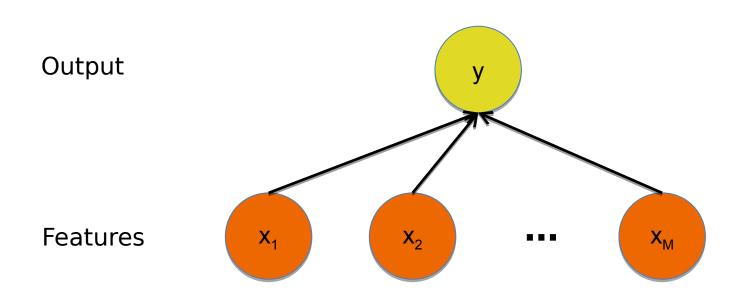
# Neural Network

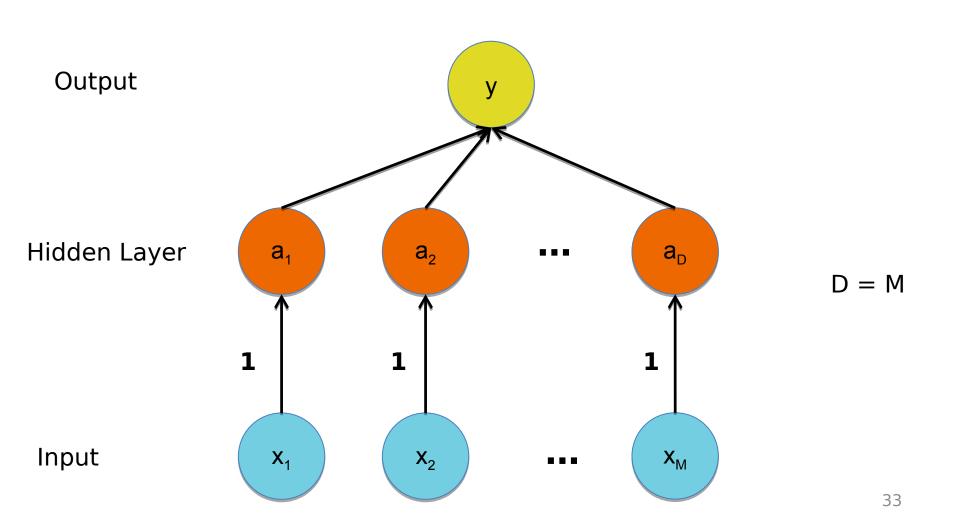


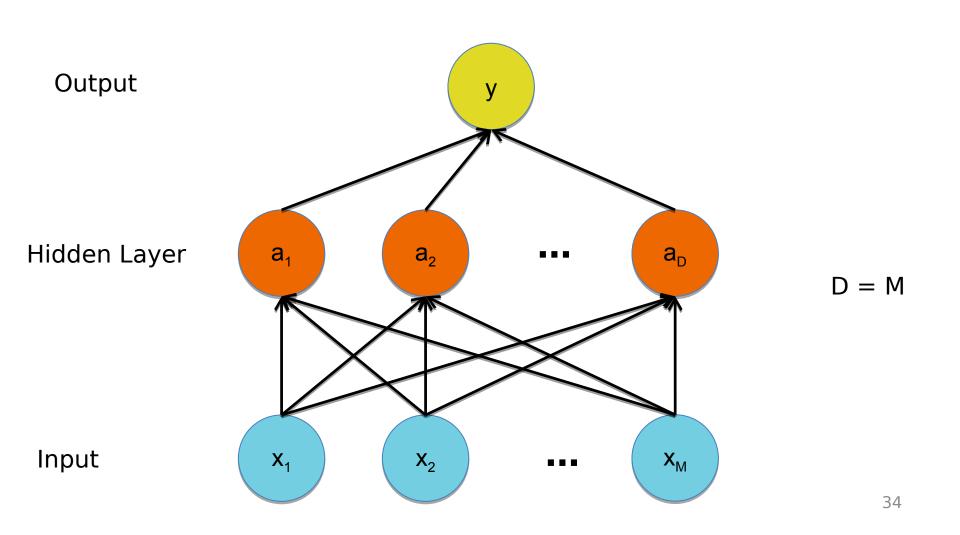
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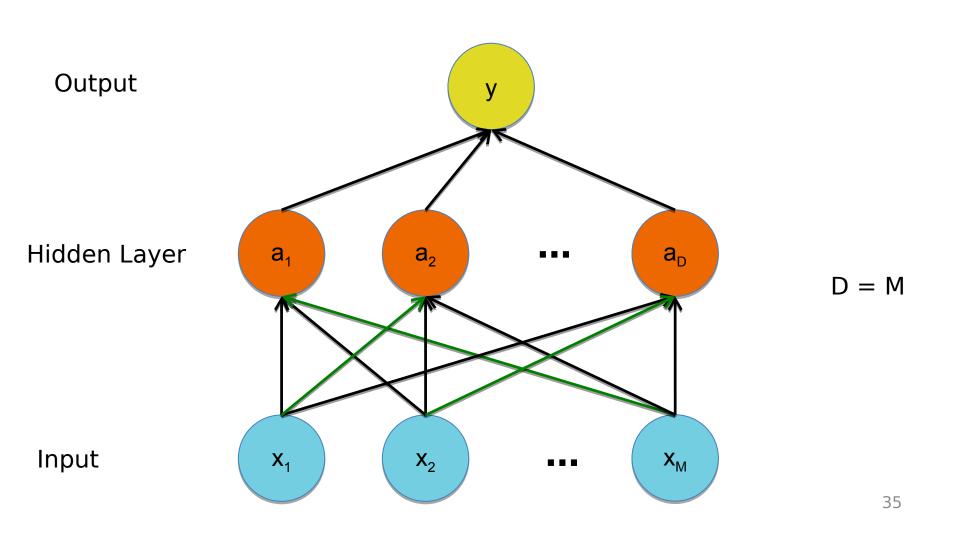


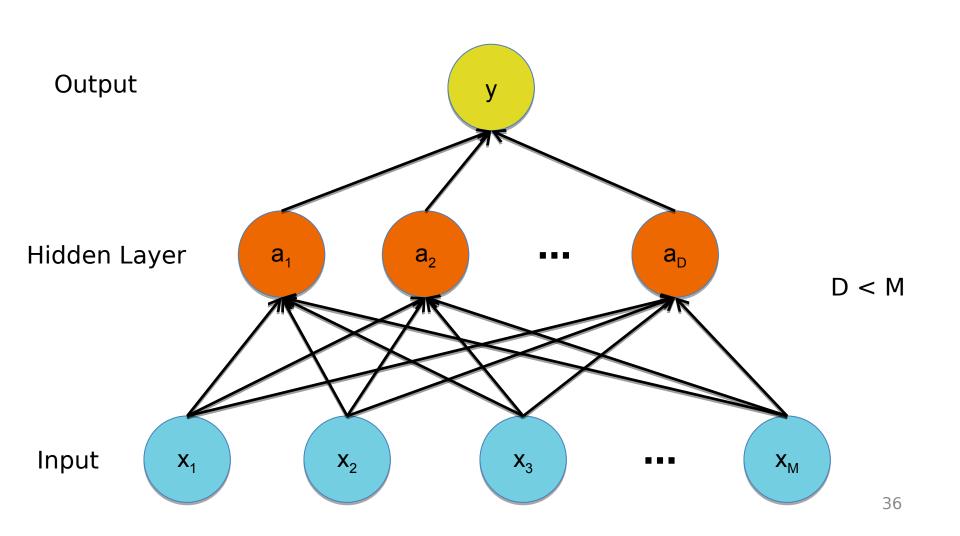






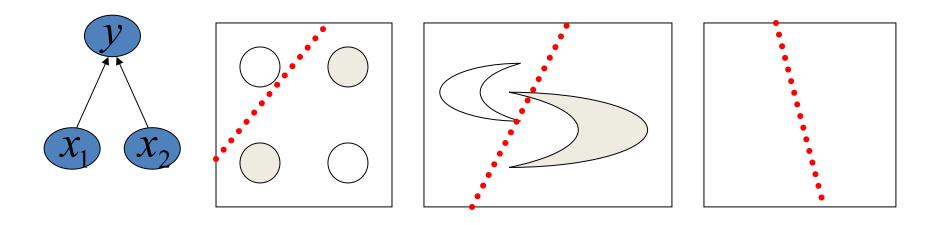






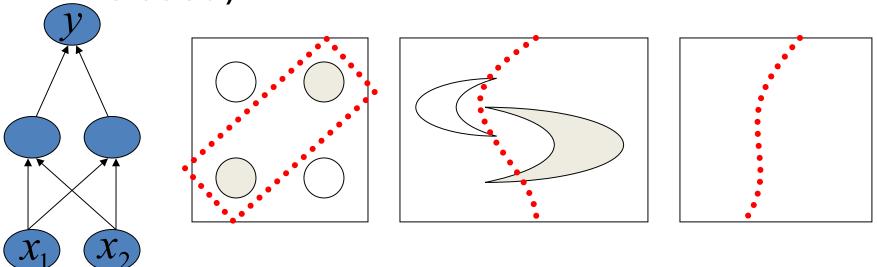
# **Decision Boundary**

- 0 hidden layers: linear classifier
  - Hyperplanes

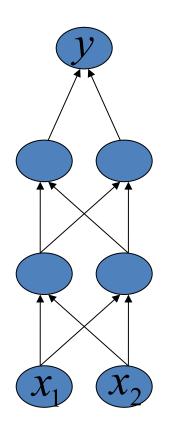


# **Decision Boundary**

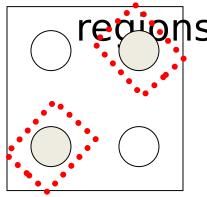
- 1 hidden layer
  - Boundary of convex region (open or closed)

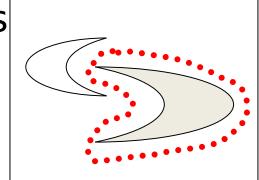


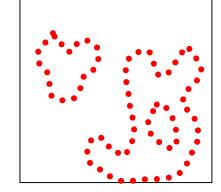
# **Decision Boundary**



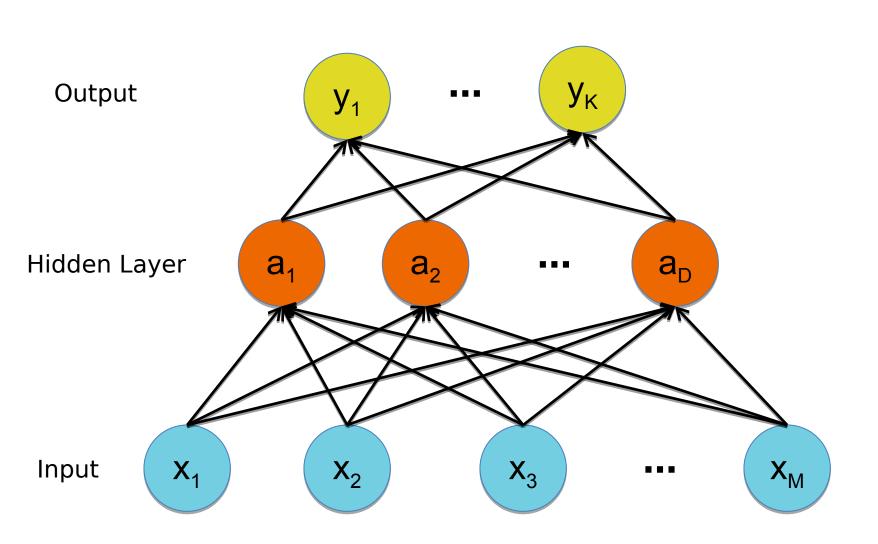
- 2 hidden layers
  - Combinations of convex





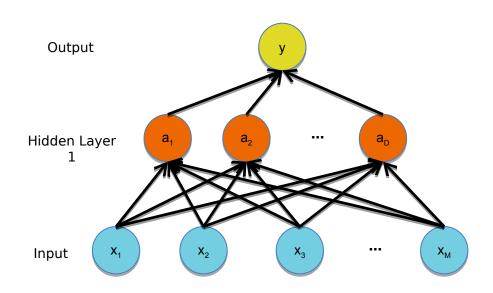


# Multi-Class Output



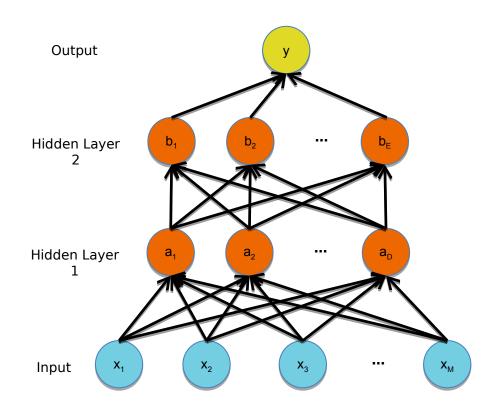
# Deeper Networks

#### Next lecture:

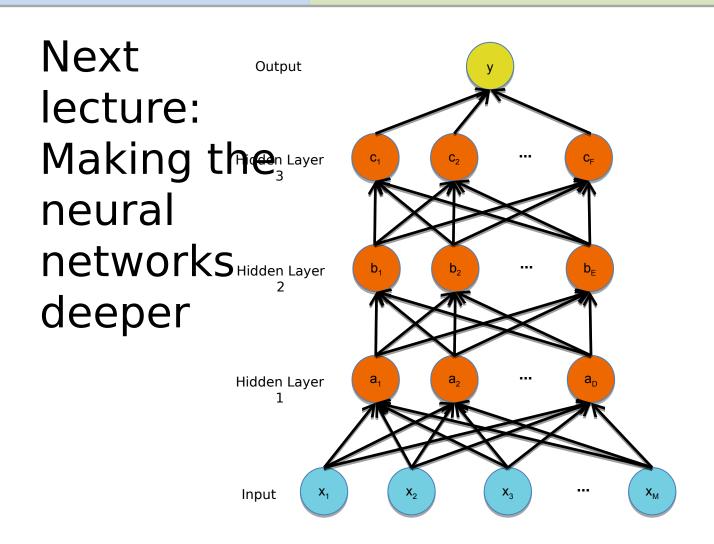


# Deeper Networks

#### Next lecture:



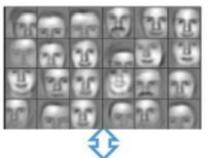
# Deeper Networks



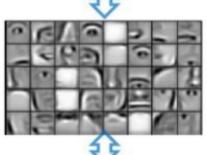
# Different Levels of Abstraction

- We don't know the "right" levels of abstraction
- So let the model figure it out!

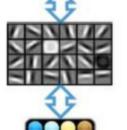
#### Feature representation



3rd layer "Objects"



2nd layer "Object parts"



1st layer "Edges"

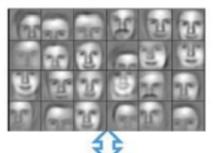
**Pixels** 

# Different Levels of Abstraction

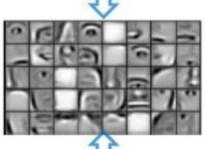
# Face Recognition:

- Deep
   Network can build up increasingly higher levels of abstraction
- Lines, parts,regionsExample from Honglak Lee (NIPS)

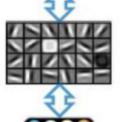
#### Feature representation



3rd layer "Objects"



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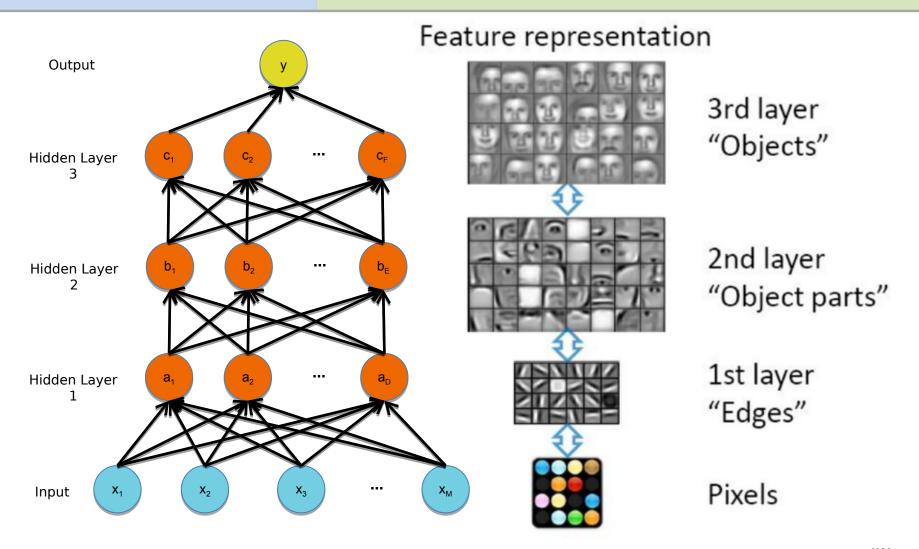


1st layer "Edges"



**Pixels** 

# Different Levels of Abstraction



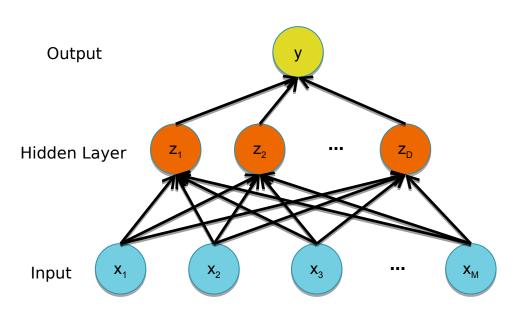
# **ARCHITECTURES**

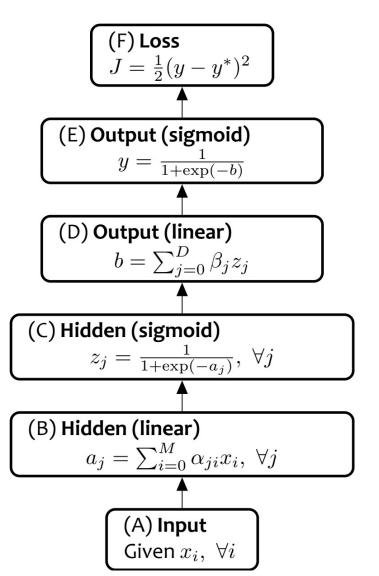
### Neural Network Architectures

Even for a basic Neural Network, there are many design decisions to make:

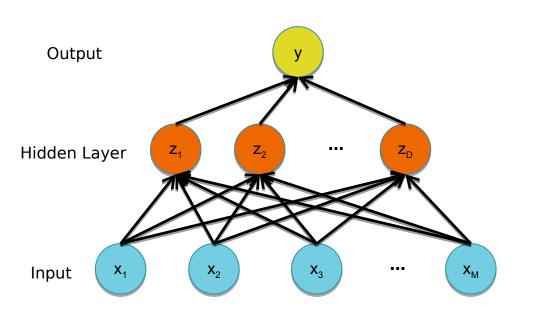
- 1. # of hidden layers (depth)
- 2. # of units per hidden layer (width)
- 3. Type of activation function (nonlinearity)
- 4. Form of objective function

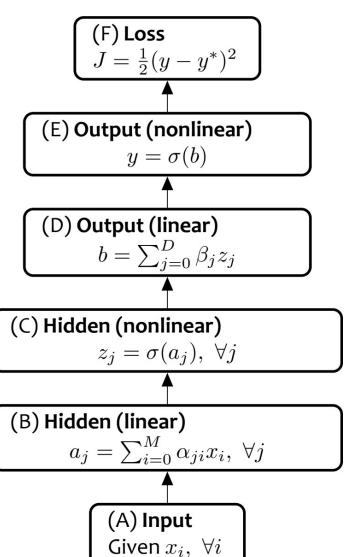
Neural Network with sigmoid activation functions

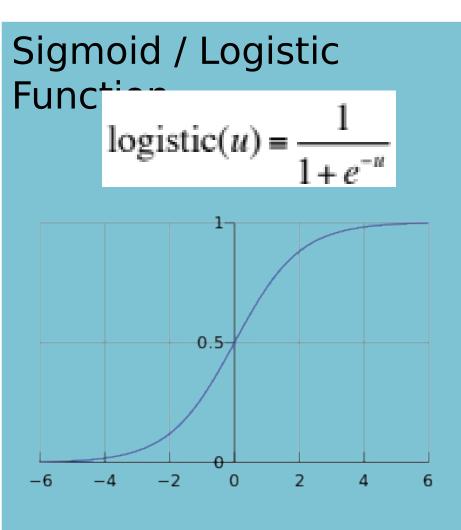




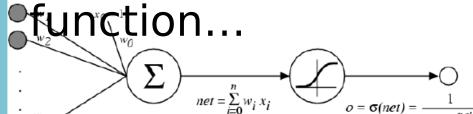
Neural Network with arbitrary nonlinear activation functions



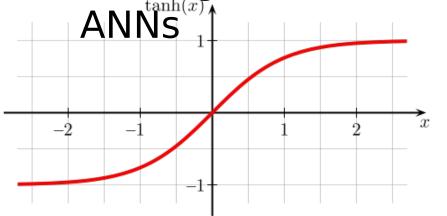




So far, we've assumed that the activation function (nonlinearity) is always the sigmoid



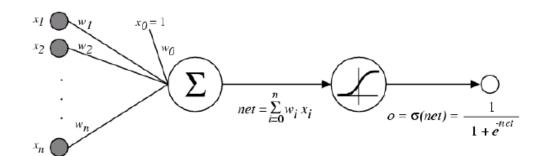
- A new change: modifying the nonlinearity
  - The logistic is not widely used in modern ANNS ↑



**Alternate** 

1: tanh

Like logistic function but shifted to range [-1, +1]



#### Understanding the difficulty of training deep feedforward neural networks

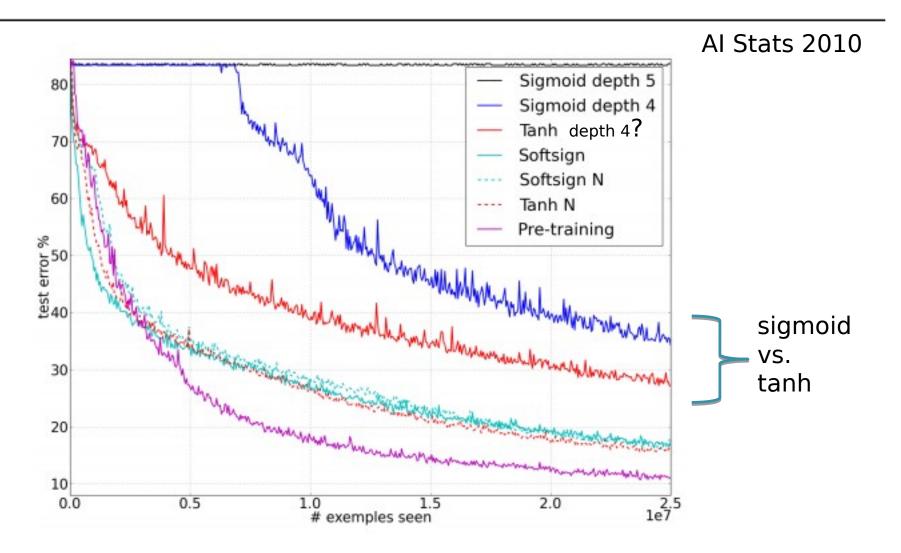
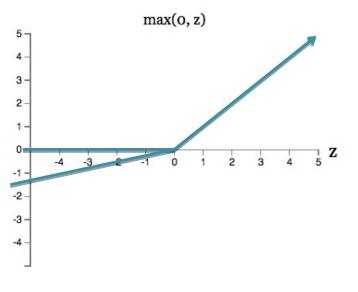


Figure from Glorot & Bentio (2010)

A new change: modifying the nonlinearity

ralli often used in vision tasks

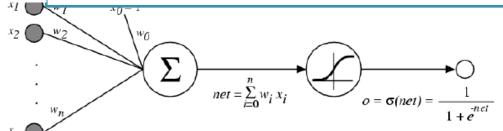


 $\max(0, w \cdot x + b)$ .

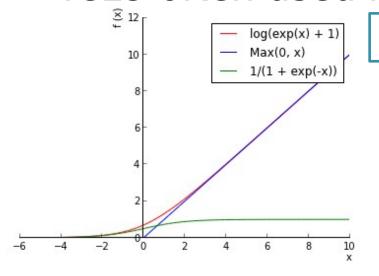
Iternate 2: rectified linear unit

Linear with a cutoff at zero

(Implementation: clip the gradient when you pass zero)



- A new change: modifying the nonlinearity
  - reLU often used in vision tasks



Alternate 2: rectified linear unit

Soft version: log(exp(x)+1)

Doesn't saturate (at one end)

Sparsifies outputs Helps with vanishing gradient



# Objective Functions for NNs

#### Regression:

- Use the same objective as Linear Regression
- Quadratic loss (i.e. mean squared error)

#### Classification:

- Use the same objective as Logistic Regression
- Cross-entropy (i.e. negative log likelihood)
- This requires probabilities, so we add an additional "softmax" layer at the end of our network

#### Forward

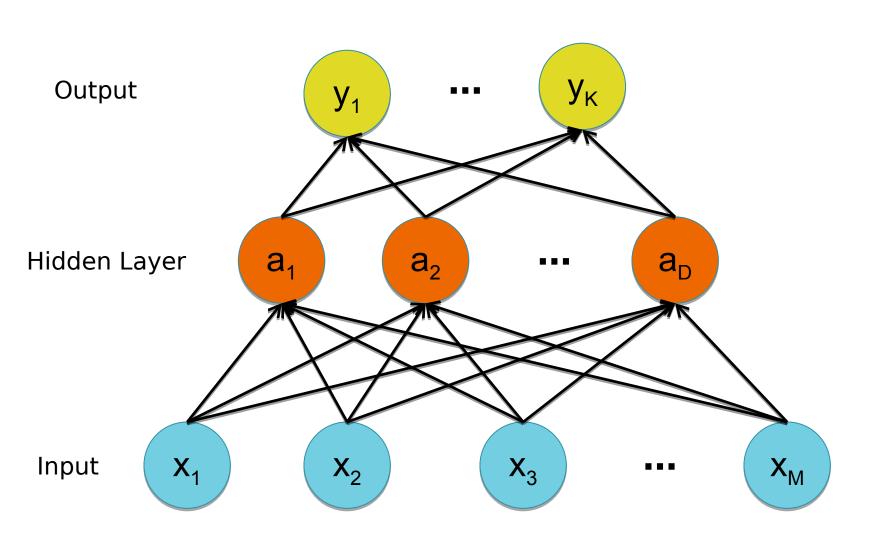
Quadratic 
$$J = \frac{1}{2}(y - y^*)^2$$

Cross Entropy 
$$J = y^* \log(y) + (1 - y^*) \log(1 - y)$$

#### Backward

Quadratic 
$$J=\frac{1}{2}(y-y^*)^2$$
 
$$\frac{dJ}{dy}=y-y^*$$
 Cross Entropy 
$$J=y^*\log(y)+(1-y^*)\log(1-y)$$
 
$$\frac{dJ}{dy}=y^*\frac{1}{y}+(1-y^*)\frac{1}{y-1}$$

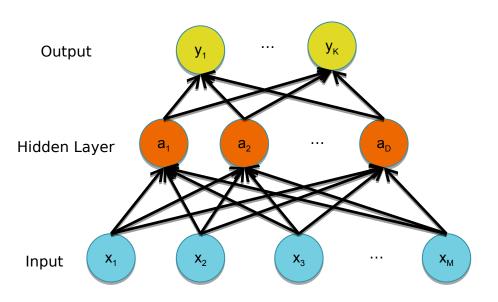
# Multi-Class Output

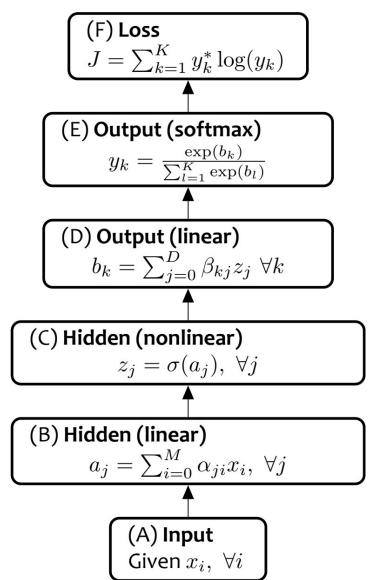


# Multi-Class Output

### Softmax:

$$y_k = \frac{\exp(b_k)}{\sum_{l=1}^K \exp(b_l)}$$





Cross-entropy vs. Quadratic loss

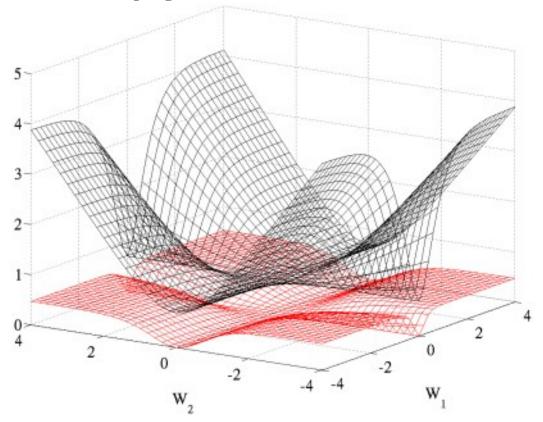


Figure 5: Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers,  $W_1$  respectively on the first layer and  $W_2$  on the second, output layer.

# Background

# A Recipe for Machine Learning

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# 3. Define goal:

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### 4. Train with SGD:

(take small steps opposite the gradient)

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abla \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

# **Objective Functions**

**Matching Quiz:** Suppose you are given a neural net with a single output, y, and one hidden layer.

gives...

- 1) Minimizing sum of squared errors...
- 2) Minimizing sum of squared errors plus squared Euclidean norm of weights...
- 3) Minimizing crossentropy...
- 4) Minimizing hinge loss...

- 5) ...MLE estimates of weights assuming target follows a Bernoulli with parameter given by the output value
- 6) ...MAP estimates of weights assuming weight priors are zero mean Gaussian
- 7) ...estimates with a large margin on the training data
- 8) ...MLE estimates of weights assuming zero mean Gaussian noise on the output value

B. 
$$1=5$$
,  $2=7$ ,  $3=8$ ,

B. 
$$1=8$$
,  $2=6$ ,  $3=8$ ,

## **BACKPROPAGATION**

# Background

# A Recipe for Machine Learning

# 1. Given training $\mathsf{data}_{\{\boldsymbol{x}_i,\boldsymbol{y}_i\}_{i=1}^N}$

### 3. Define goal:

$$oldsymbol{ heta}^* = rg\min_{oldsymbol{ heta}} \sum_{i=1}^N \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

# 2. Choose each of these:

- Recision function  $\hat{m{y}} = f_{m{ heta}}(m{x}_i)$
- Loss function  $\ell(\hat{m{y}},m{y}_i)\in\mathbb{R}$

#### 4. Train with SGD:

(take small steps opposite the gradient)

$$oldsymbol{ heta}^{(t+1)} = oldsymbol{ heta}^{(t)} - \eta_t 
abla \ell(f_{oldsymbol{ heta}}(oldsymbol{x}_i), oldsymbol{y}_i)$$

# Backpropagation

### Question 1:

When can we compute the gradients of the parameters of an arbitrary neural network?

### Question 2:

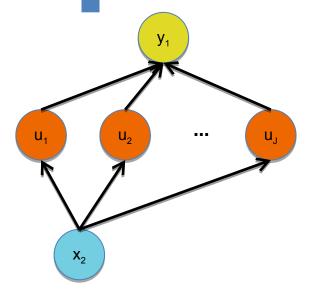
When can we make the gradient computation efficient?

# Chain Rule

Given: y = g(u) and u = h(x)

### Chain Rule:

$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j} \frac{du_j}{dx_k}, \quad \forall i, k$$



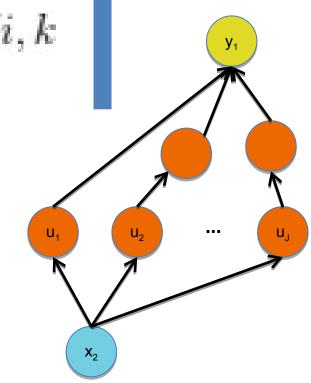
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Backpropaga tion is just repeated application of the chain rule from Calculus 101.

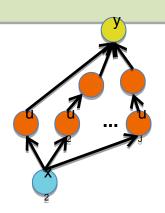


# Chain Rule

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#### **Backpropagation:**

- 1. Instantiate the computation as a directed acyclic graph, where each intermediate quantity is a node
- 2. At each node, store (a) the quantity computed in the forward pass and (b) the **partial derivative** of the goal with respect to that node's intermediate quantity.
- **3. Initialize** all partial derivatives to 0.
- 4. Visit each node in **reverse topological order**. At each node, add its contribution to the partial derivatives of its parents

This algorithm is also called **automatic differentiation in the** reverse-mode

# Backpropagation

**Simple Example:** The goal is to compute  $J = \cos(\sin(x^2) + 3x^2)$  on the forward pass and the derivative  $\frac{dJ}{dx}$  on the backward pass.

#### **Forward**

$$J = cos(u)$$

$$u = u_1 + u_2$$

$$u_1 = sin(t)$$

$$u_2 = 3t$$

$$t = x^2$$

# Backpropagation

**Simple Example:** The goal is to compute  $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative  $\frac{dJ}{dx}$  on the backward pass.

#### Forward

$$J = cos(u)$$

$$u = u_1 + u_2$$

$$u_1 = \sin(t)$$

$$u_2 = 3t$$

$$t = x^2$$

#### Backward

$$J = cos(u) \qquad \frac{dJ}{du} += -sin(u)$$

$$u = u_1 + u_2 \quad \frac{dJ}{du_1} += \frac{dJ}{du} \frac{du}{du_1}, \quad \frac{du}{du_1} = 1 \qquad \qquad \frac{dJ}{du_2} += \frac{dJ}{du} \frac{du}{du_2}, \quad \frac{du}{du_2} = 1$$

$$\frac{au}{du_1} = 1$$

$$\frac{dJ}{du_2} += \frac{dJ}{du_2}$$

$$\frac{du}{du_2} = 1$$

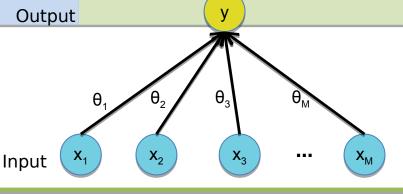
$$u_1 = sin(t)$$
  $\frac{dJ}{dt} += \frac{dJ}{du_1} \frac{du_1}{dt}, \quad \frac{du_1}{dt} = \cos(t)$ 

$$u_2 = 3t$$
 
$$\frac{dJ}{dt} += \frac{dJ}{du_2} \frac{du_2}{dt}, \quad \frac{du_2}{dt} = 3$$

$$\frac{dJ}{dx} += \frac{dJ}{dt}\frac{dt}{dx}, \quad \frac{dt}{dx} = 2x$$

# Backpropagation

Case 1: Logistic Regression



#### **Forward**

$$J = y^* \log y + (1 - y^*) \log(1 - y) \quad \frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$y = \frac{1}{1 + \exp(-a)}$$

$$a = \sum_{j=0}^{D} \theta_j x_j$$

#### Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

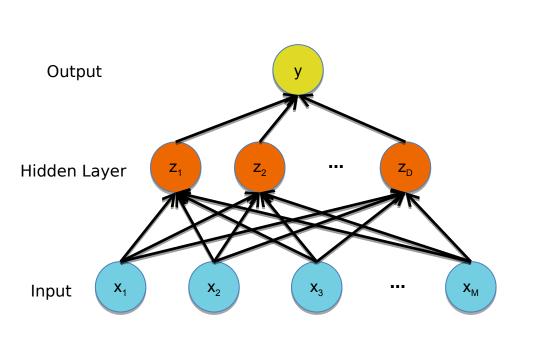
$$\frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da}, \frac{dy}{da} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$$

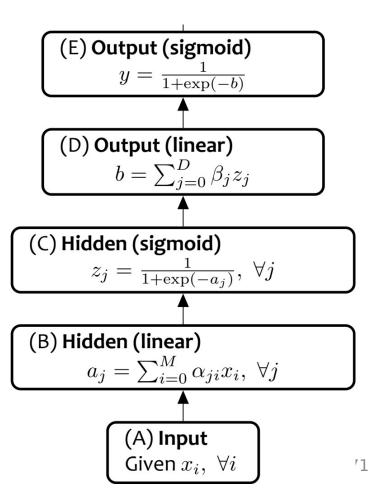
$$\frac{dJ}{d\theta_i} = \frac{dJ}{da} \frac{da}{d\theta_i}, \ \frac{da}{d\theta_i} = x_j$$

$$\frac{dJ}{dx_j} = \frac{dJ}{da}\frac{da}{dx_j}, \, \frac{da}{dx_j} = \theta_j$$

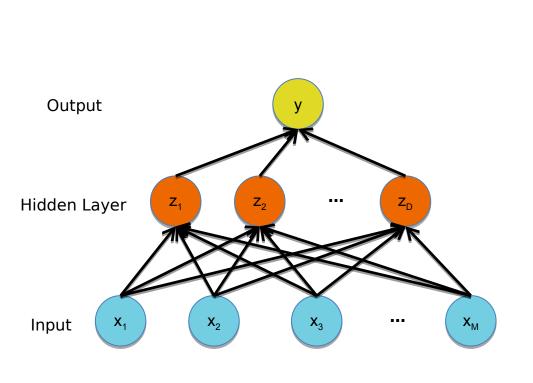
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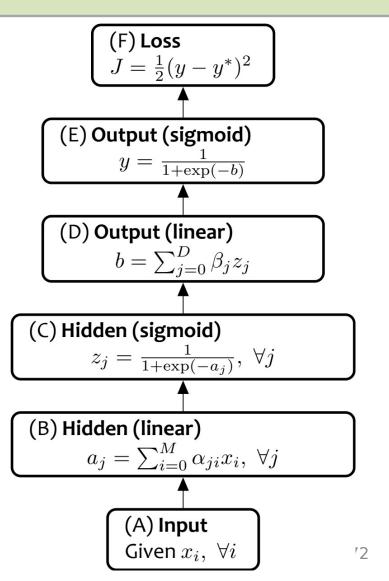
# Backpropagation





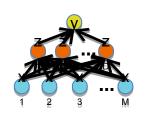
# Backpropagation





# Backpropagation

#### Case 2: Neural Network



#### **Forward**

$$J = y^* \log y + (1 - y^*) \log(1 - y) \quad \frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$y = \frac{1}{1 + \exp(-b)}$$

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

#### Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$$

$$\frac{dJ}{d\beta_i} = \frac{dJ}{db} \frac{db}{d\beta_i}, \frac{db}{d\beta_i} = z_j$$

$$\frac{dJ}{dz_i} = \frac{dJ}{db} \frac{db}{dz_i}, \frac{db}{dz_i} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j} \frac{dz_j}{da_j}, \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$$

$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j} \frac{da_j}{d\alpha_{ji}}, \ \frac{da_j}{d\alpha_{ji}} = x_i$$

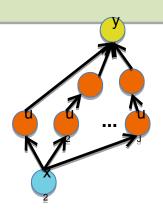
$$\frac{dJ}{dx_i} = \frac{dJ}{da_j} \frac{da_j}{dx_i}, \ \frac{da_j}{dx_i} = \sum_{i=0}^{D} \alpha_{ji}$$

# Chain Rule

Given:  $\boldsymbol{y} = g(\boldsymbol{u})$  and  $\boldsymbol{u} = h(\boldsymbol{x})$ 

**Chain Rule:** 

$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j} \frac{du_j}{dx_k}, \quad \forall i, k$$



#### **Backpropagation:**

- 1. Instantiate the computation as a directed acyclic graph, where each intermediate quantity is a node
- 2. At each node, store (a) the quantity computed in the forward pass and (b) the **partial derivative** of the goal with respect to that node's intermediate quantity.
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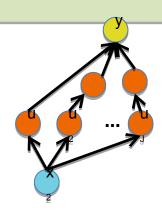
This algorithm is also called **automatic differentiation in the** reverse-mode

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$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j} \frac{du_j}{dx_k}, \quad \forall i, k$$



#### **Backpropagation:**

- 1. Instantiate the computation as a directed acyclic graph, where each node represents a Tensor.
- 2. At each node, store (a) the quantity computed in the forward pass and (b) the **partial derivatives** of the goal with respect to that node's Tensor.
- 3. Initialize all partial derivatives to 0.
- 4. Visit each node in **reverse topological order**. At each node, add its contribution to the partial derivatives of its parents

This algorithm is also called **automatic differentiation in the** reverse-mode

# Backpropagation

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Module 5

Module 4

Module 3

Module 2

Module 1

**Forward** 

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

$$y = \frac{1}{1 + \exp(-b)}$$

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Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1-y^*)}{y-1}$$

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# Background

### A Recipe for

## Gradients

1. Given training data $\{oldsymbol{x}_i,oldsymbol{y}_i\}_{i=1}^N$ 

**Backpropagation** can compute this gradient!

And it's a special case of a more general algorithm called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

2. Choose each these:

$$\hat{y} = f_{m{ heta}}(x_i)$$
 function efficiently!

- Loss function  $\ell(\hat{m{y}}, m{y}_i) \in \mathbb{R}$ 

opposite the gradient) 
$$\boldsymbol{\theta}^{(t)} = \boldsymbol{\eta}_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

# Summary

#### 1. Neural Networks...

- provide a way of learning features
- are highly nonlinear prediction functions
- (can be) a highly parallel network of logistic regression classifiers
- discover useful hidden representations of the input

### 2. Backpropagation...

- provides an efficient way to compute gradients
- is a special case of reverse-mode automatic differentiation