School of Computer Science
Carnegie Mellon

# 10-601B Introduction to Machine Learning

# Neural Networks

Matt Gormley
Lecture 15
October 19, 2016

**Readings:**
Bishop Ch. 5
Murphy Ch. 16.5, Ch. 28
Mitchell Ch. 4

# Reminders

# Outline

- Logistic Regression (Recap)
- Neural Networks
- Backpropagation

# RECALL: LOGISTIC REGRESSION

# Using gradient ascent for linear classifiers

Recall…

Key idea behind today's lecture:

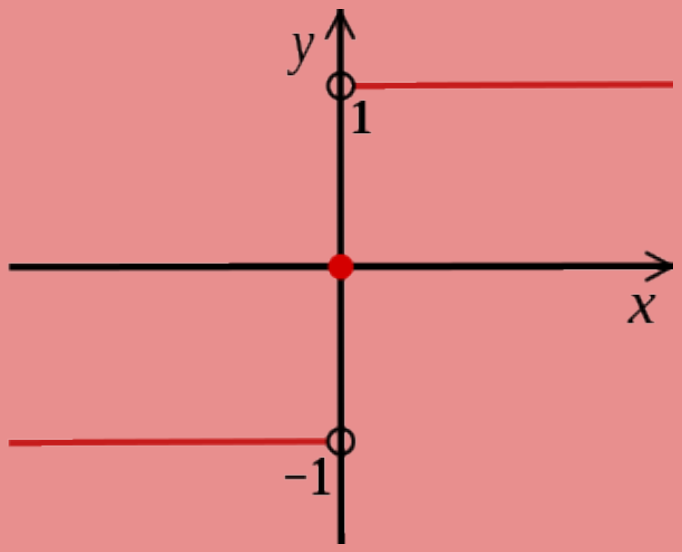
1. Define a linear classifier (logistic regression)
2. Define an objective function (likelihood)
3. Optimize it with gradient descent to learn parameters
4. Predict the class with highest probability under the model

# Using gradient ascent for linear classifiers

Recall…

This decision function isn't differentiable:

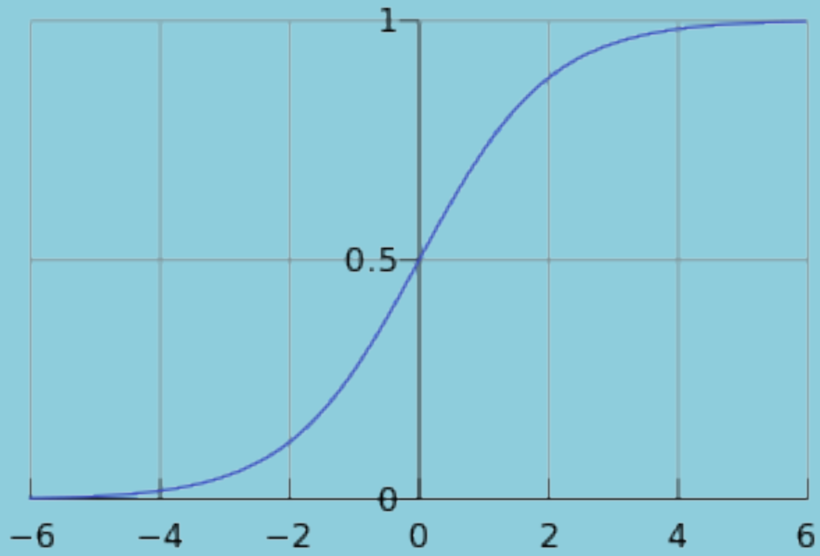
$$h(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^T \mathbf{x})$$




sign(x)

Use a differentiable function instead:

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




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

# Using gradient ascent for linear classifiers

Recall…

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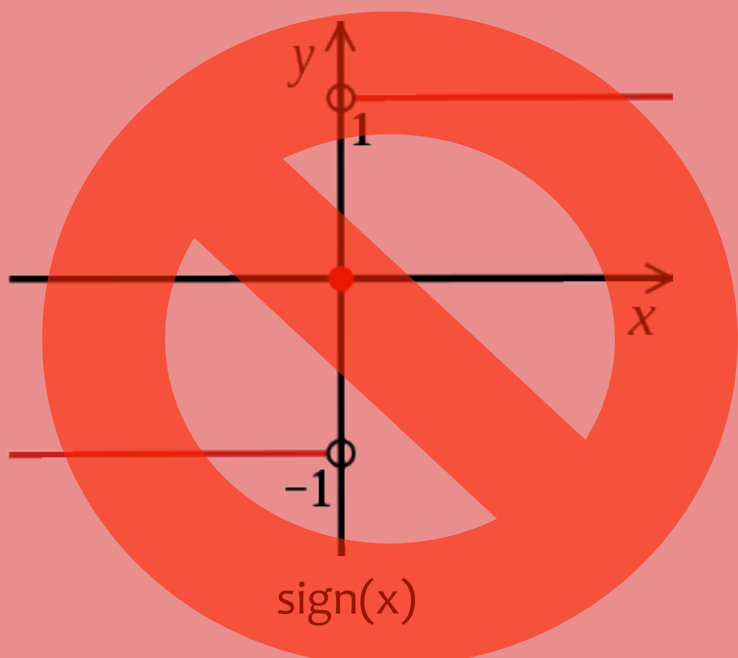


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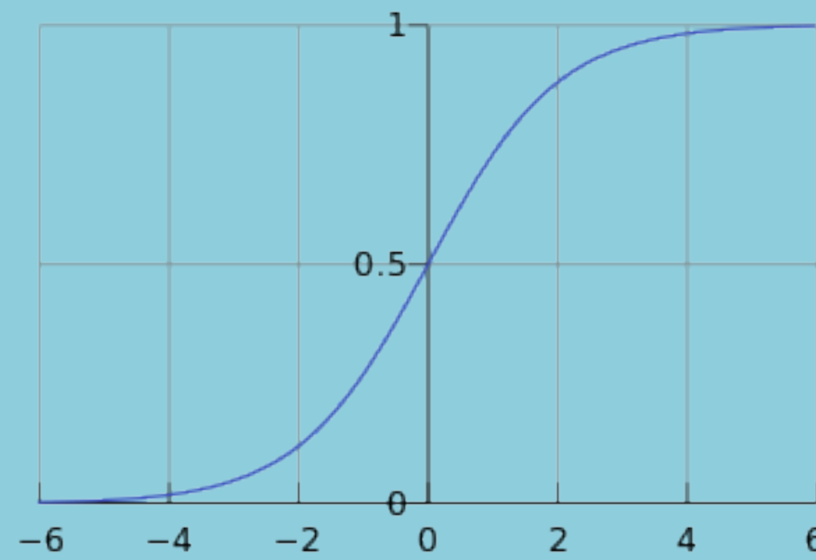



$$\text{logistic}(u) \equiv \frac{1}{1 + e^{-u}}$$

Recall…

# Logistic Regression

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

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

**Model:** Logistic function applied to dot product of parameters with input vector.

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

**Learning:** finds the parameters that minimize some objective function. $\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\text{argmin}}\, J(\boldsymbol{\theta})$

**Prediction:** Output is the most probable class.

$$\hat{y} = \underset{y \in \{0,1\}}{\text{argmax}}\, p_{\boldsymbol{\theta}}(y|\mathbf{x})$$

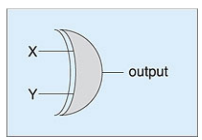
# NEURAL NETWORKS

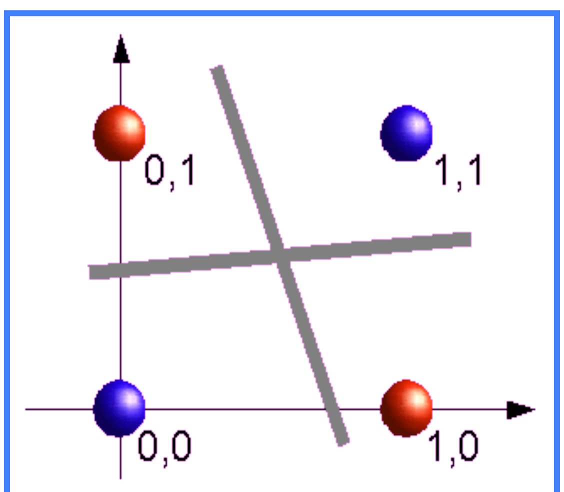
# Learning highly non-linear functions

f: X → Y

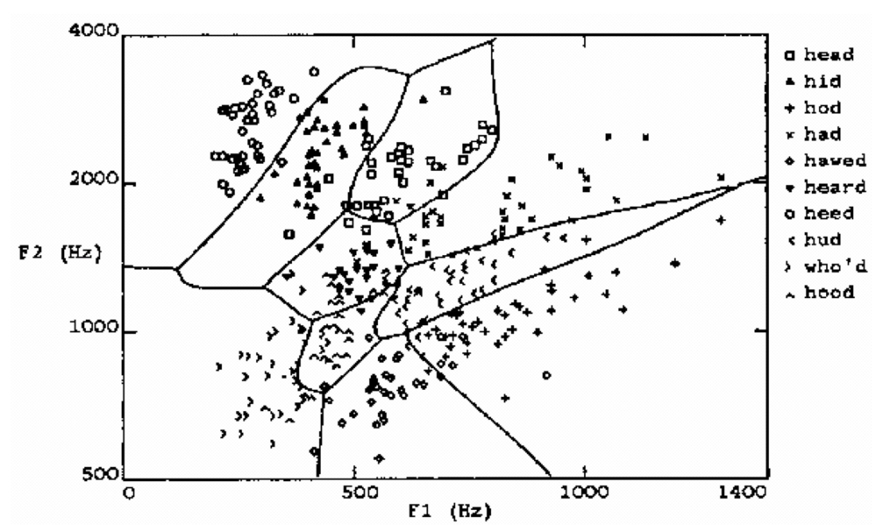
- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

The XOR gate



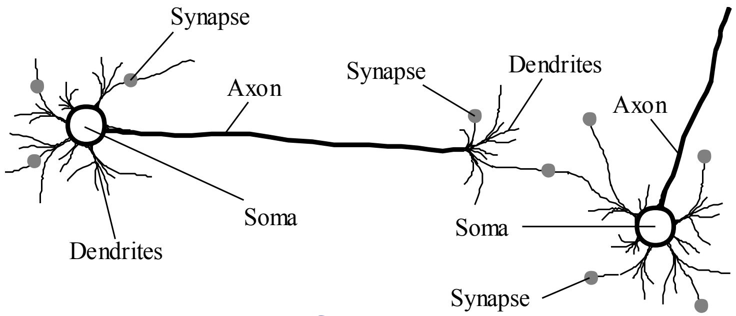



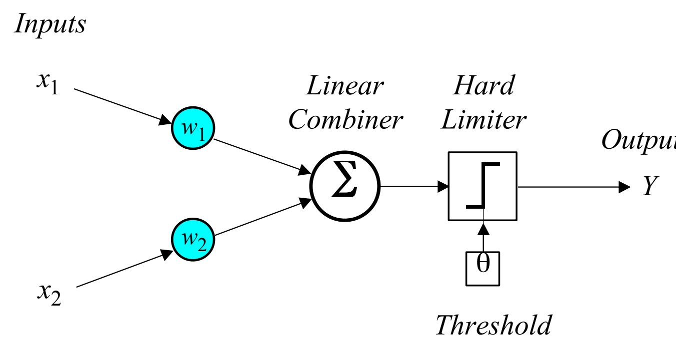

Speech recognition



# Perceptron and Neural Nets

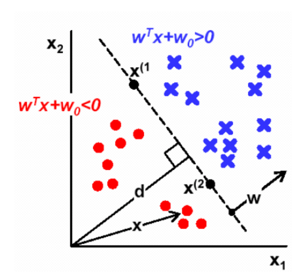
- From biological neuron to artificial neuron (perceptron)



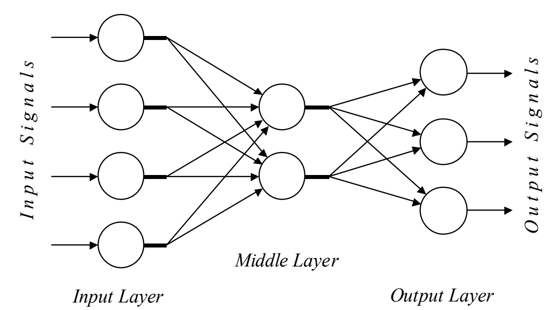




- Activation function

$$X = \sum_{i=1}^{n} x_i w_i \qquad Y = \begin{cases} +1, & \text{if } X \geq \omega_0 \\ -1, & \text{if } X < \omega_0 \end{cases}$$

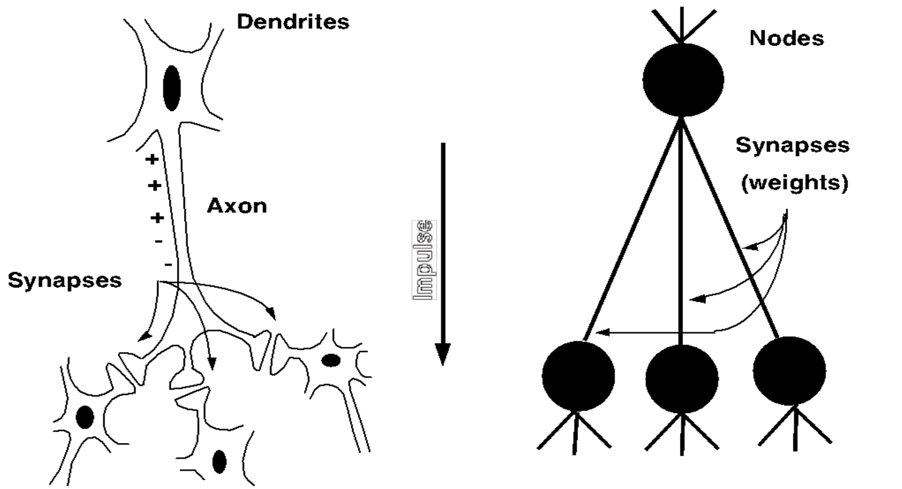



- Artificial neuron networks
  - supervised learning
  - gradient descent



# Connectionist Models

- Consider humans:
  - Neuron switching time
    ~ 0.001 second
  - Number of neurons
    ~ $10^{10}$
  - Connections per neuron
    ~ $10^{4-5}$
  - Scene recognition time
    ~ 0.1 second
  - 100 inference steps doesn't seem like enough
    → much parallel computation

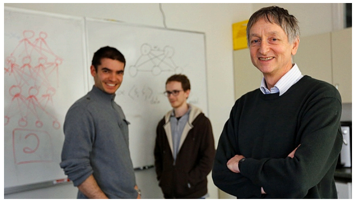



- Properties of artificial neural nets (ANN)
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed processes

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

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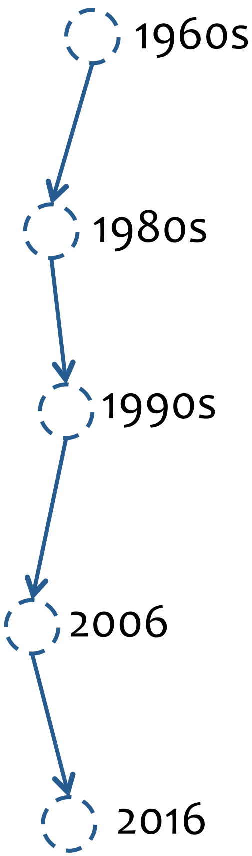


Deep learning:

- 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 data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

*Face* *Face* *Not a face*

2. Choose each of these:
   – Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

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

   – Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

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

# Background

# A Recipe for Machine Learning

1. Given training data:

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– Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Background

A Recipe for

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^{N}$$

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# Gradients

**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!

opp site the gradient)

$$\boldsymbol{\theta}^{(t} \quad {}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

# Goals for Today's Lecture

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

A Recipe for

2. Choose each of these:
   - Decision function

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

Train with SGD:

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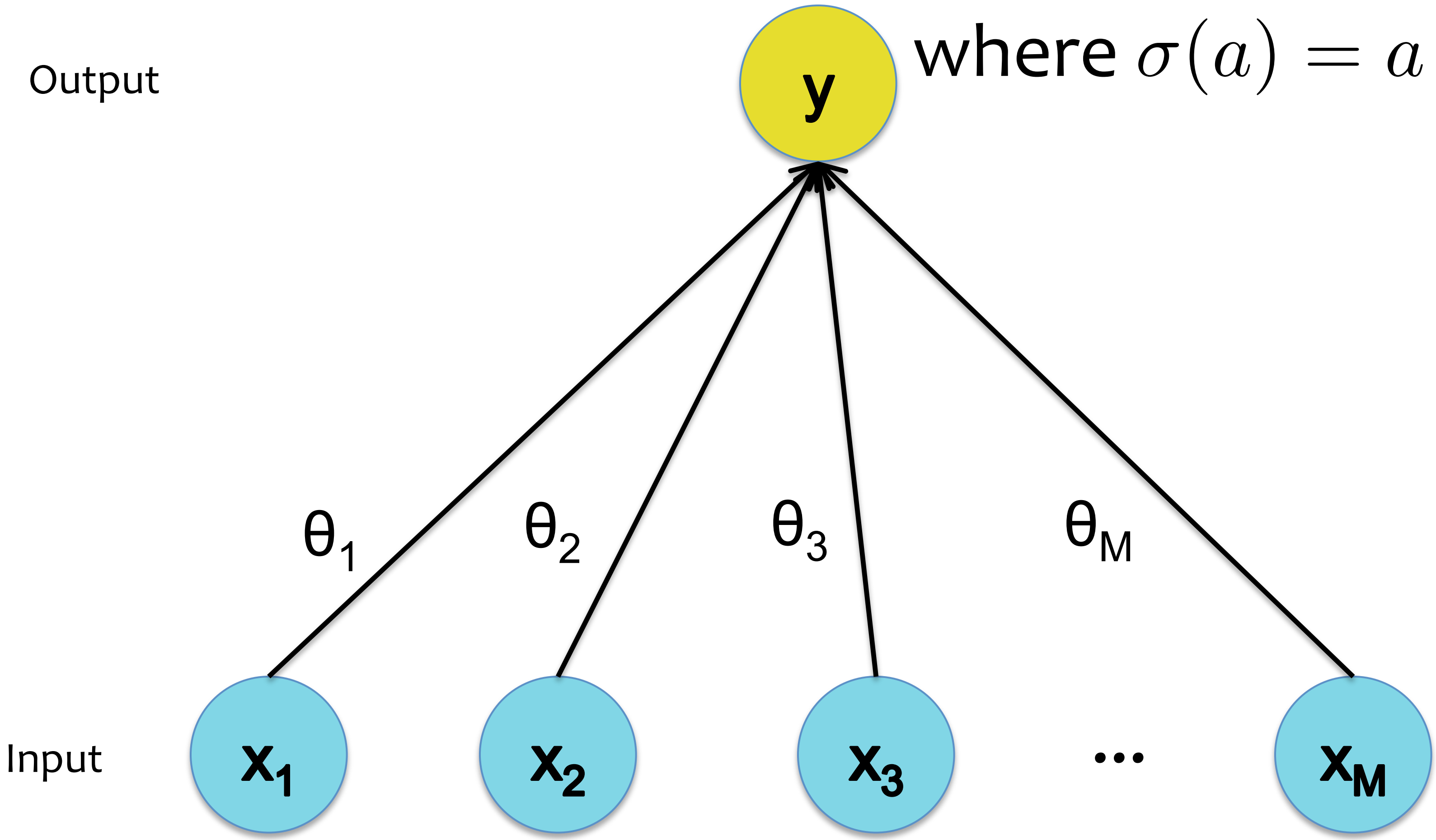
# Decision Functions

# Linear Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = a$

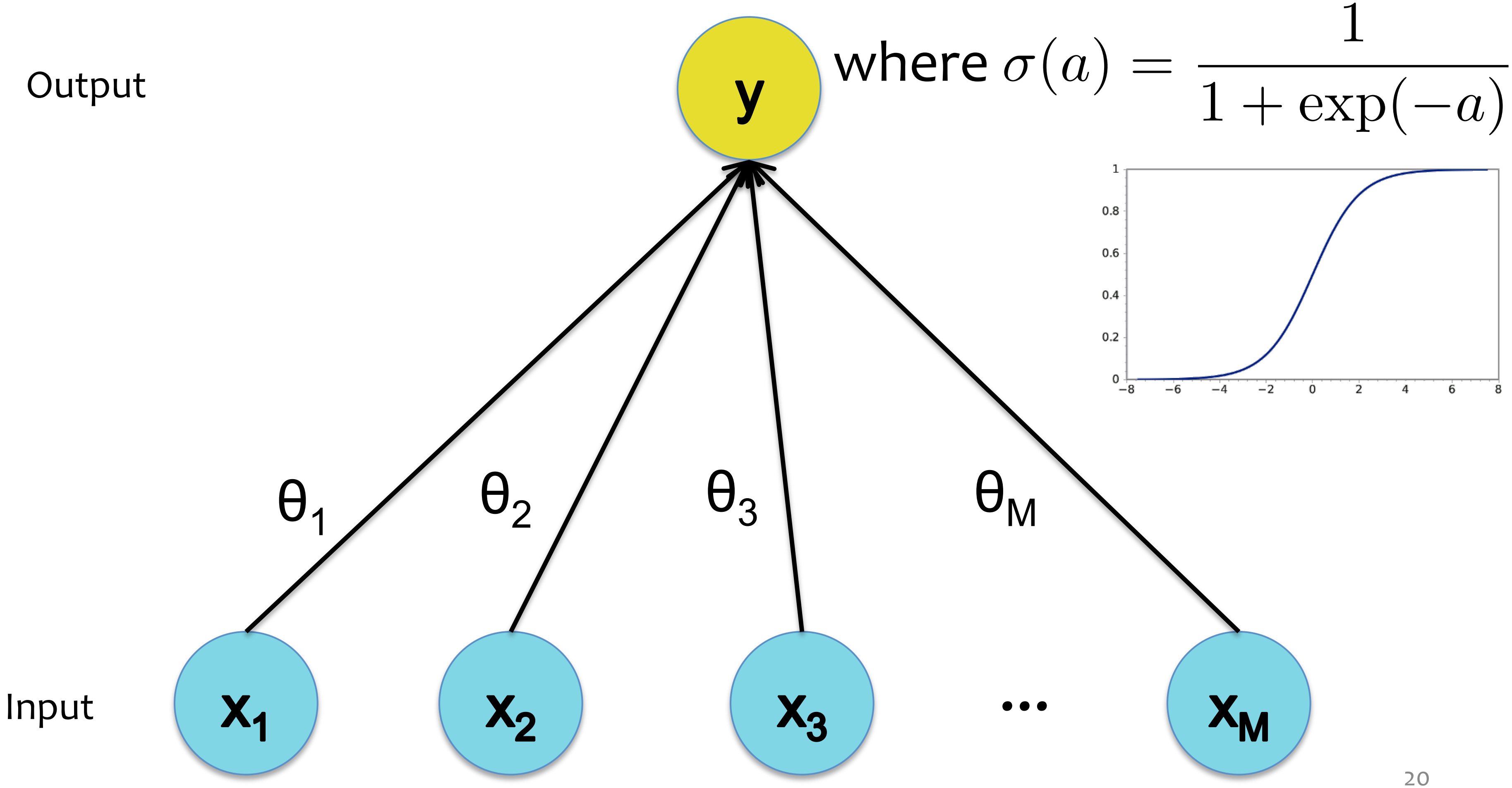


Decision Functions

# Logistic Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = \dfrac{1}{1 + \exp(-a)}$



Decision Functions

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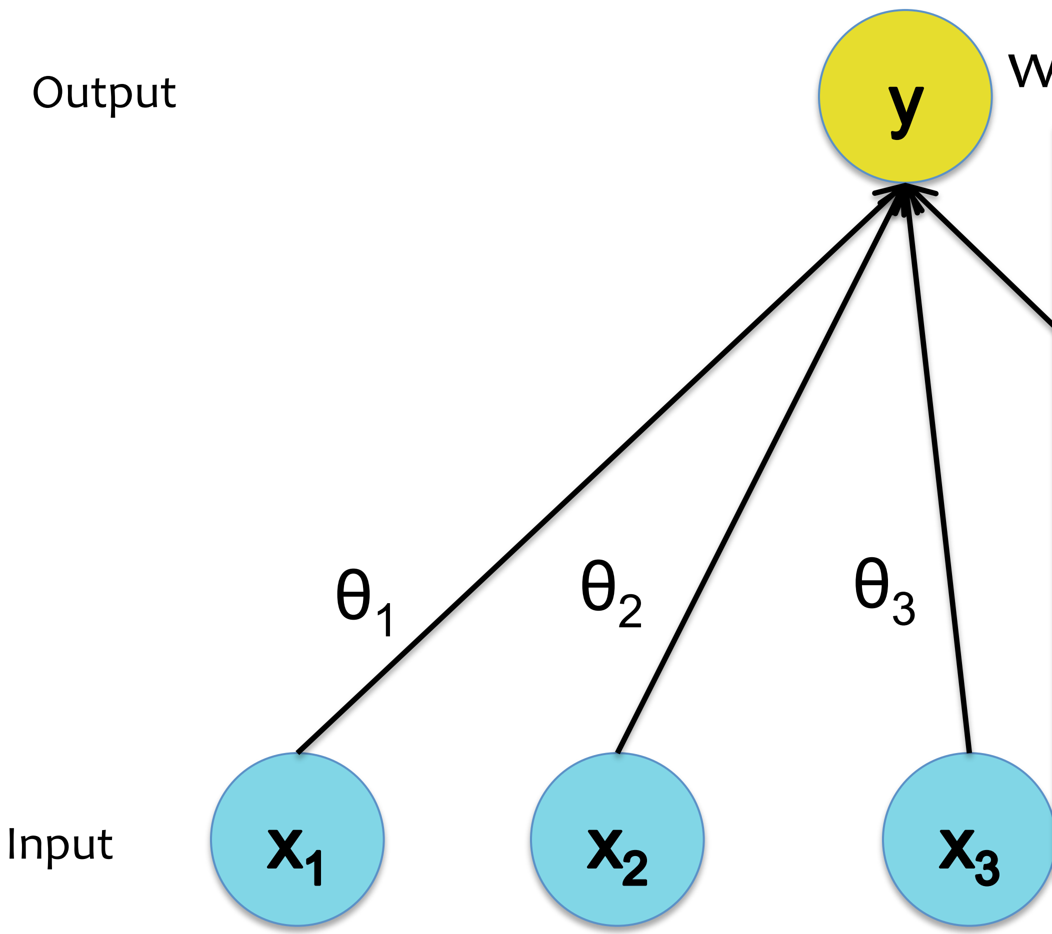


# Logistic Regression

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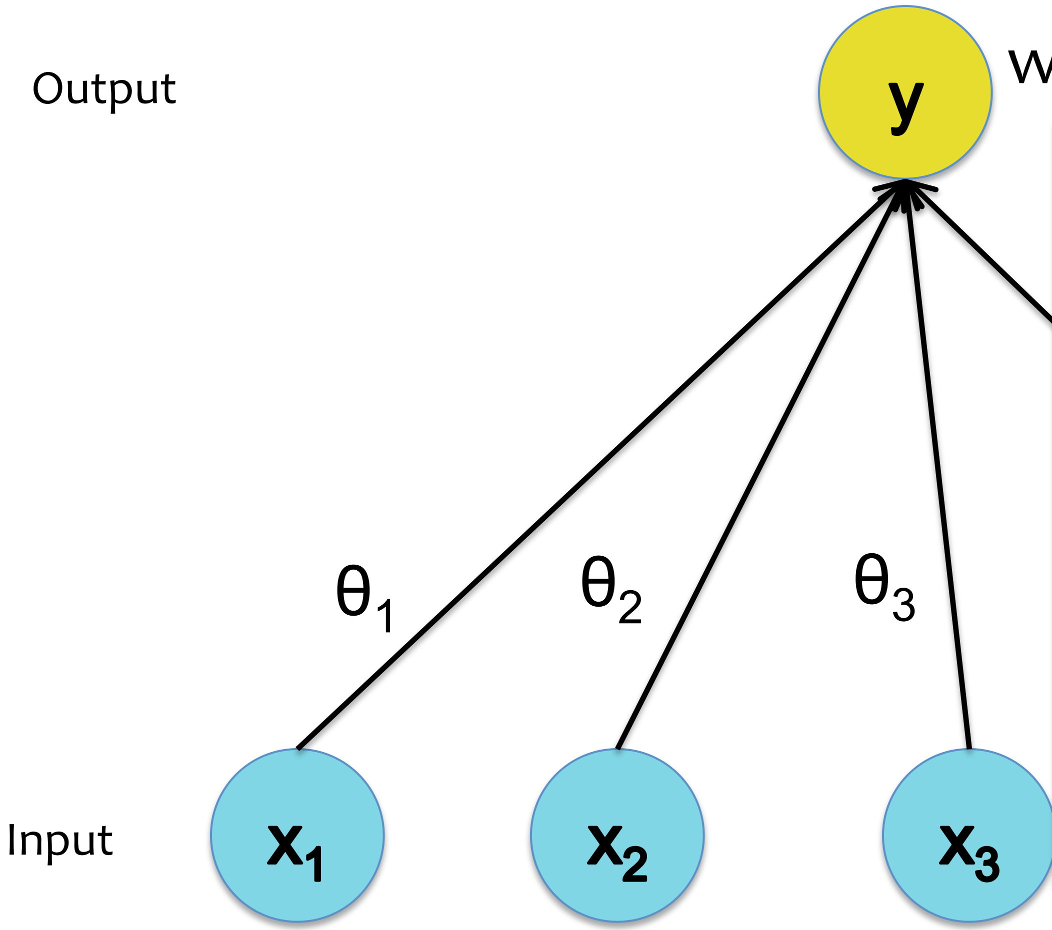


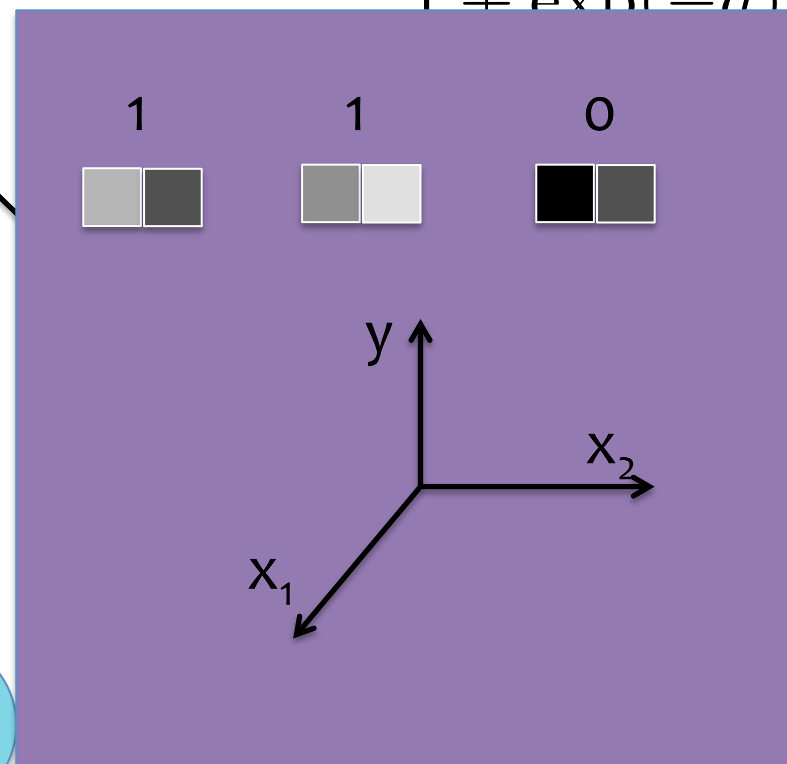

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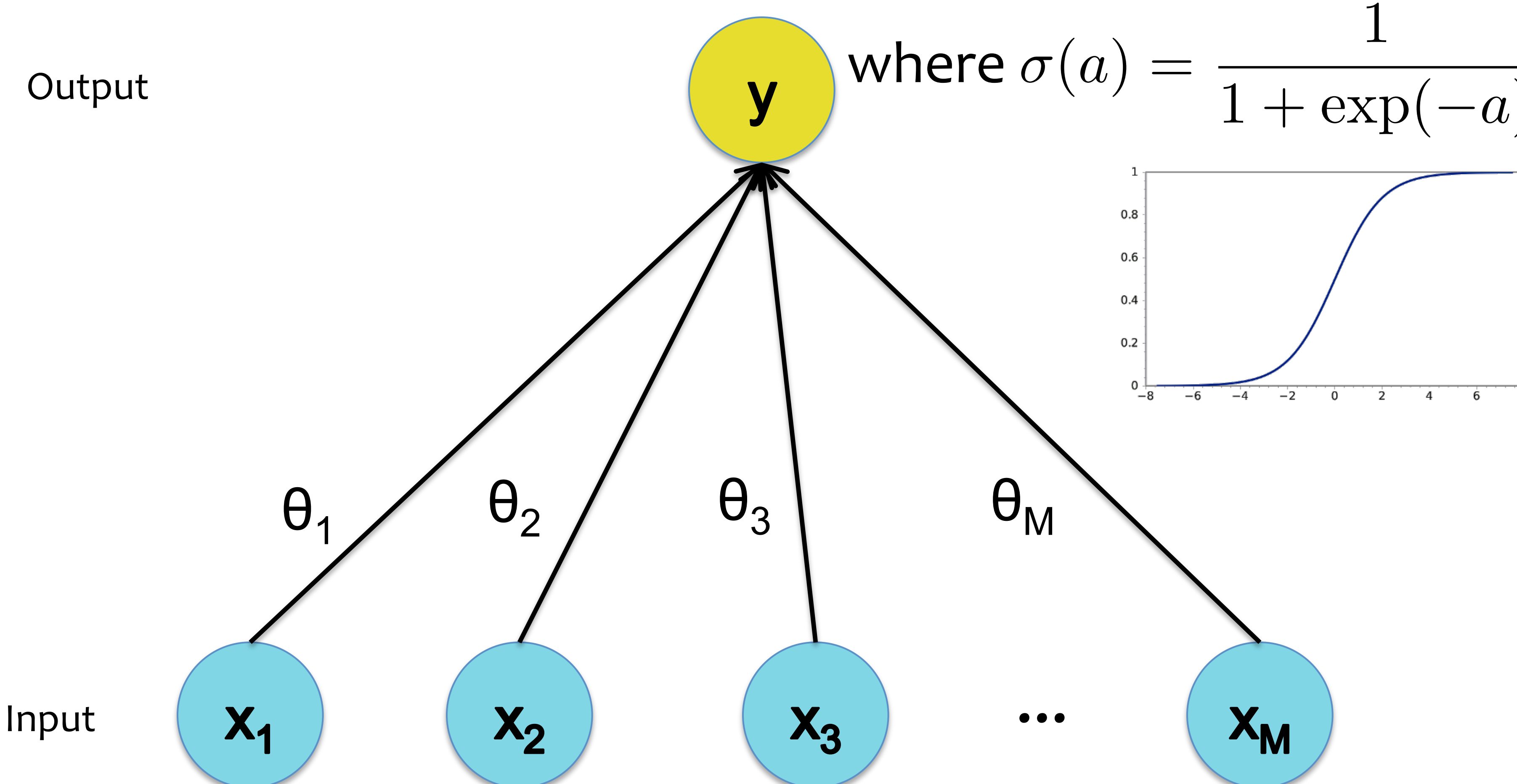
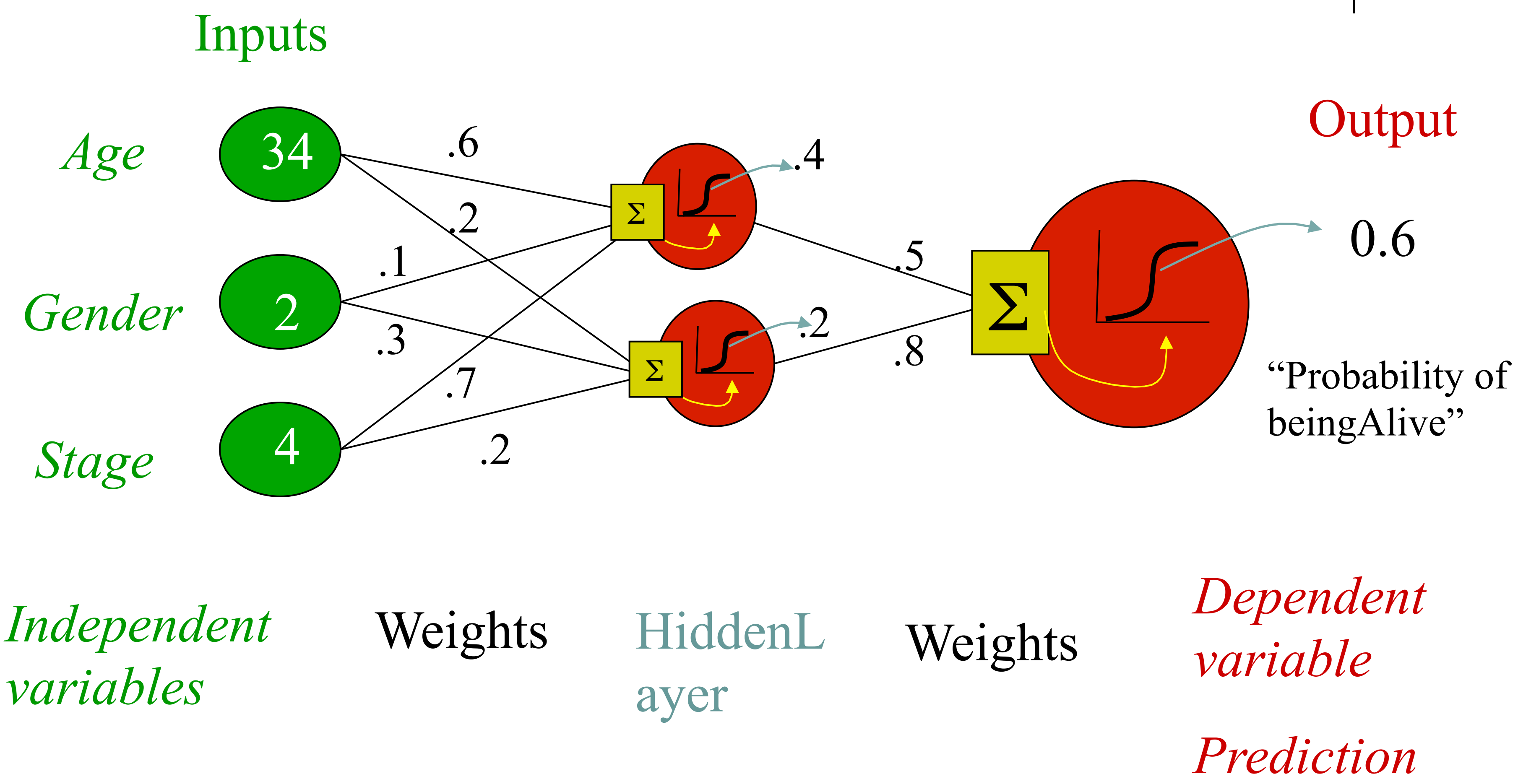
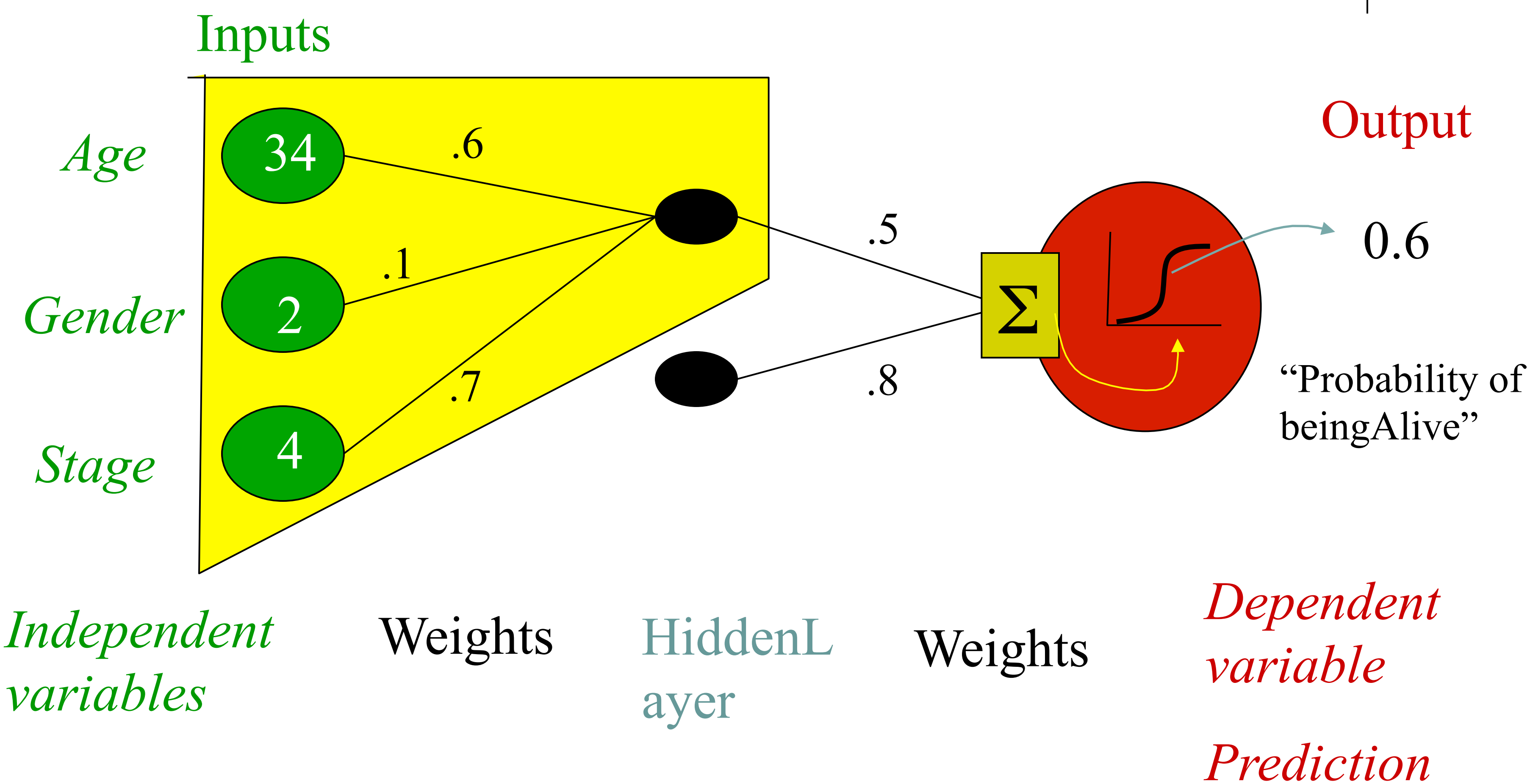
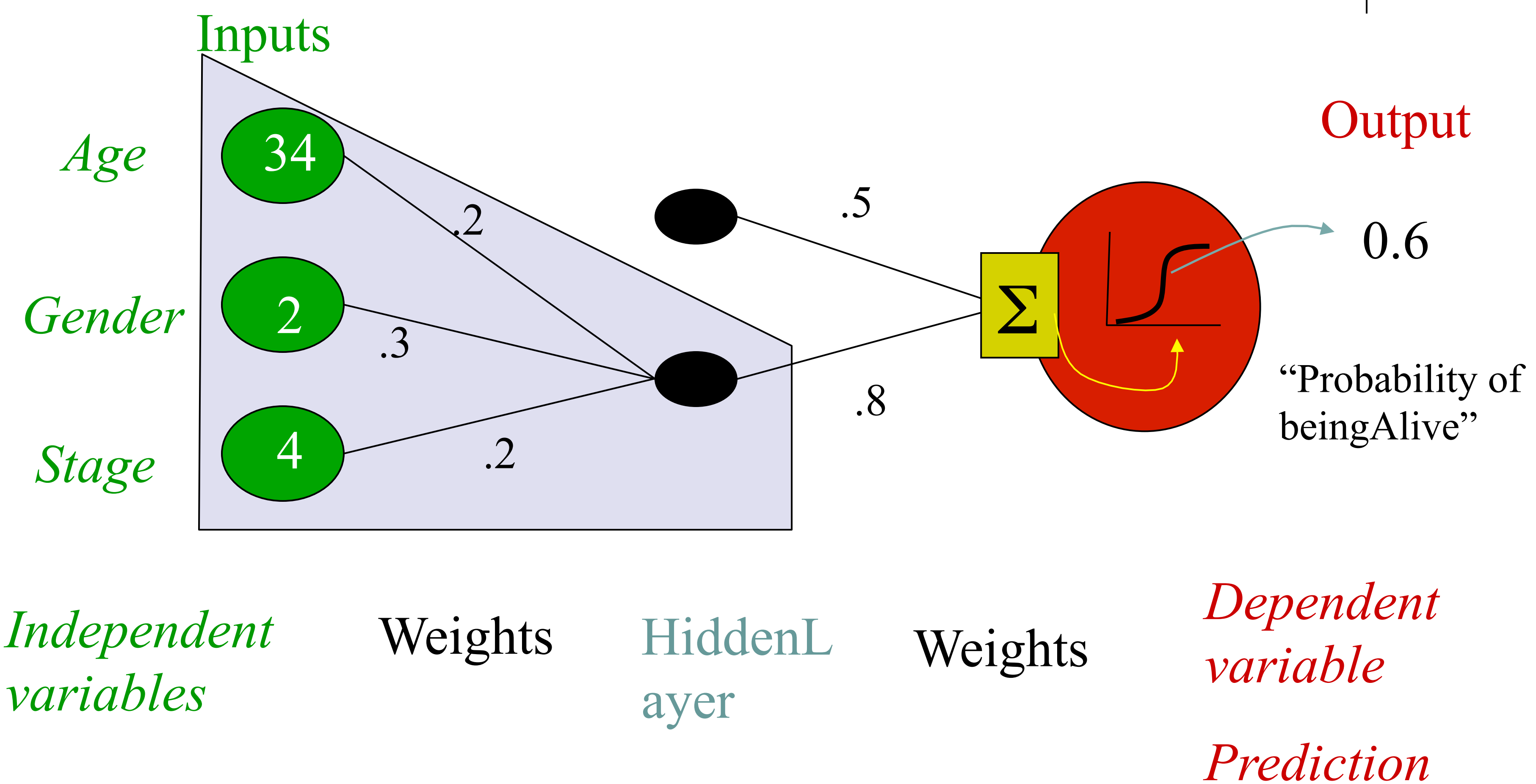


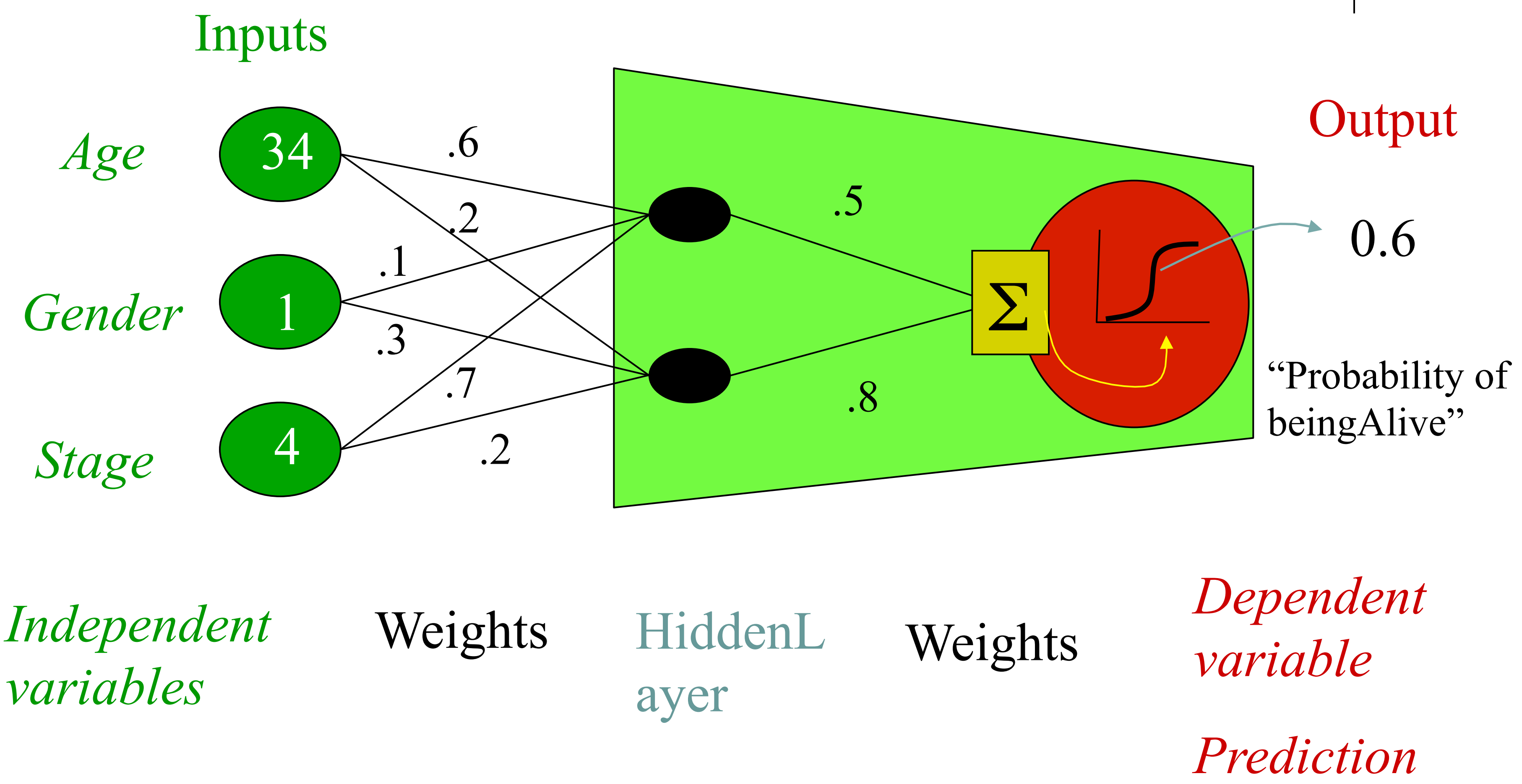
# Neural Network Model



# "Combined logistic models"




Inputs
Age
Gender
Stage
34
2
4
.2
.3
.2
.5
.8
Σ
Output
0.6
"Probability of beingAlive"
Independent variables
Weights
HiddenLayer
Weights
Dependent variable
Prediction


Inputs
Output
Age
34
Gender
1
Stage
4
.6
.2
.1
.3
.7
.2
.5
.8
Σ
0.6
"Probability of beingAlive"
Independent variables
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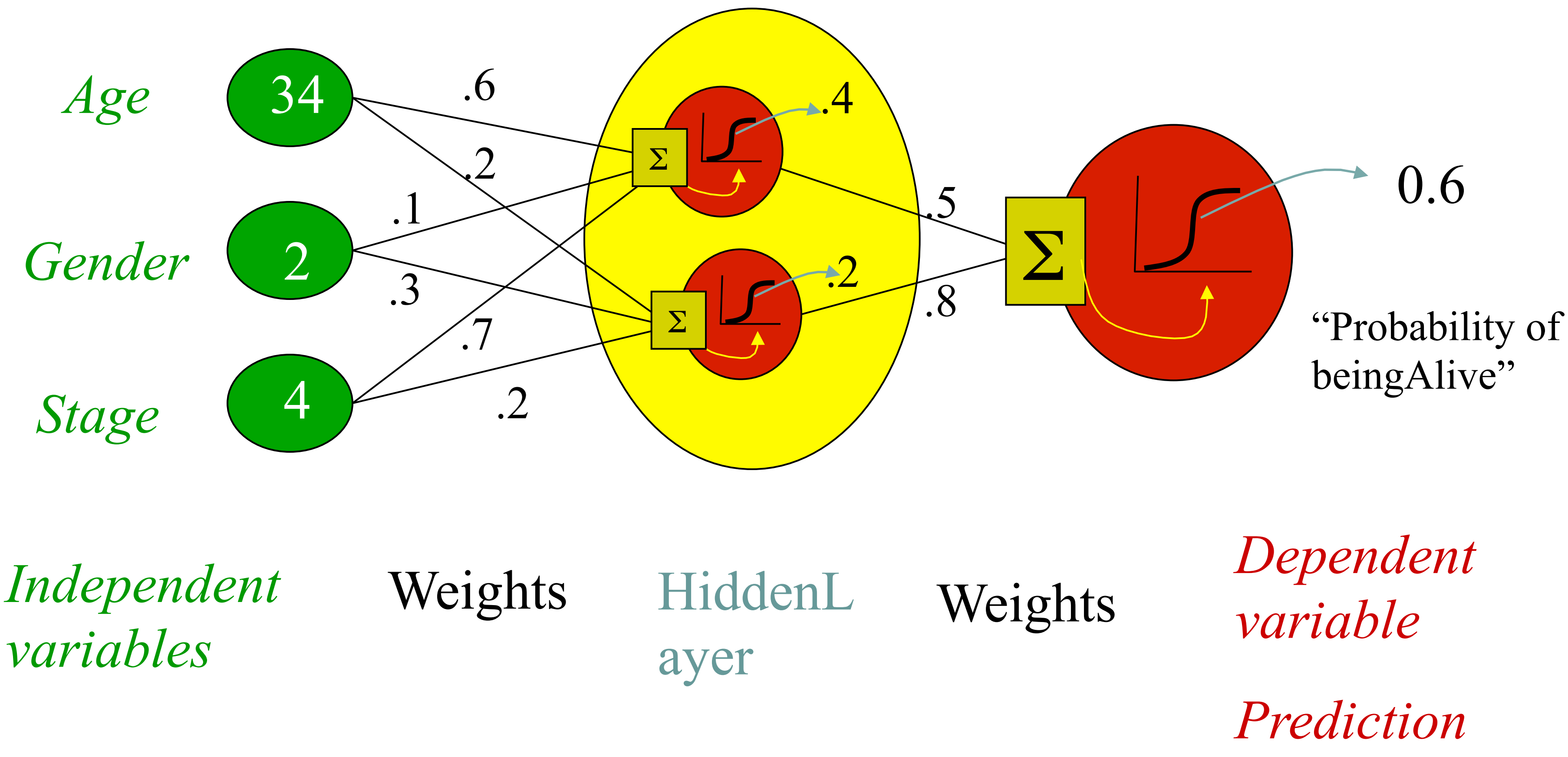
Prediction

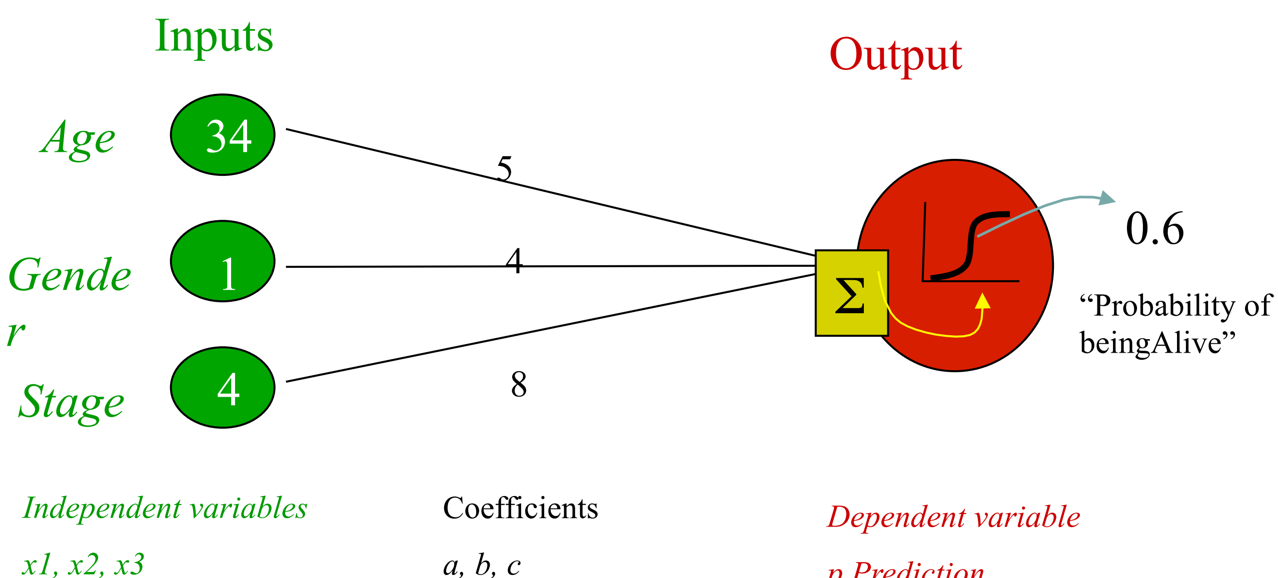
# Not really, no target for hidden units...



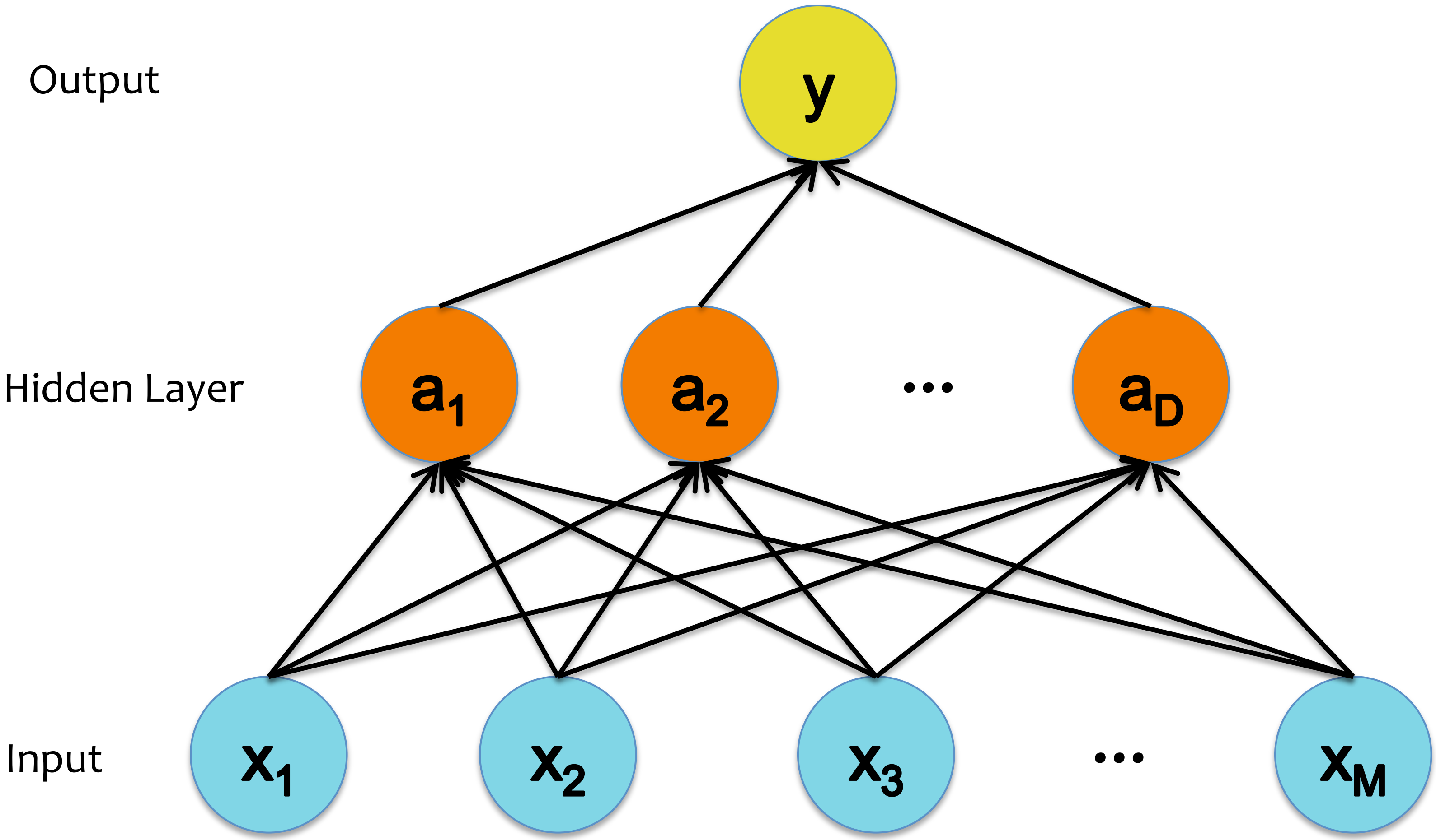
# Jargon Pseudo-Correspondence

- Independent variable = input variable
- Dependent variable = output variable
- Coefficients = “weights”
- Estimates = “targets”

## Logistic Regression Model (the sigmoid unit)

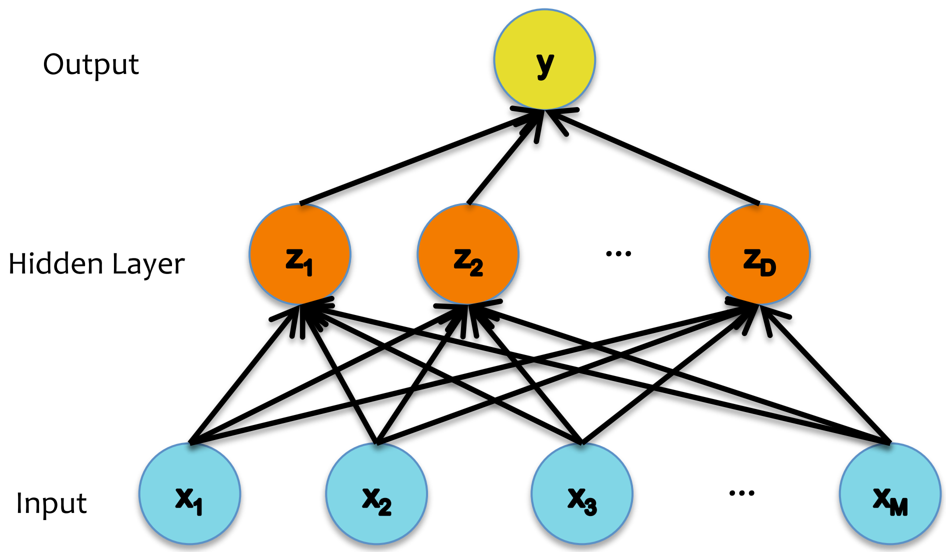


# Neural Network



# Decision Functions

# Neural Network




(E) **Output (sigmoid)**
$$y = \frac{1}{1+\exp(-b)}$$

(D) **Output (linear)**
$$b = \sum_{j=0}^{D} \beta_j z_j$$

(C) **Hidden (sigmoid)**
$$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$$

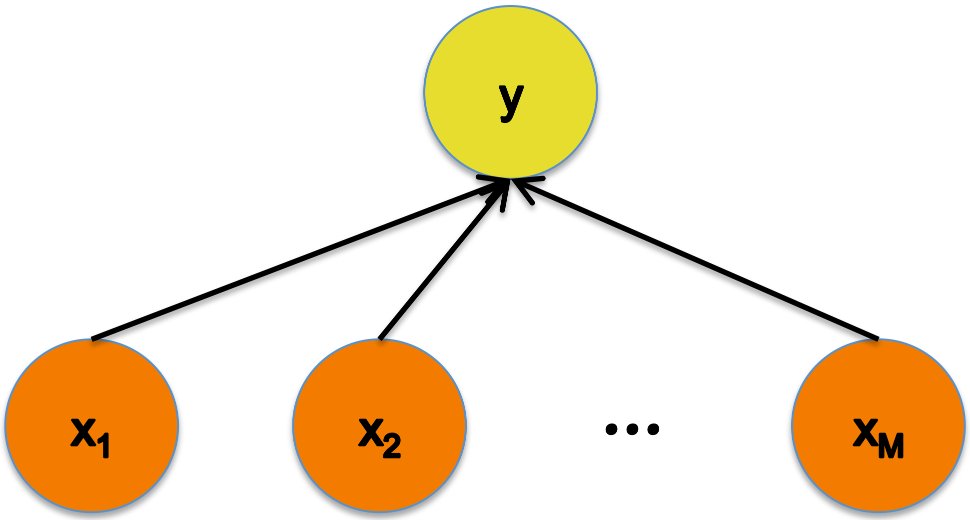
(B) **Hidden (linear)**
$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$$

(A) **Input**
Given $x_i, \ \forall i$

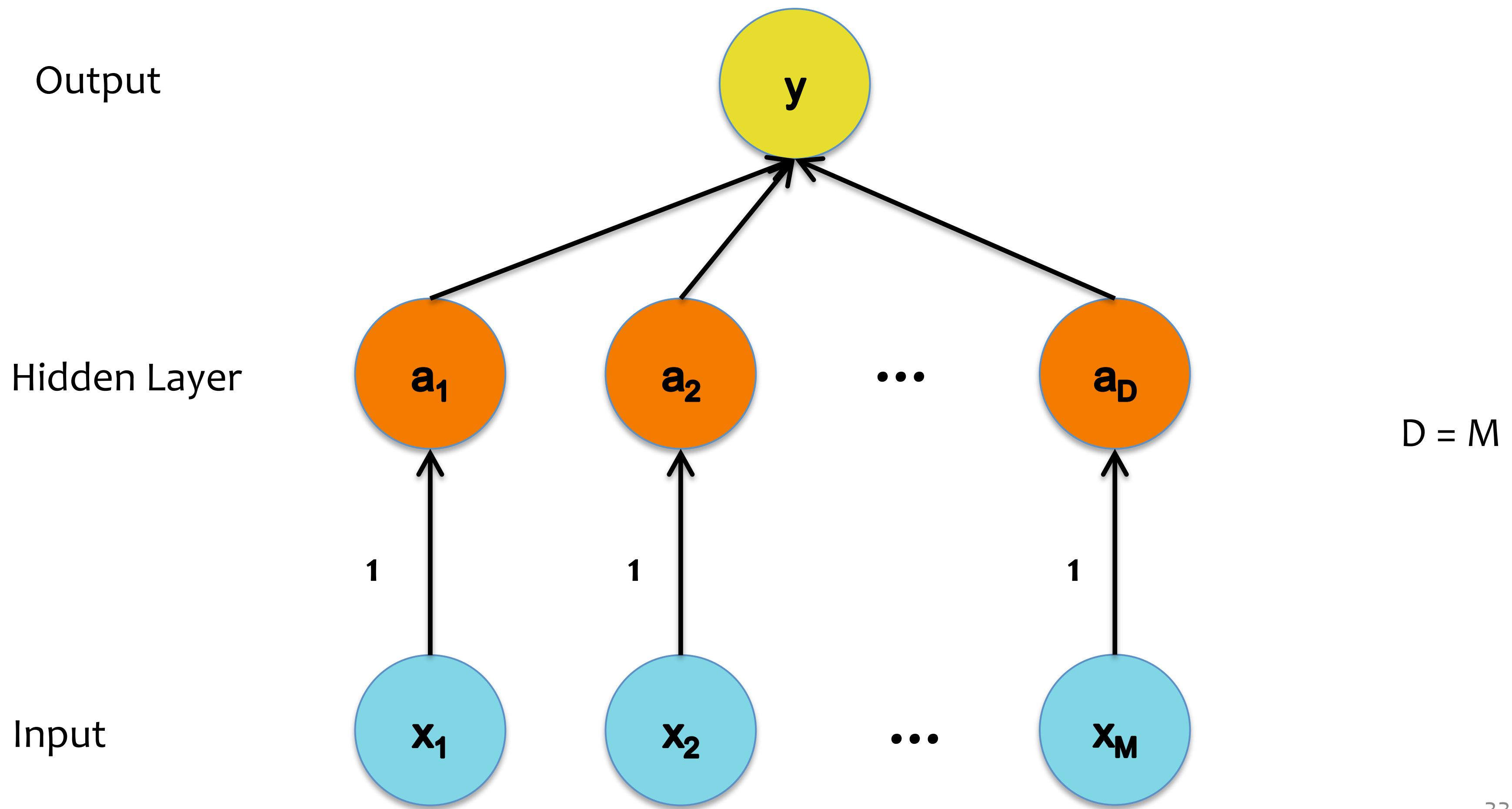
# Building a Neural Net

Output

Features



# Building a Neural Net



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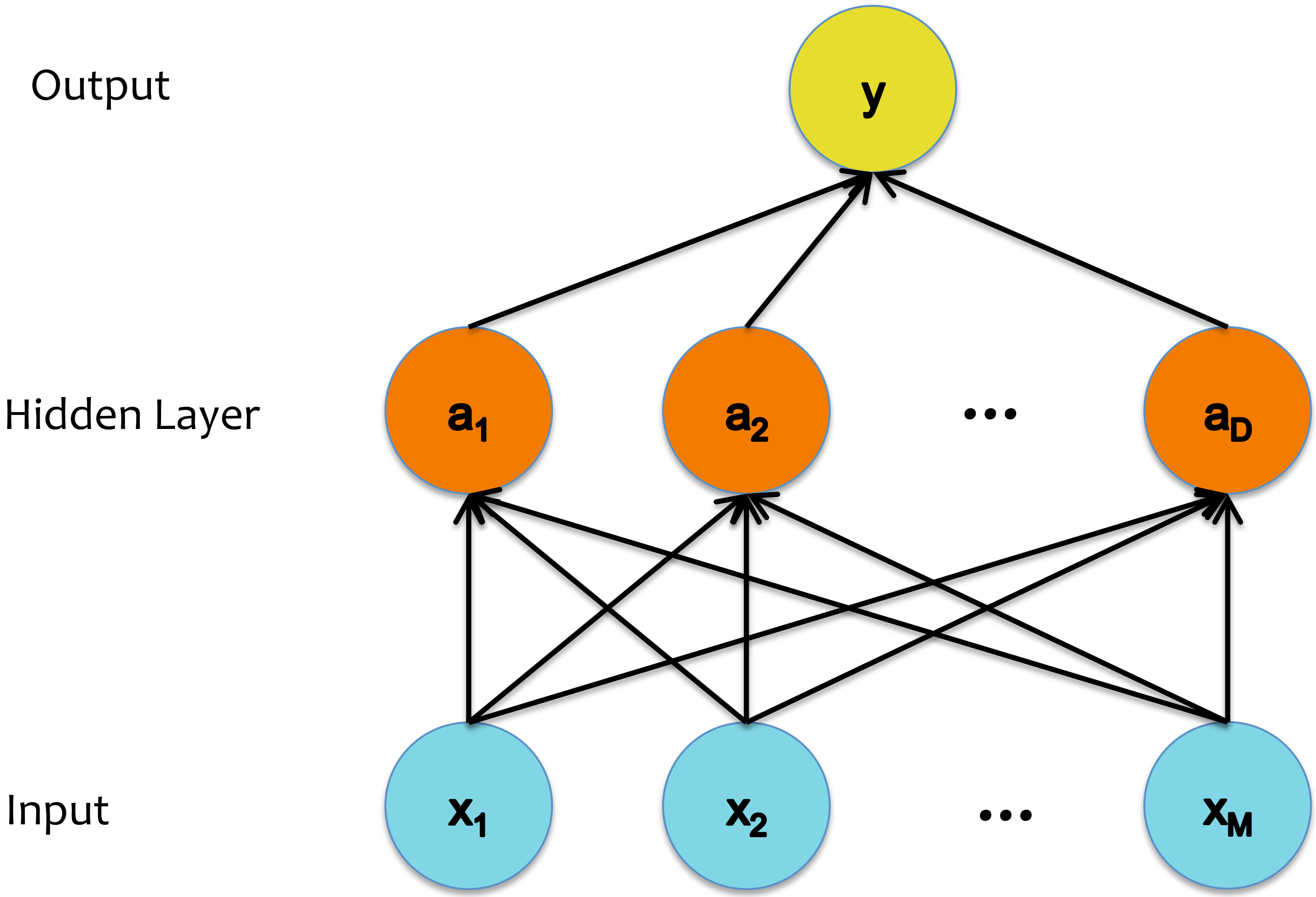
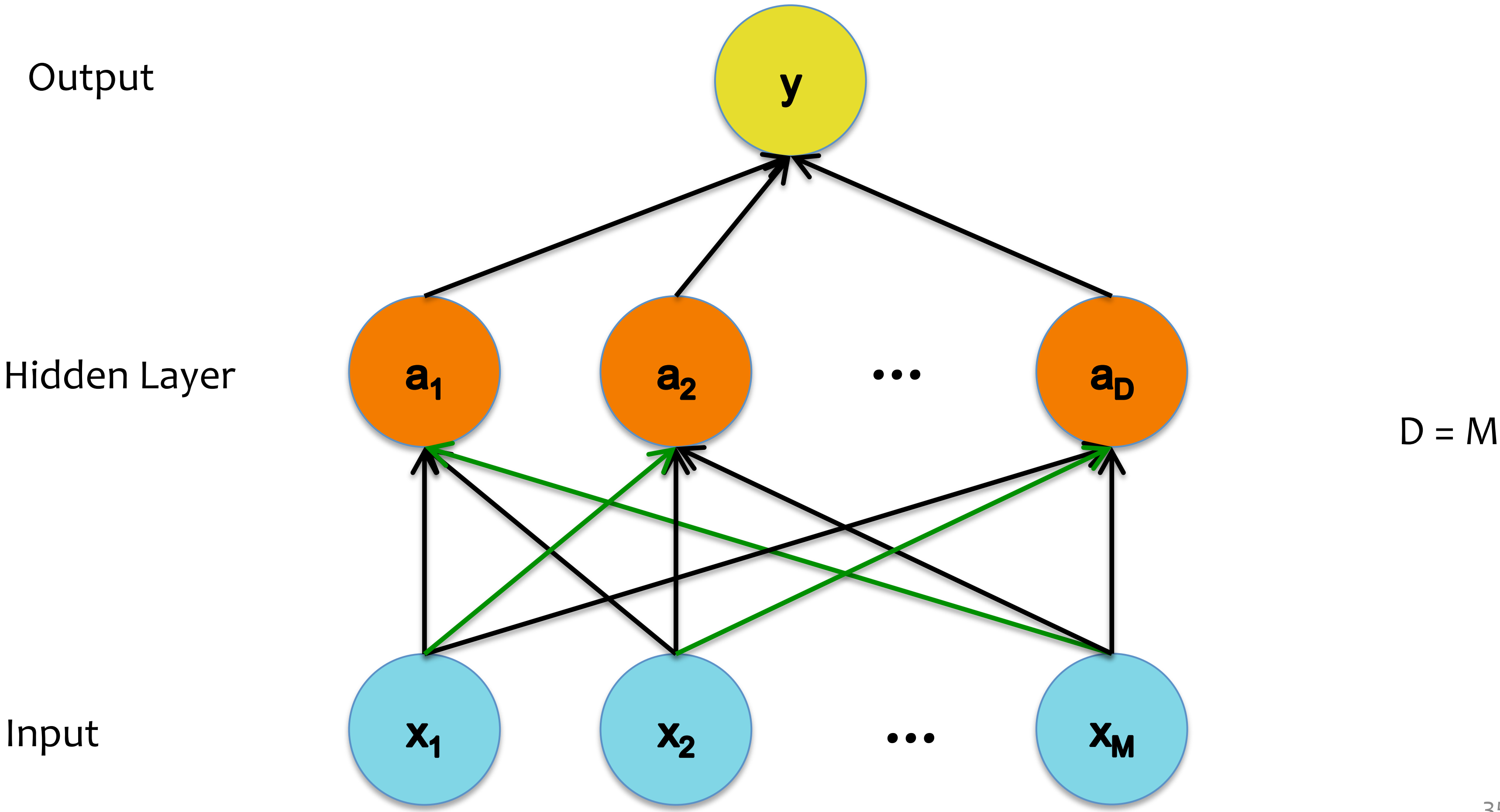
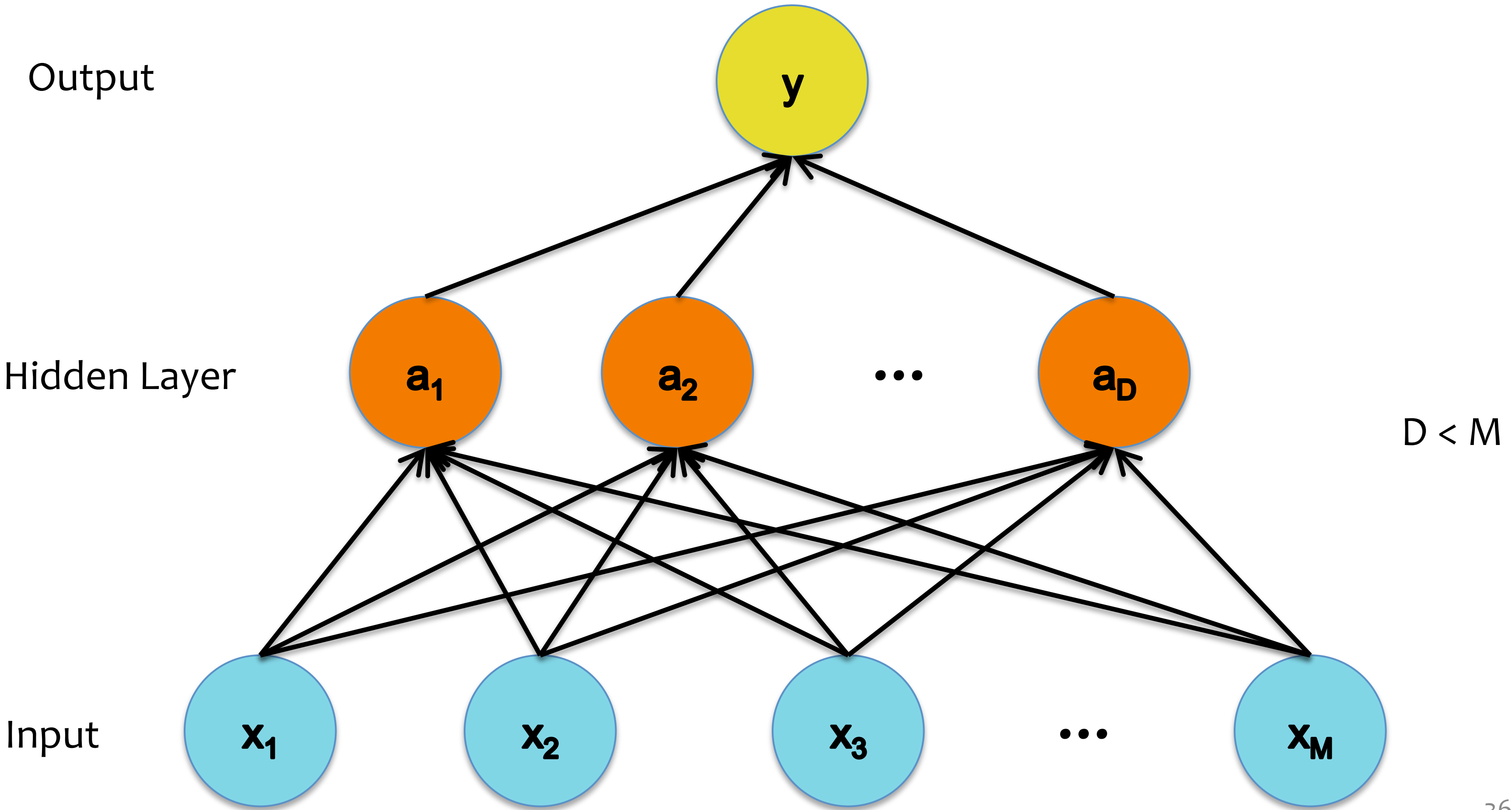



D = M

# Building a Neural Net

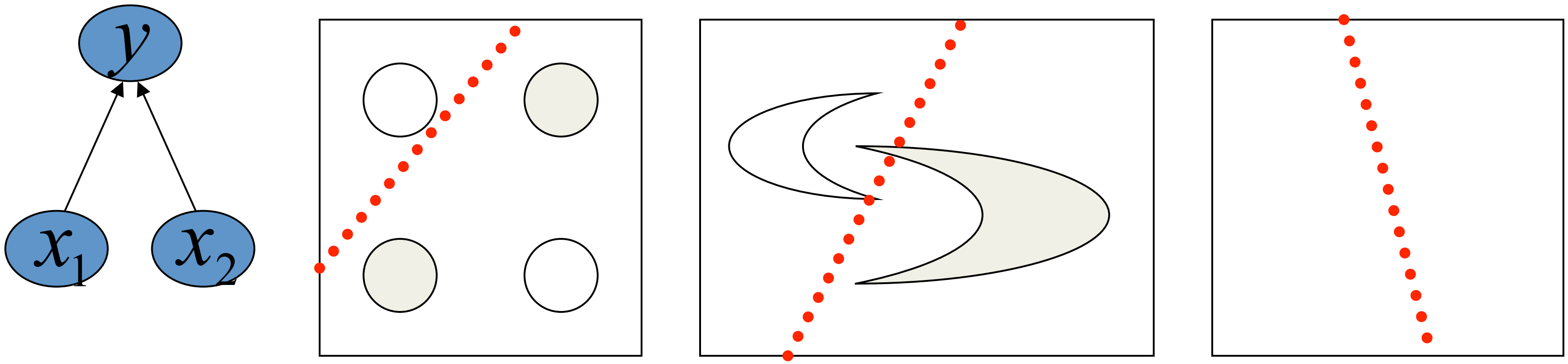


# Building a Neural Net



# Decision Boundary

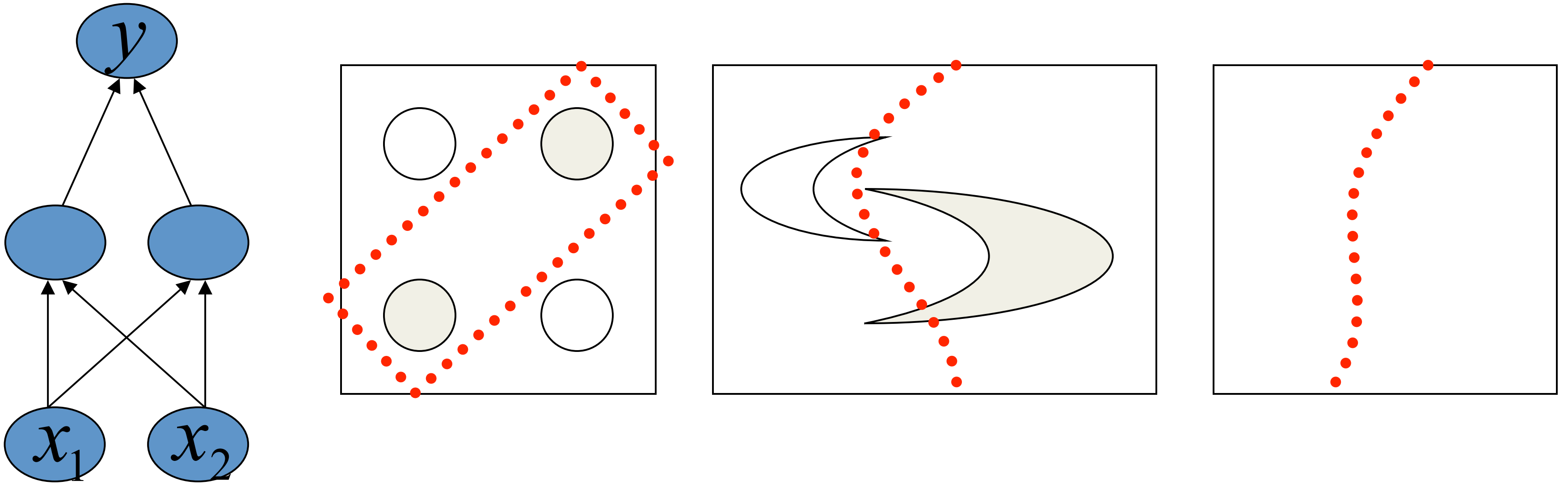
- 0 hidden layers: linear classifier
  - Hyperplanes




Example from to Eric Postma via Jason Eisner

# Decision Boundary

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

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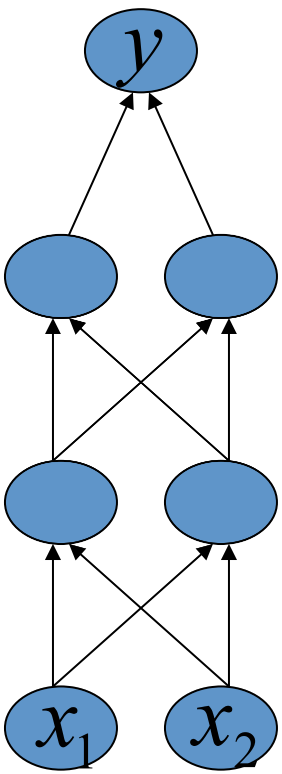
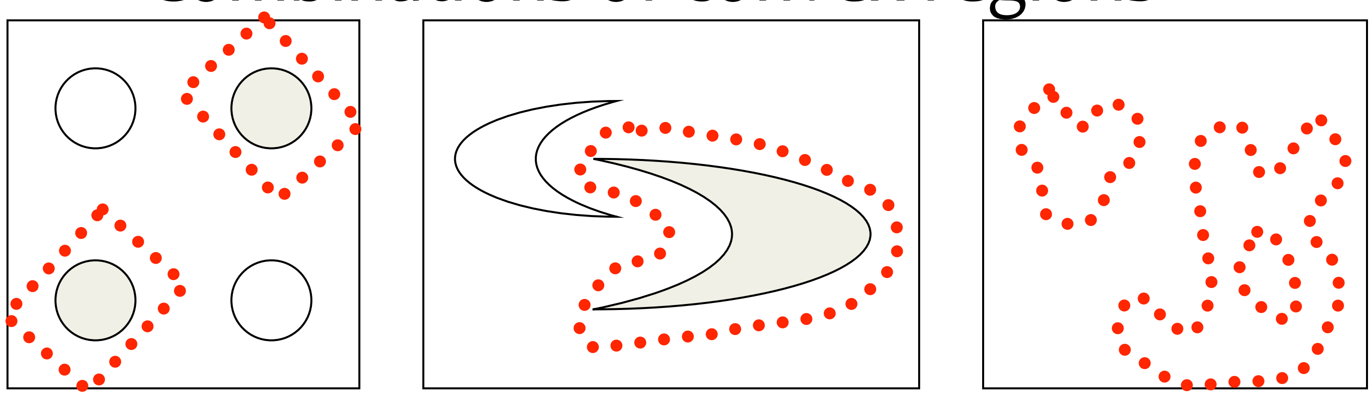
# Decision Boundary




- 2 hidden layers
  - Combinations of convex regions



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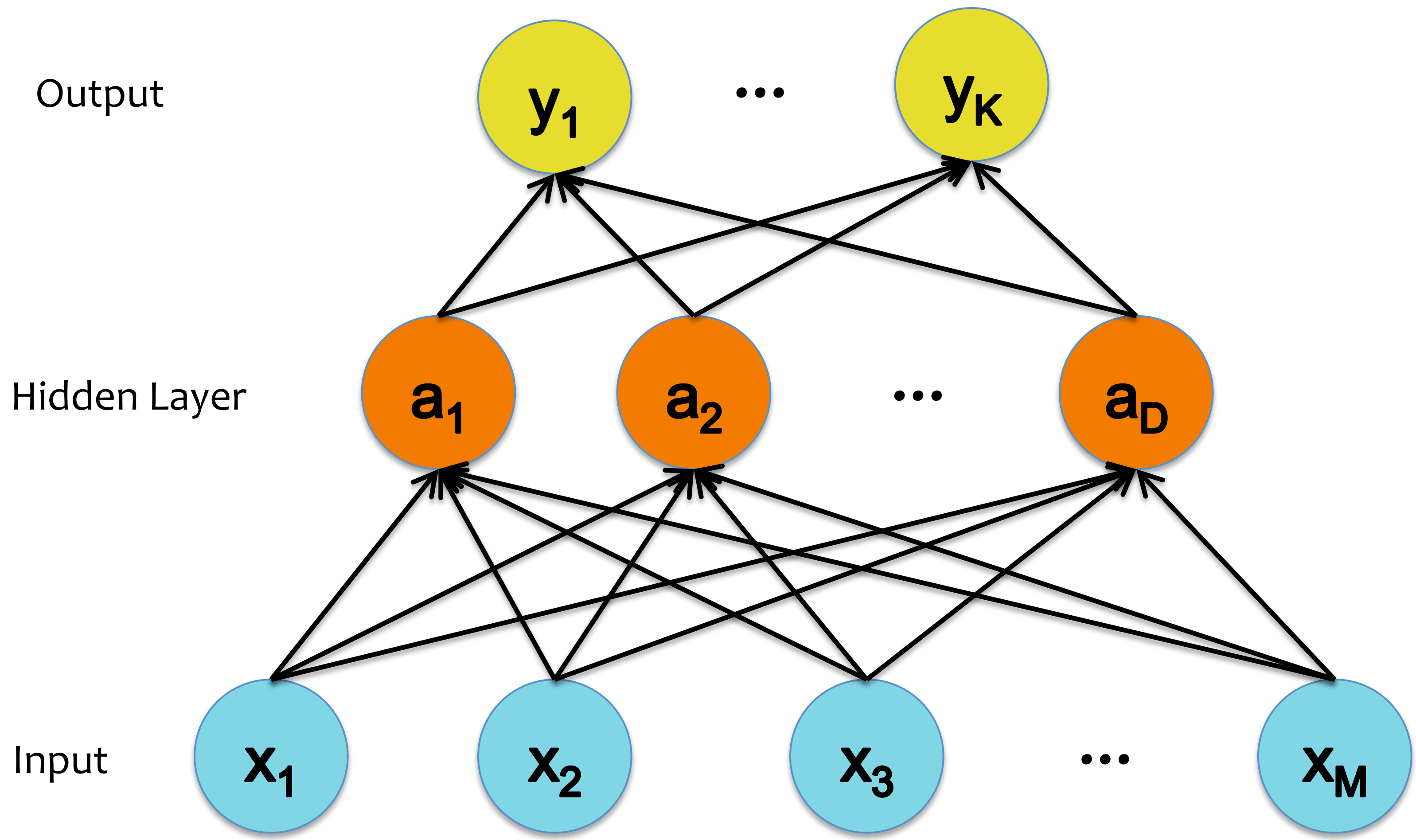
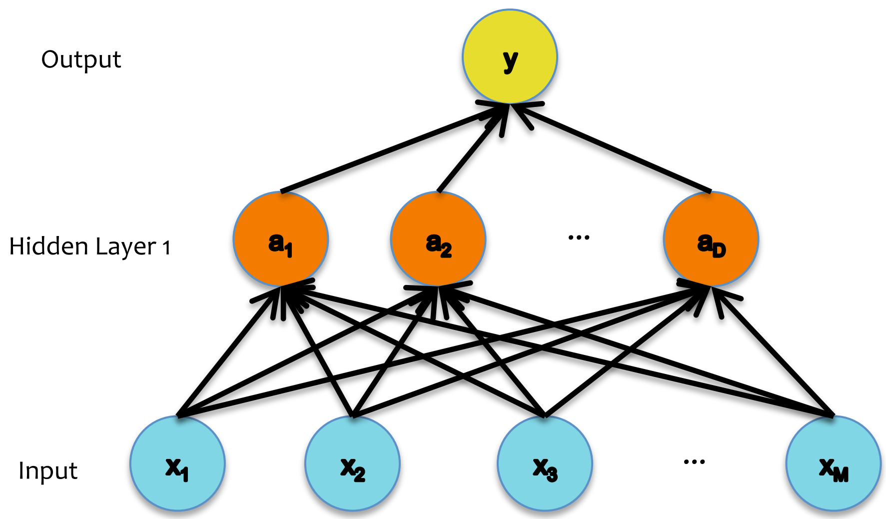
# Multi-Class Output



Decision Functions

# Deeper Networks

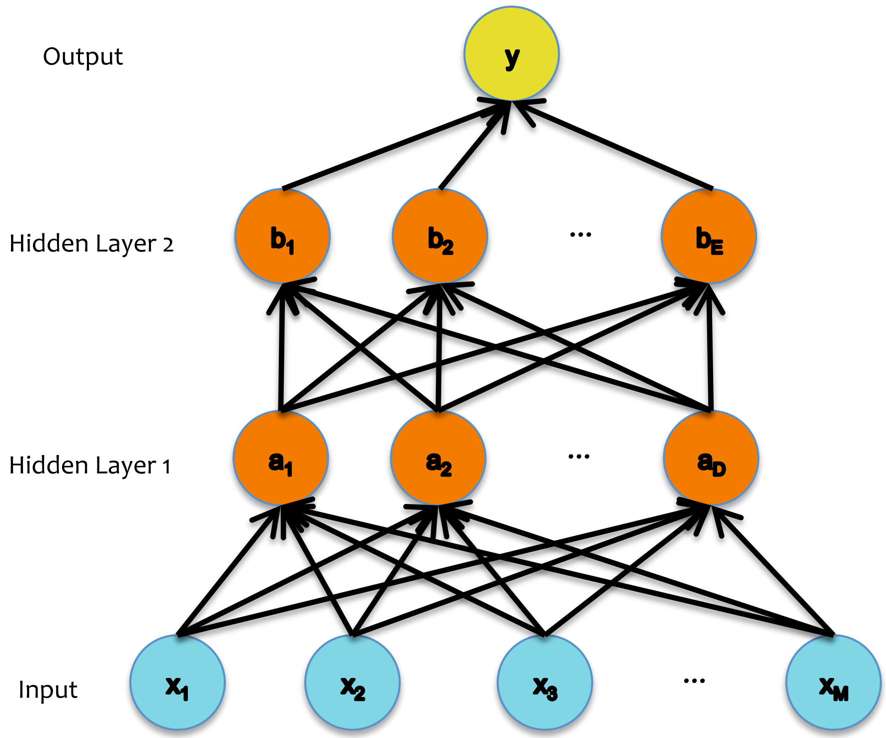
Next lecture:



Decision Functions

# Deeper Networks

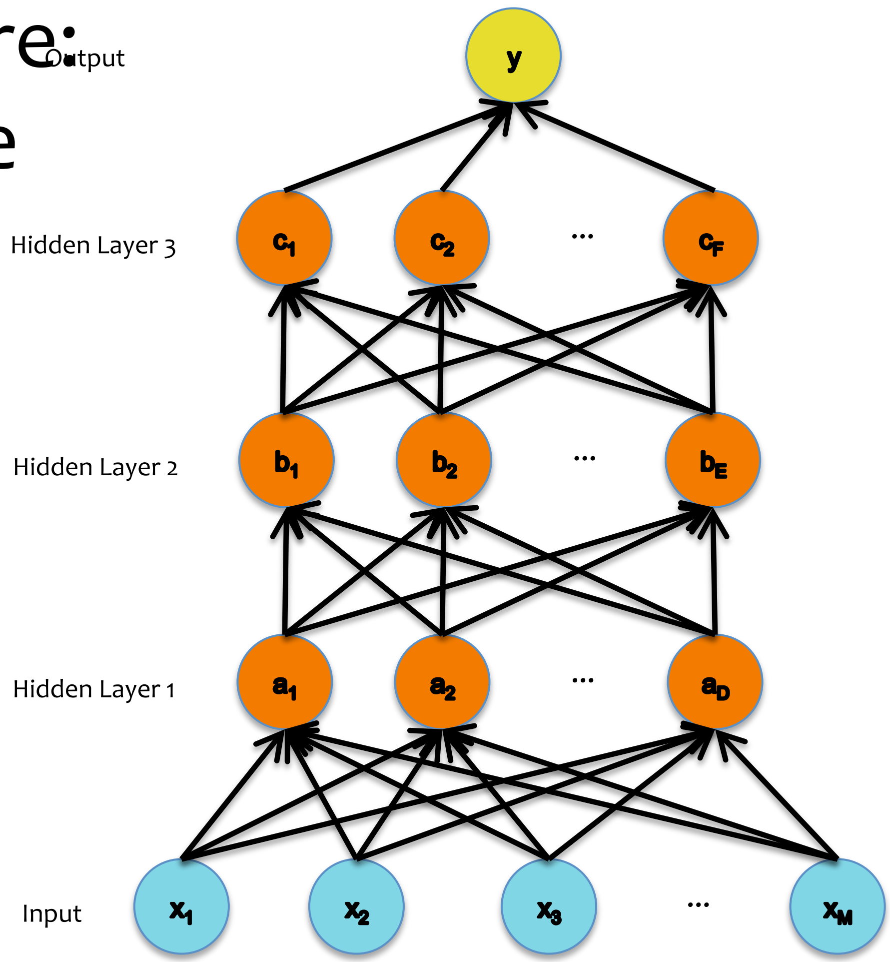
## Next lecture:



Decision Functions

# Deeper Networks

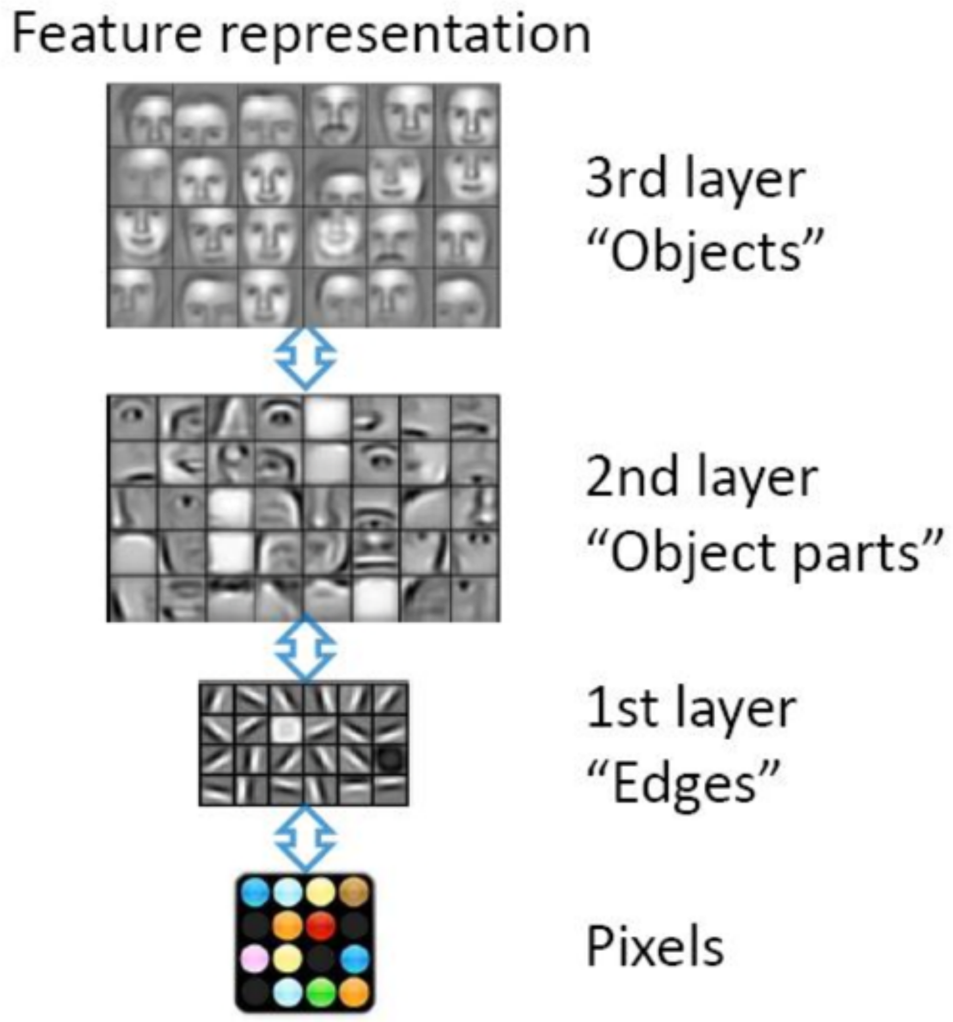
Next lecture: Making the neural networks deeper



Decision Functions

# Different Levels of Abstraction

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



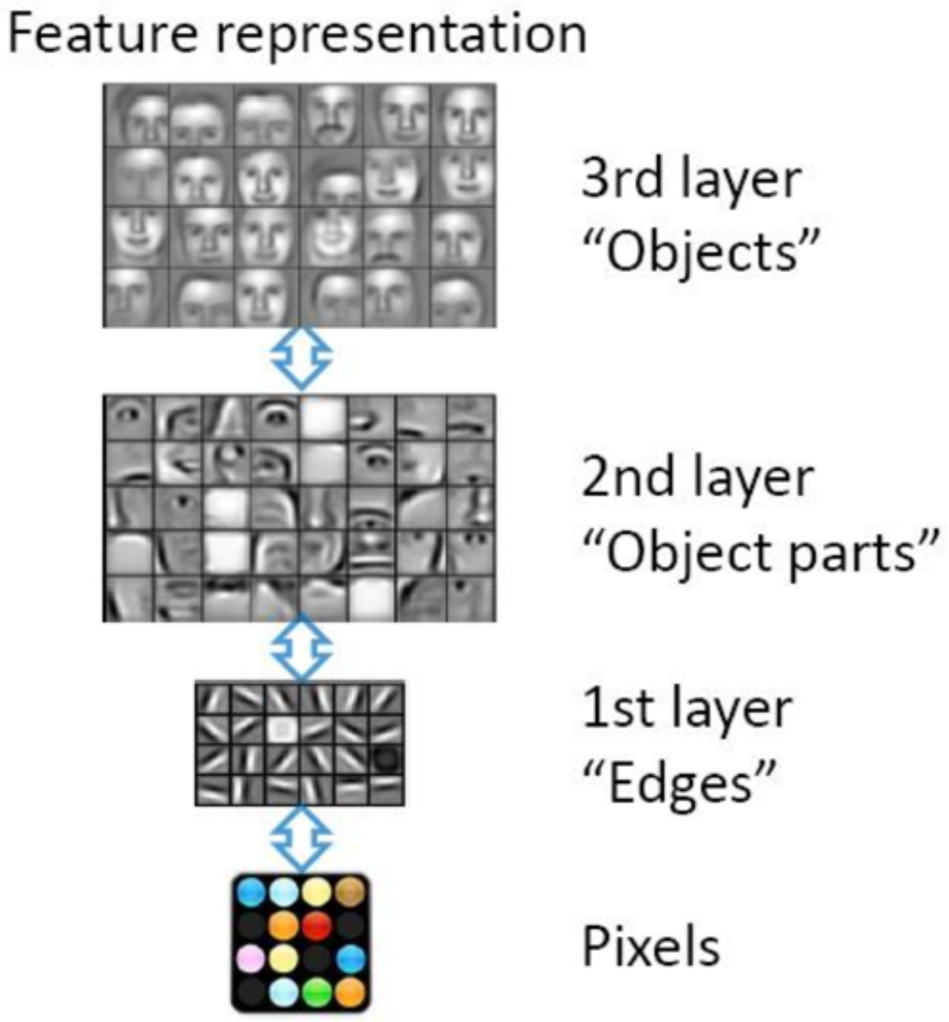

Example from Honglak Lee (NIPS 2010)

Decision Functions

# Different Levels of Abstraction

**Face Recognition:**

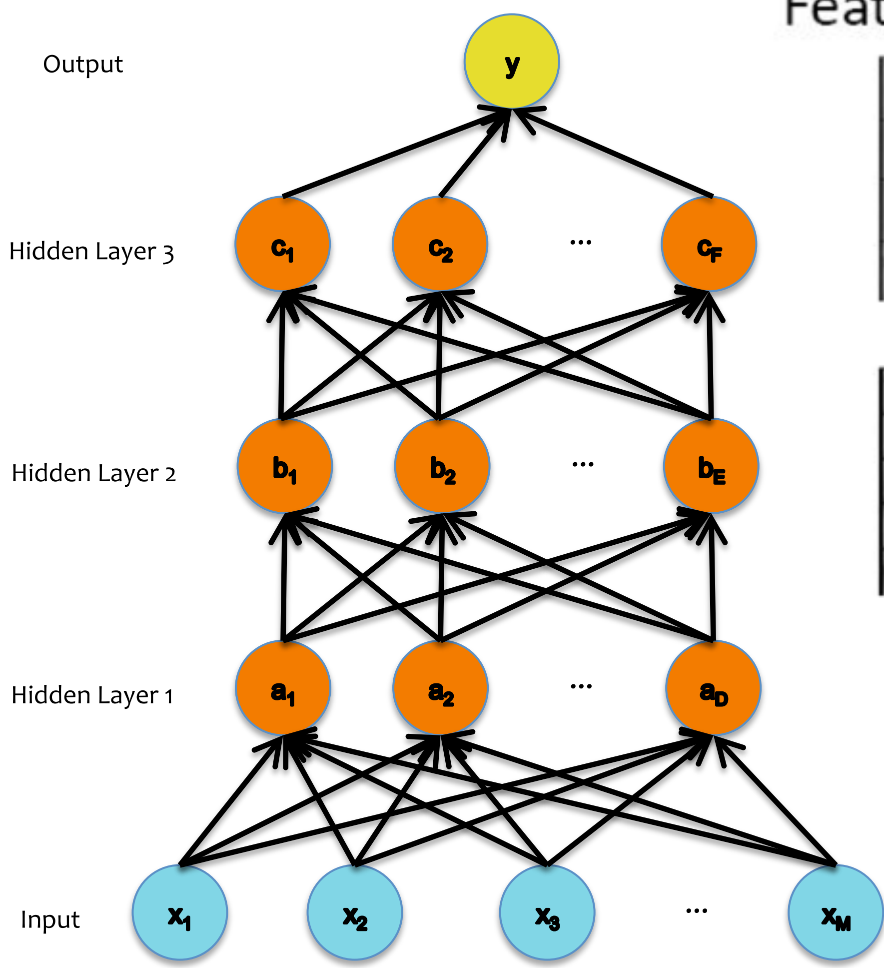
- Deep Network can build up increasingly higher levels of abstraction
- Lines, parts, regions

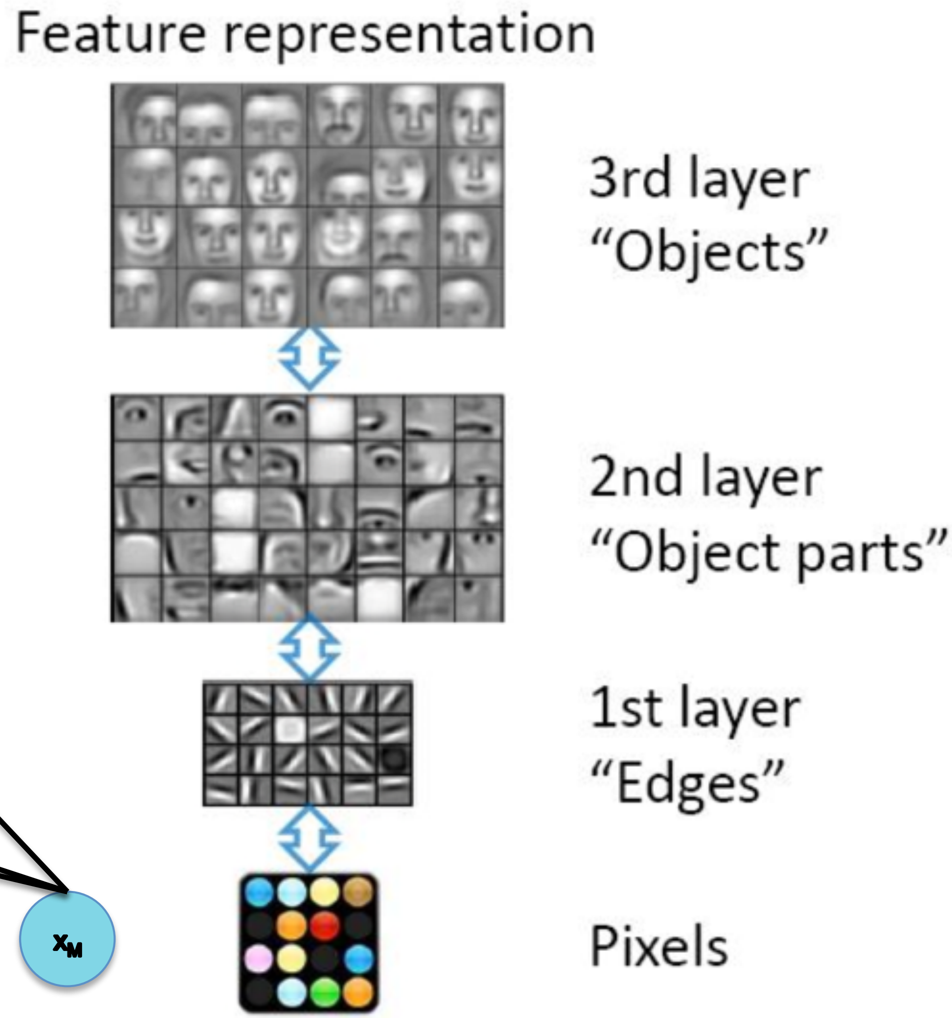



Example from Honglak Lee (NIPS 2010)

Decision Functions

# Different Levels of Abstraction




Example from Honglak Lee (NIPS 2010)

# ARCHITECTURES

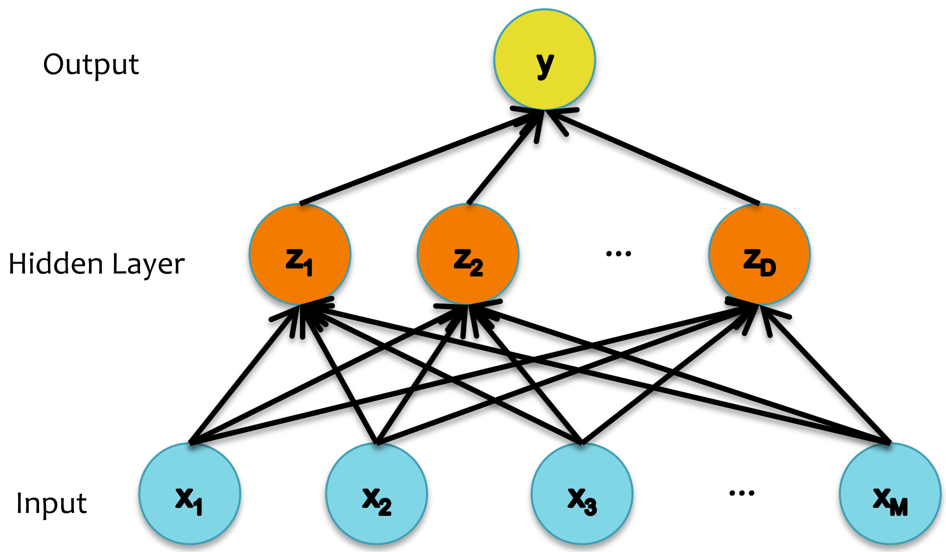
# Neural Network Architectures

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

# Activation Functions

Neural Network with sigmoid activation functions




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

**(E) Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$

**(D) Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

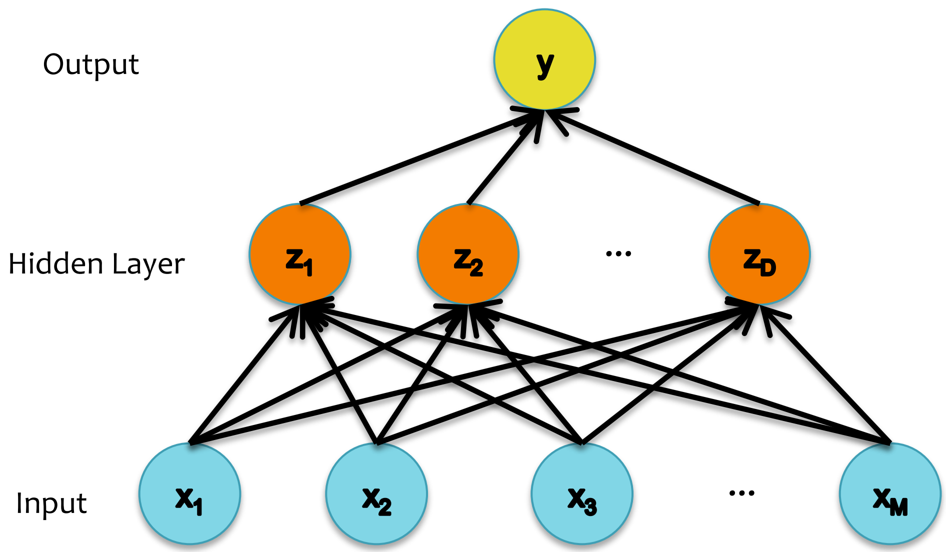
**(C) Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

**(B) Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

**(A) Input**
Given $x_i, \ \forall i$

# Activation Functions

Neural Network with arbitrary nonlinear activation functions




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

(E) **Output (nonlinear)**
$y = \sigma(b)$

(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

(C) **Hidden (nonlinear)**
$z_j = \sigma(a_j), \ \forall j$

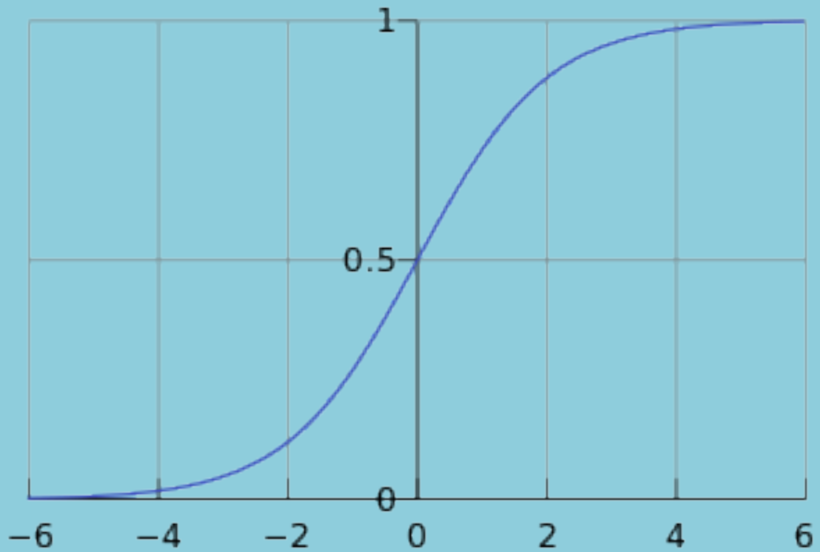
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

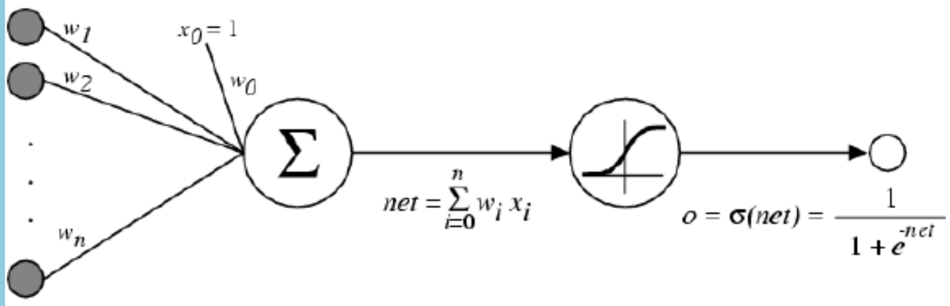
# Activation Functions

## Sigmoid / Logistic Function

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

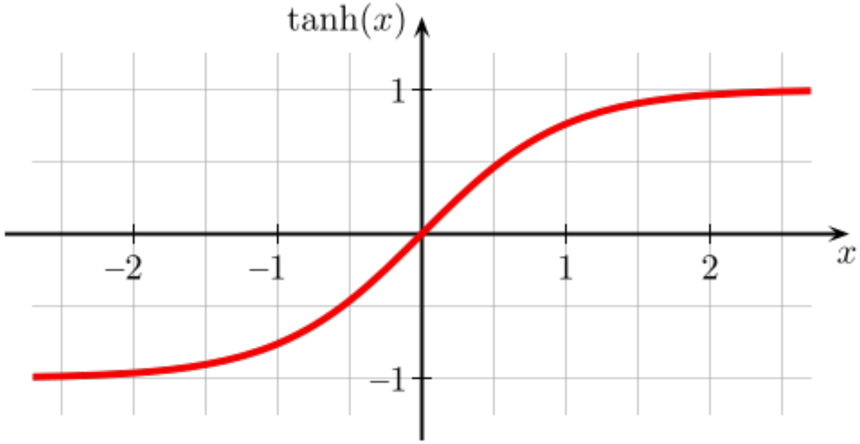



So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function…



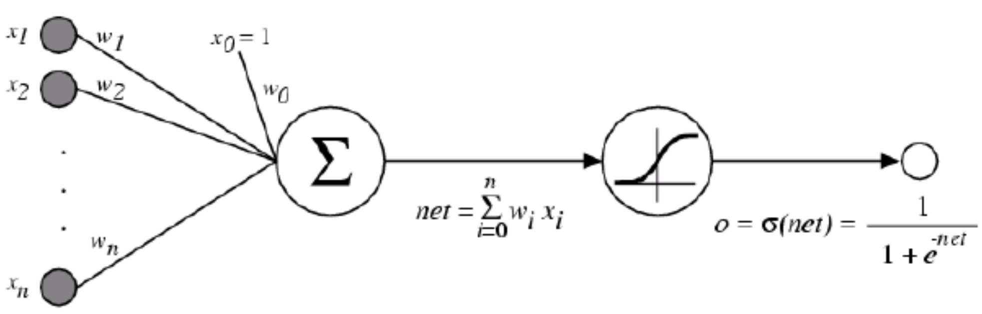
# Activation Functions

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




Alternate 1: tanh

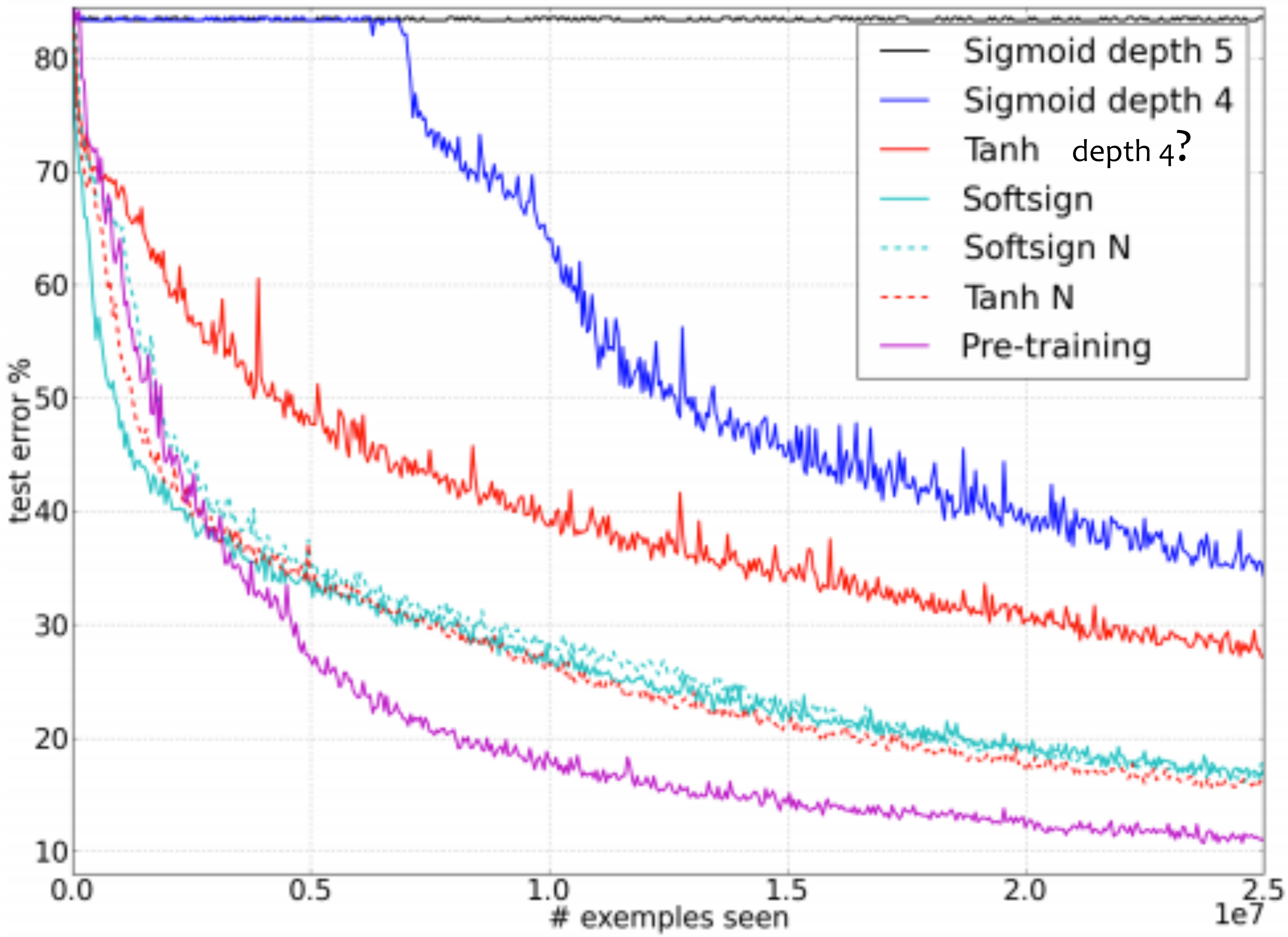
Like logistic function but shifted to range [-1, +1]




Slide from William Cohen

# Understanding the difficulty of training deep feedforward neural networks

AI Stats 2010

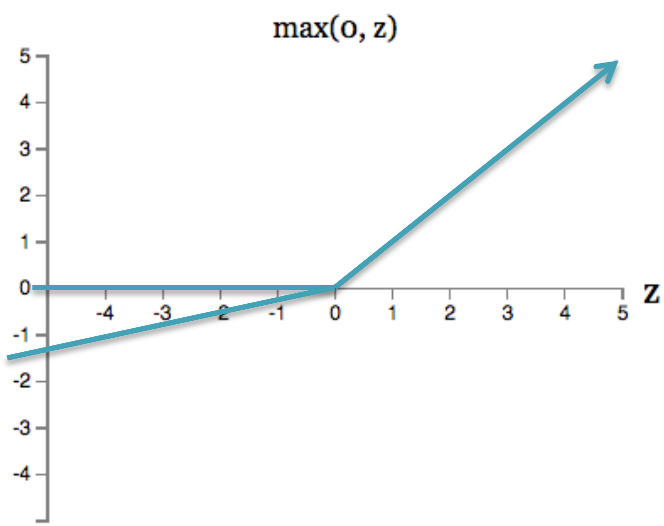



sigmoid
vs.
tanh

Figure from Glorot & Bentio (2010)

# Activation Functions

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

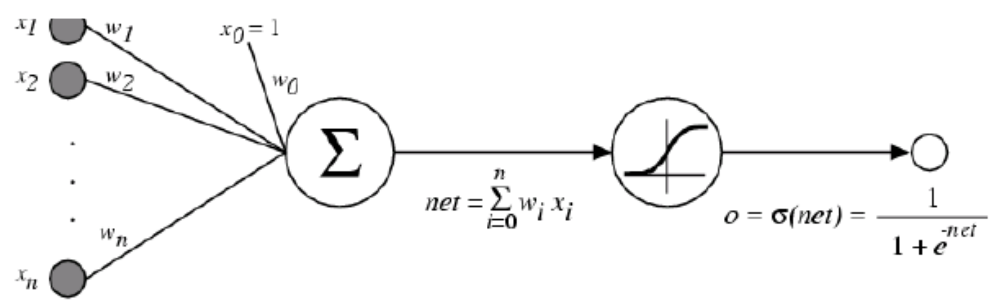



Alternate 2: rectified linear unit

Linear with a cutoff at zero

(Implementation: clip the gradient when you pass zero)

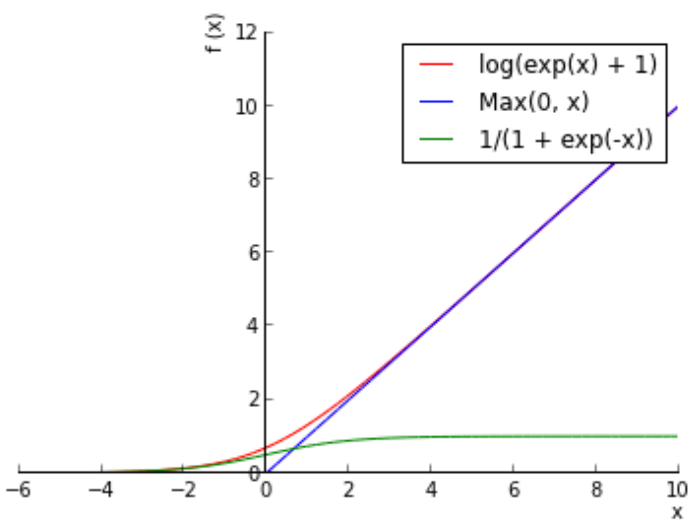
$$\max(0, w \cdot x + b).$$




Slide from William Cohen

# Activation Functions

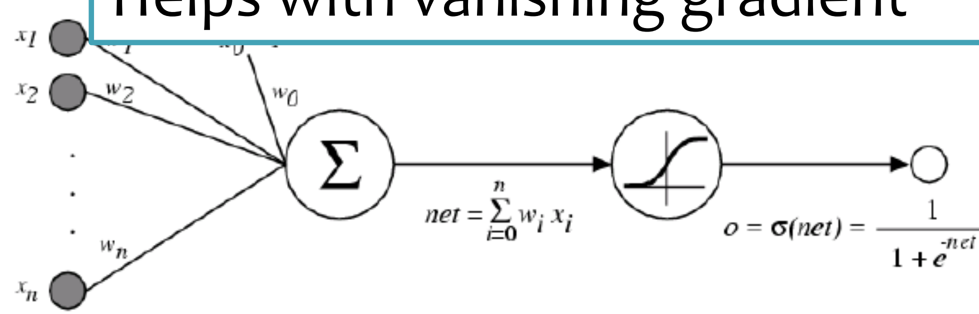
- A new change: modifying the nonlinearity
  - reLU often used in vision tasks




Alternate 2: rectified linear unit

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

Doesn't saturate (at one end)
Sparsifies outputs
Helps with vanishing gradient



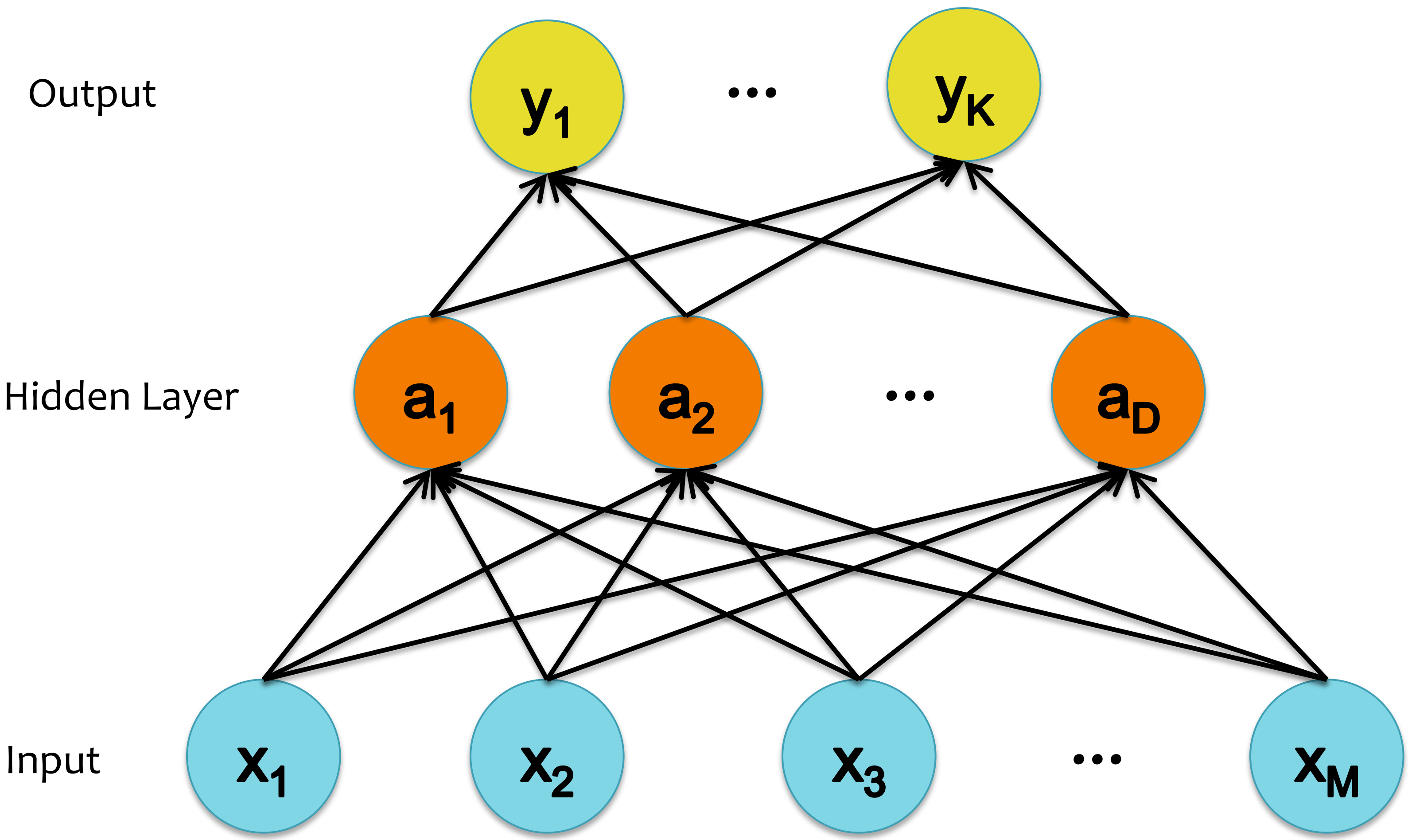

Slide from William Cohen

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

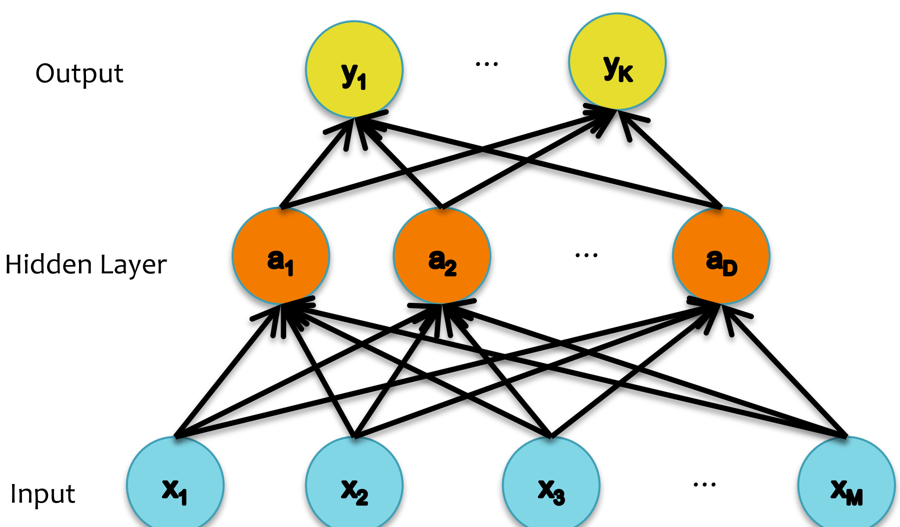
# Multi-Class Output



# Multi-Class Output

## Softmax:

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




**(F) Loss**
$J = \sum_{k=1}^{K} y_k^* \log(y_k)$

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

**(D) Output (linear)**
$b_k = \sum_{j=0}^{D} \beta_{kj} z_j \;\; \forall k$

**(C) Hidden (nonlinear)**
$z_j = \sigma(a_j), \;\; \forall j$

**(B) Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \;\; \forall j$

**(A) Input**
Given $x_i, \;\; \forall i$

# Cross-entropy vs. Quadratic loss

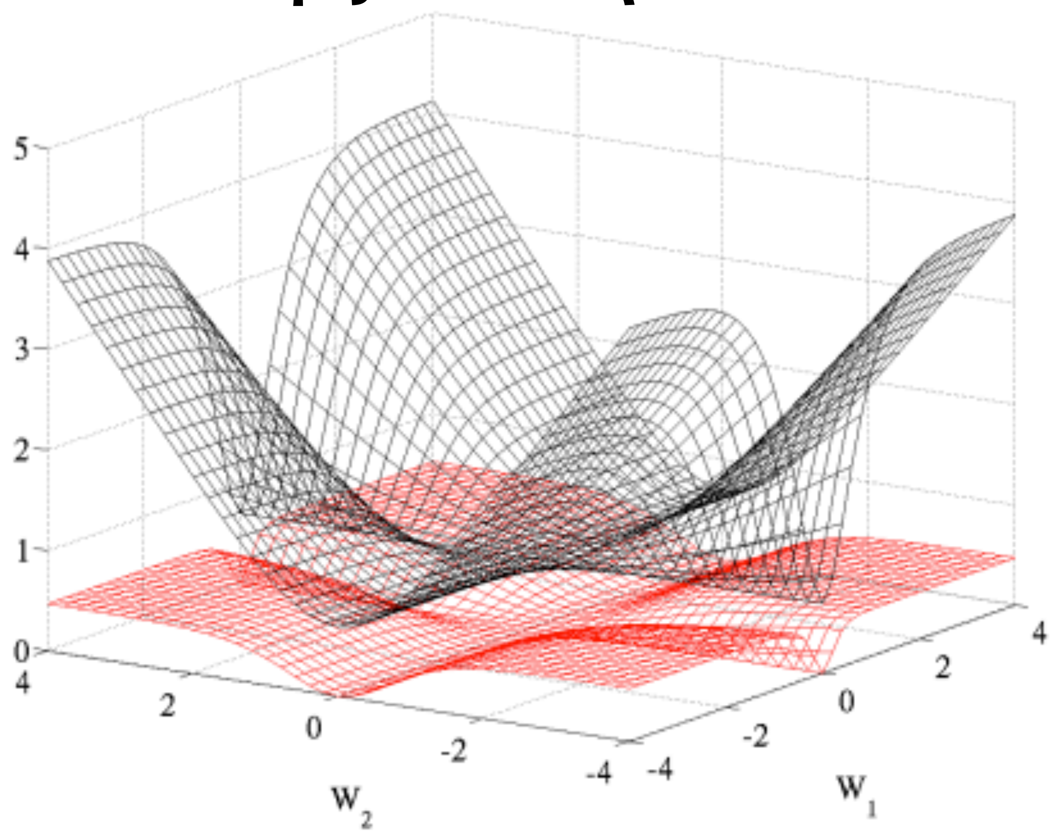



Figure 5: *Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, $W_1$ respectively on the first layer and $W_2$ on the second, output layer.*

Figure from Glorot & Bentio (2010)

Background

# A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:

– Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

# Objective Functions

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

| | | |
|---|---|---|
| 1) Minimizing sum of squared errors… | …gives… | 5) …MLE estimates of weights assuming target follows a Bernoulli with parameter given by the output value |
| 2) Minimizing sum of squared errors plus squared Euclidean norm of weights… | | 6) …MAP estimates of weights assuming weight priors are zero mean Gaussian |
| 3) Minimizing cross-entropy… | | 7) …estimates with a large margin on the training data |
| 4) Minimizing hinge loss… | | 8) …MLE estimates of weights assuming zero mean Gaussian noise on the output value |

A. 1=5, 2=7, 3=6, 4=8
B. 1=5, 2=7, 3=8, 4=6
C. 1=7, 2=5, 3=5, 4=7
D. 1=7, 2=5, 3=6, 4=8
E. 1=8, 2=6, 3=5, 4=7
F. 1=8, 2=6, 3=8, 4=6

# BACKPROPAGATION

Background

# A Recipe for Machine Learning

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# 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?

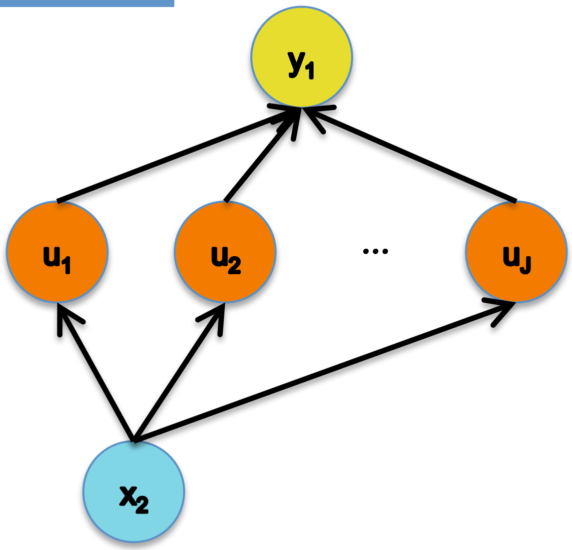
Training

# Chain Rule

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

**Chain Rule:**

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



# Training

# Chain Rule

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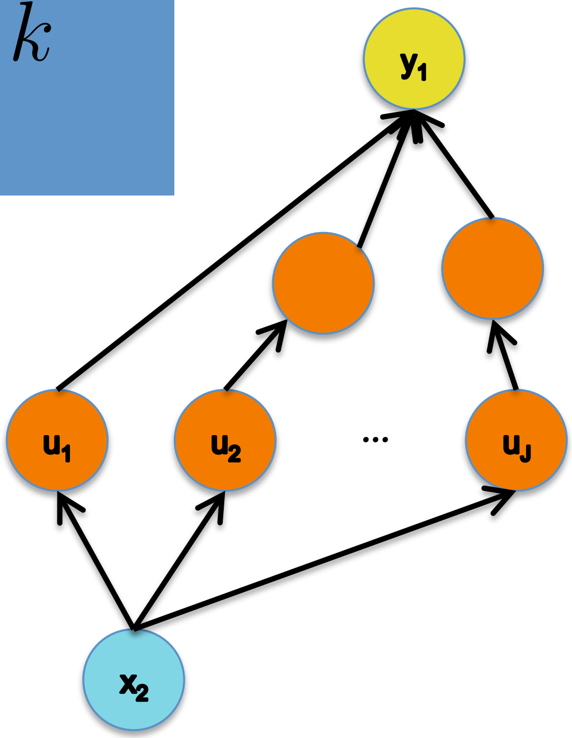
**Backpropagation** is just repeated application of the **chain rule** from Calculus 101.



# Training

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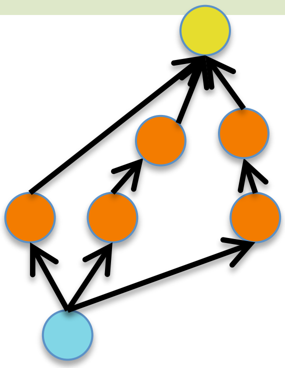


**Backpropagation:**

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

$$J = cos(u)$$

$$u = u_1 + u_2$$

$$u_1 = sin(t)$$

$$u_2 = 3t$$

$$t = x^2$$

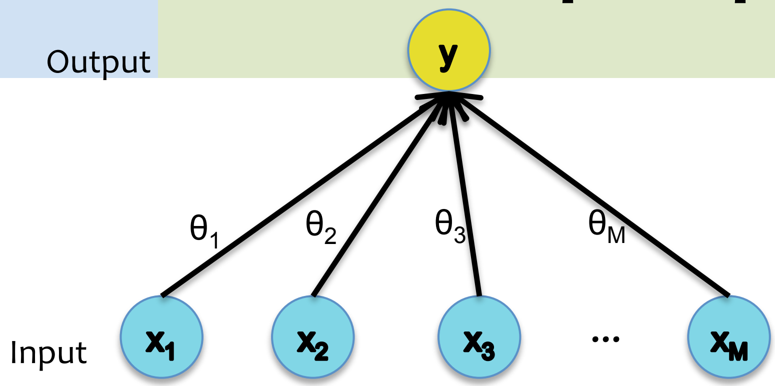
Training

# 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 | Backward |
|---|---|
| $J = cos(u)$ | $\frac{dJ}{du} \mathrel{+}= -sin(u)$ |
| $u = u_1 + u_2$ | $\frac{dJ}{du_1} \mathrel{+}= \frac{dJ}{du}\frac{du}{du_1}, \quad \frac{du}{du_1} = 1 \qquad \frac{dJ}{du_2} \mathrel{+}= \frac{dJ}{du}\frac{du}{du_2}, \quad \frac{du}{du_2} = 1$ |
| $u_1 = sin(t)$ | $\frac{dJ}{dt} \mathrel{+}= \frac{dJ}{du_1}\frac{du_1}{dt}, \quad \frac{du_1}{dt} = \cos(t)$ |
| $u_2 = 3t$ | $\frac{dJ}{dt} \mathrel{+}= \frac{dJ}{du_2}\frac{du_2}{dt}, \quad \frac{du_2}{dt} = 3$ |
| $t = x^2$ | $\frac{dJ}{dx} \mathrel{+}= \frac{dJ}{dt}\frac{dt}{dx}, \quad \frac{dt}{dx} = 2x$ |

# Training Backpropagation




**Case 1: Logistic Regression**

Forward

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

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

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

Backward

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

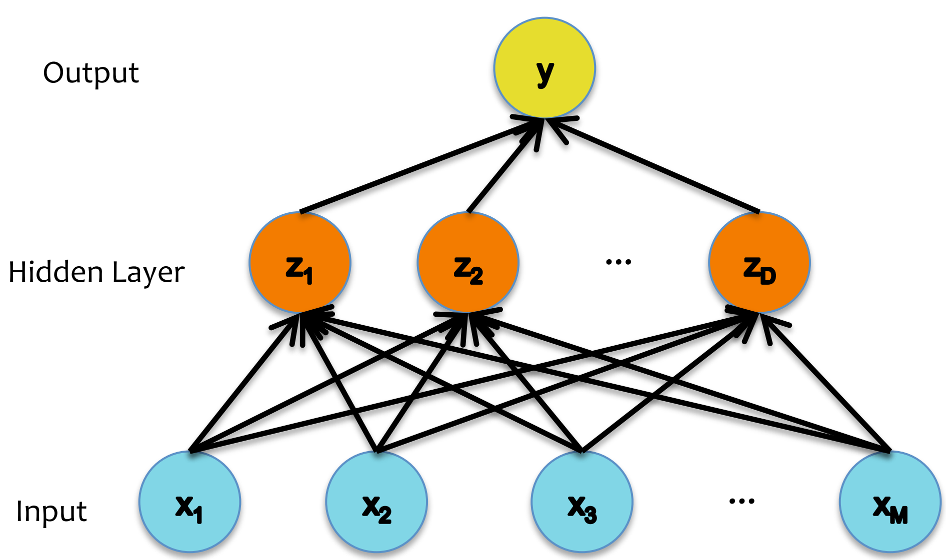
$$\frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da}, \quad \frac{dy}{da} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$$

$$\frac{dJ}{d\theta_j} = \frac{dJ}{da}\frac{da}{d\theta_j}, \quad \frac{da}{d\theta_j} = x_j$$

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

# Training

# Backpropagation




**(E) Output (sigmoid)**
$$y = \frac{1}{1+\exp(-b)}$$

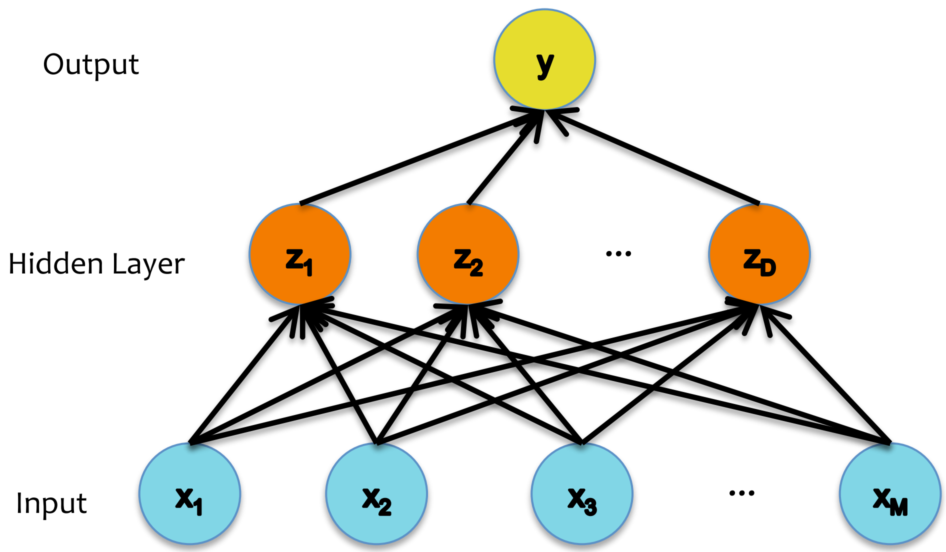
**(D) Output (linear)**
$$b = \sum_{j=0}^{D} \beta_j z_j$$

**(C) Hidden (sigmoid)**
$$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$$

**(B) Hidden (linear)**
$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$$

**(A) Input**
Given $x_i, \ \forall i$

# Training — Backpropagation




**(F) Loss**
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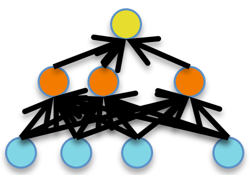
**(A) Input**
Given $x_i, \ \forall i$

# Backpropagation

**Case 2: Neural Network**



Forward

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

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

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

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

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

Backward

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

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

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

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

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

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

# Training

# Chain Rule

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

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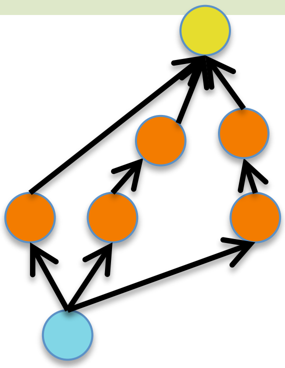

**Backpropagation:**

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**

Training

# Chain Rule

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

**Chain Rule:**

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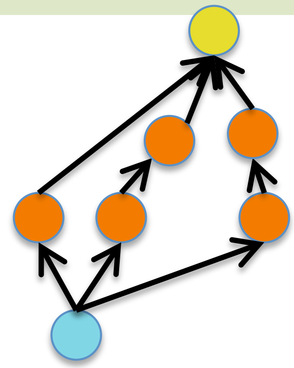

**Backpropagation:**

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**

# Training Backpropagation

Case 2:

| | Forward | Backward |
|---|---|---|
| Module 5 | $J = y^* \log y + (1 - y^*) \log(1 - y)$ | $\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$ |
| Module 4 | $y = \frac{1}{1 + \exp(-b)}$ | $\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$ |
| Module 3 | $b = \sum_{j=0}^{D} \beta_j z_j$ | $\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$ <br> $\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$ |
| Module 2 | $z_j = \frac{1}{1 + \exp(-a_j)}$ | $\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$ |
| Module 1 | $a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$ | $\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$ <br> $\frac{dJ}{dx_i} = \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \sum_{j=0}^{D} \alpha_{ji}$ |

# Gradients

**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!

Background

A Recipe for

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of t

– Decision functio

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

opp site the gradient)

$$- \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

# 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