Neural Networks

Outline

- Logistic Regression (Recap)
- Neural Networks
- Backpropagation

RECALL: LOGISTIC REGRESSION

Using gradient ascent for linear classifiers

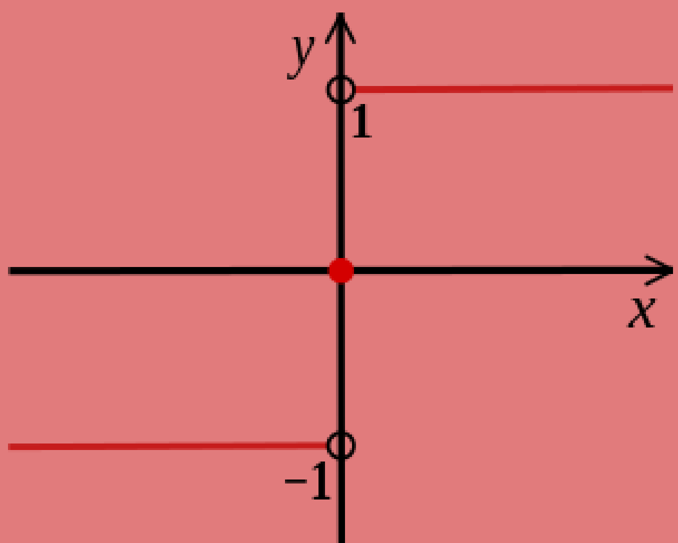
Key idea behind today's lecture:

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:

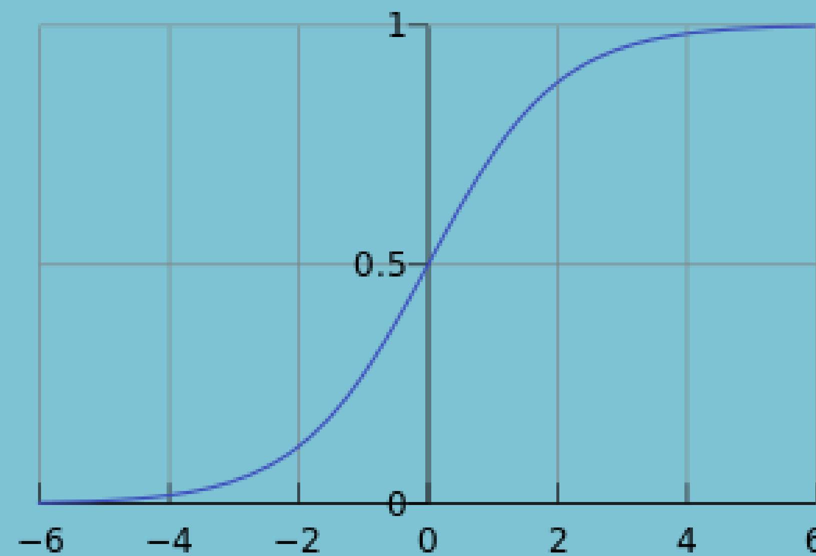
$$h(\mathbf{x}) = \text{sign}(\boldsymbol{\theta}^T \mathbf{x})$$



sign(x)

Use a differentiable function instead:

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



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

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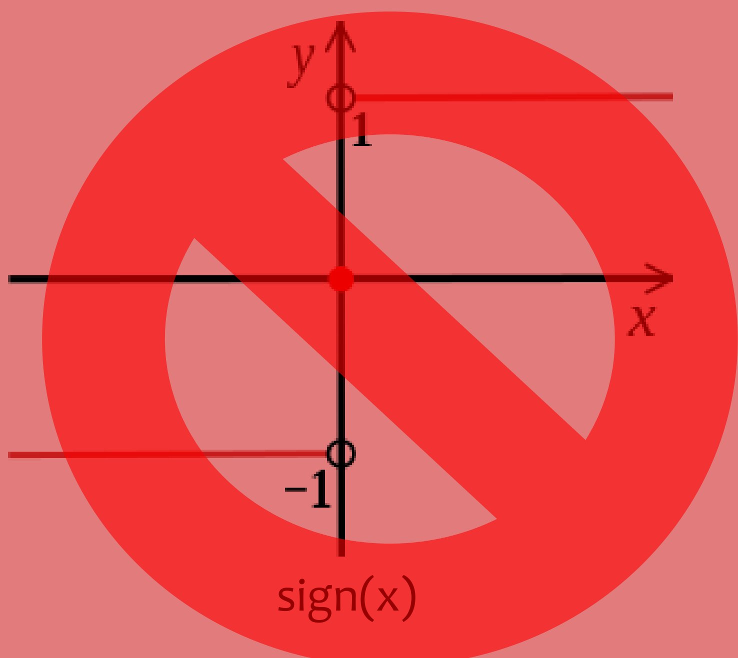

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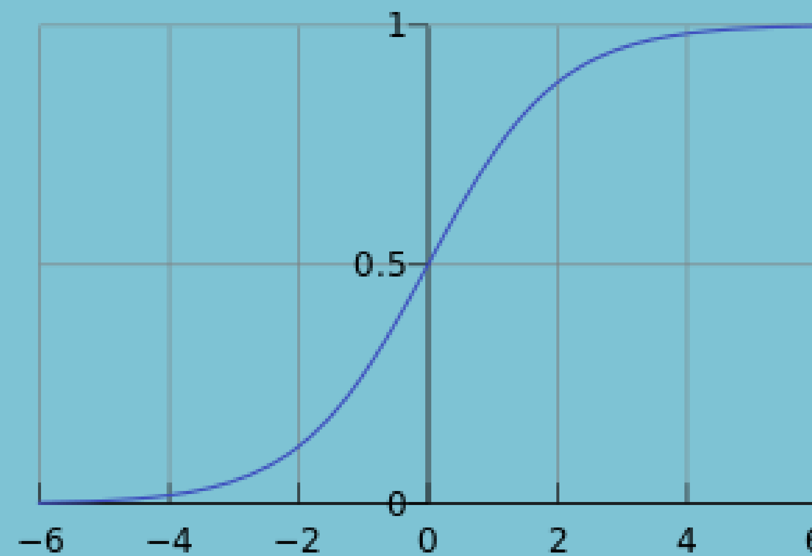


$$\text{logistic}(u) \circ \frac{1}{1+e^{-u}}$$

Logistic Regression

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

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

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. $\boldsymbol{\theta}^* = \operatorname*{argmin}_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

Prediction: Output is the most probable class.

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

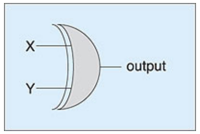
NEURAL NETWORKS

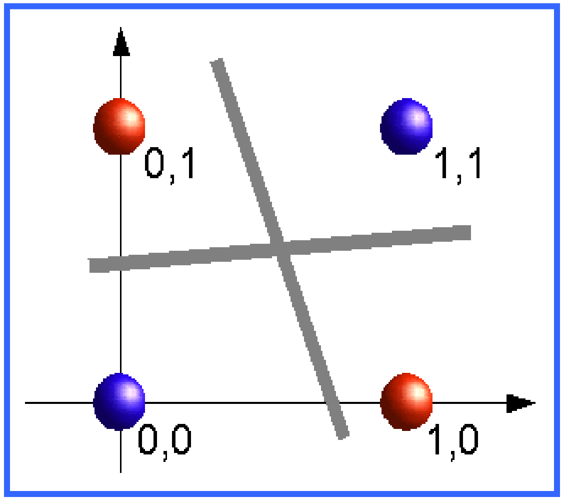
Learning highly non-linear functions

f: X → Y

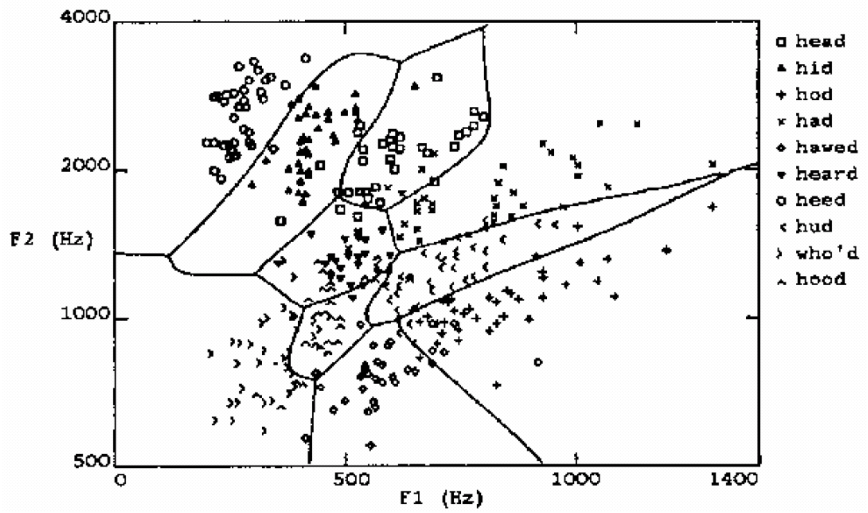
- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars

The XOR gate



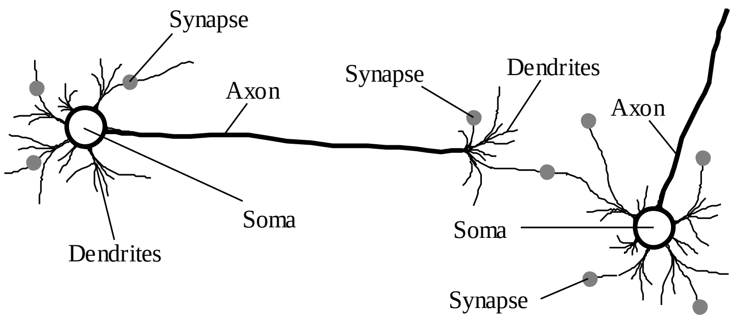


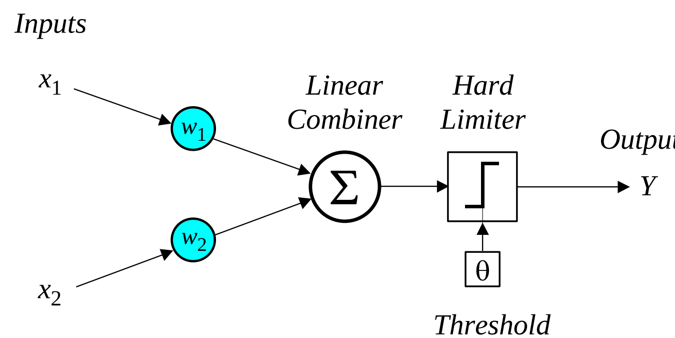
Speech recognition



Perceptron and Neural Nets

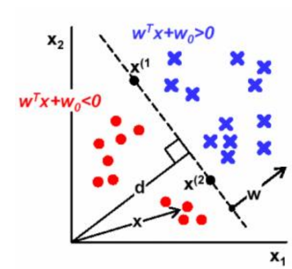
- From biological neuron to artificial neuron (perceptron)



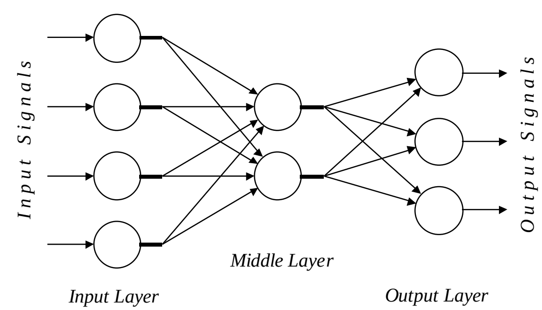


- Activation function

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

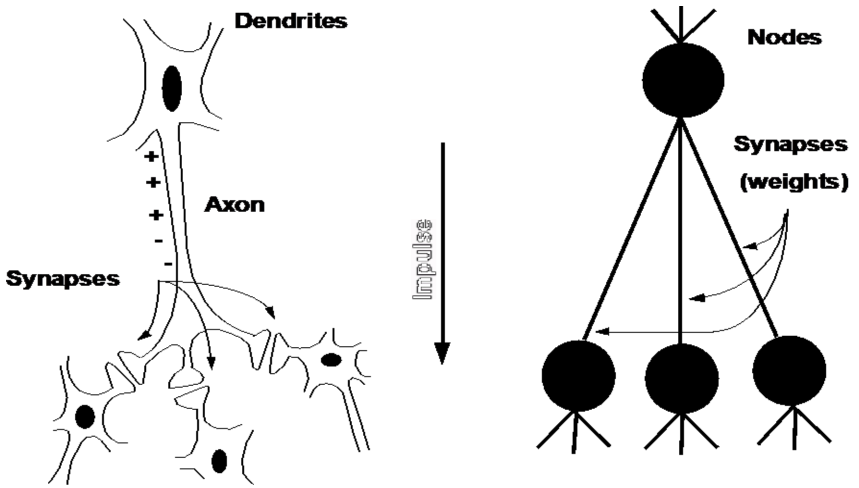


- Artificial neuron networks
  - supervised learning
  - gradient descent



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



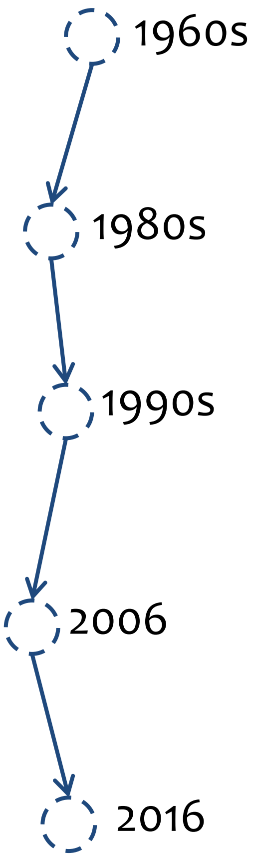
Motivation

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

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 data:

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

Face *Face* *Not a face*

2. Choose each of these:
   – Decision function

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

   – Loss function

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

Examples: Linear regression, Logistic regression, Neural Network

Examples: Mean-squared error, Cross Entropy

Background

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

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!

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

B

1.

2. Choose each of these:

– Decision function

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

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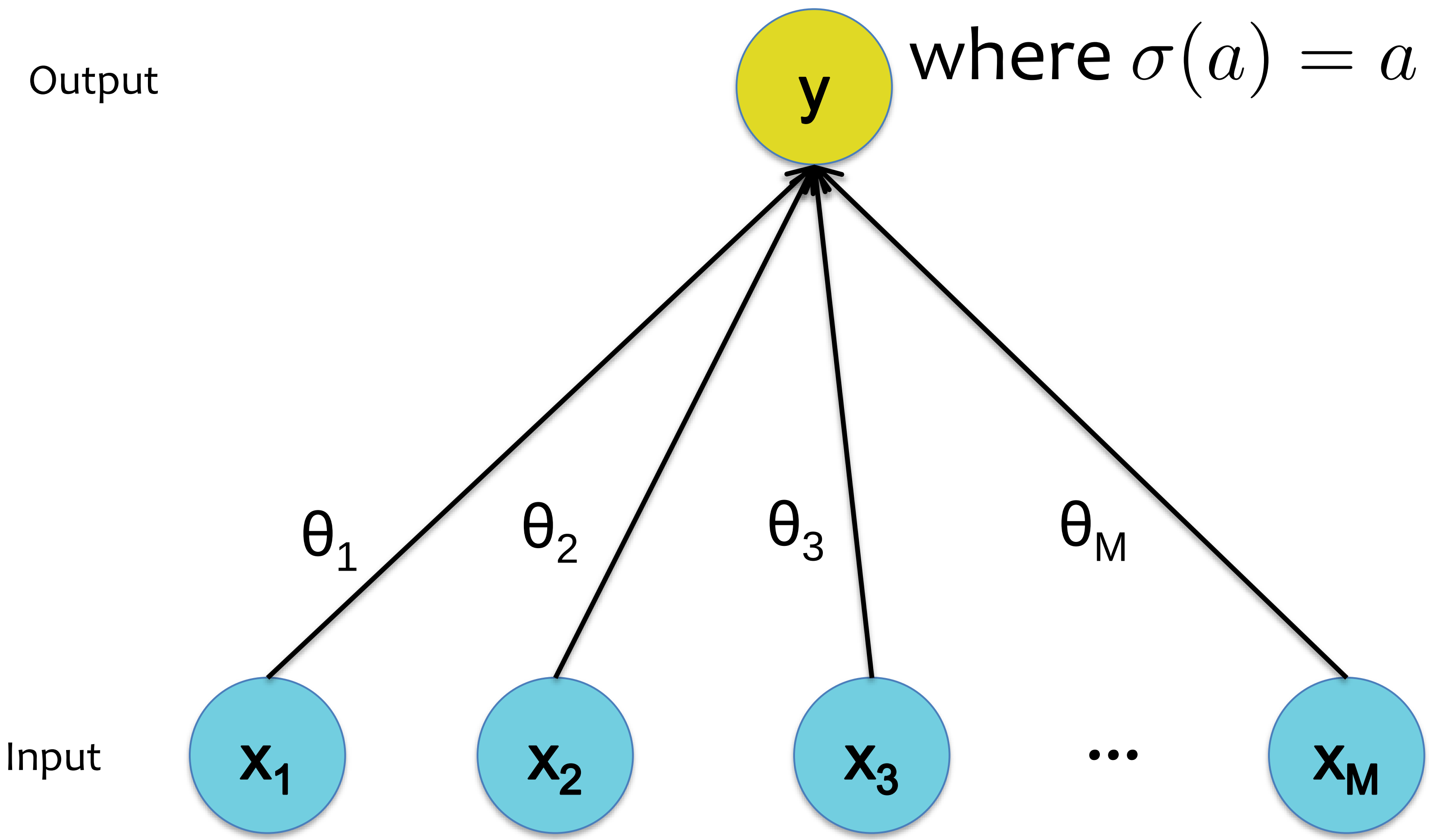
Linear Regression

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

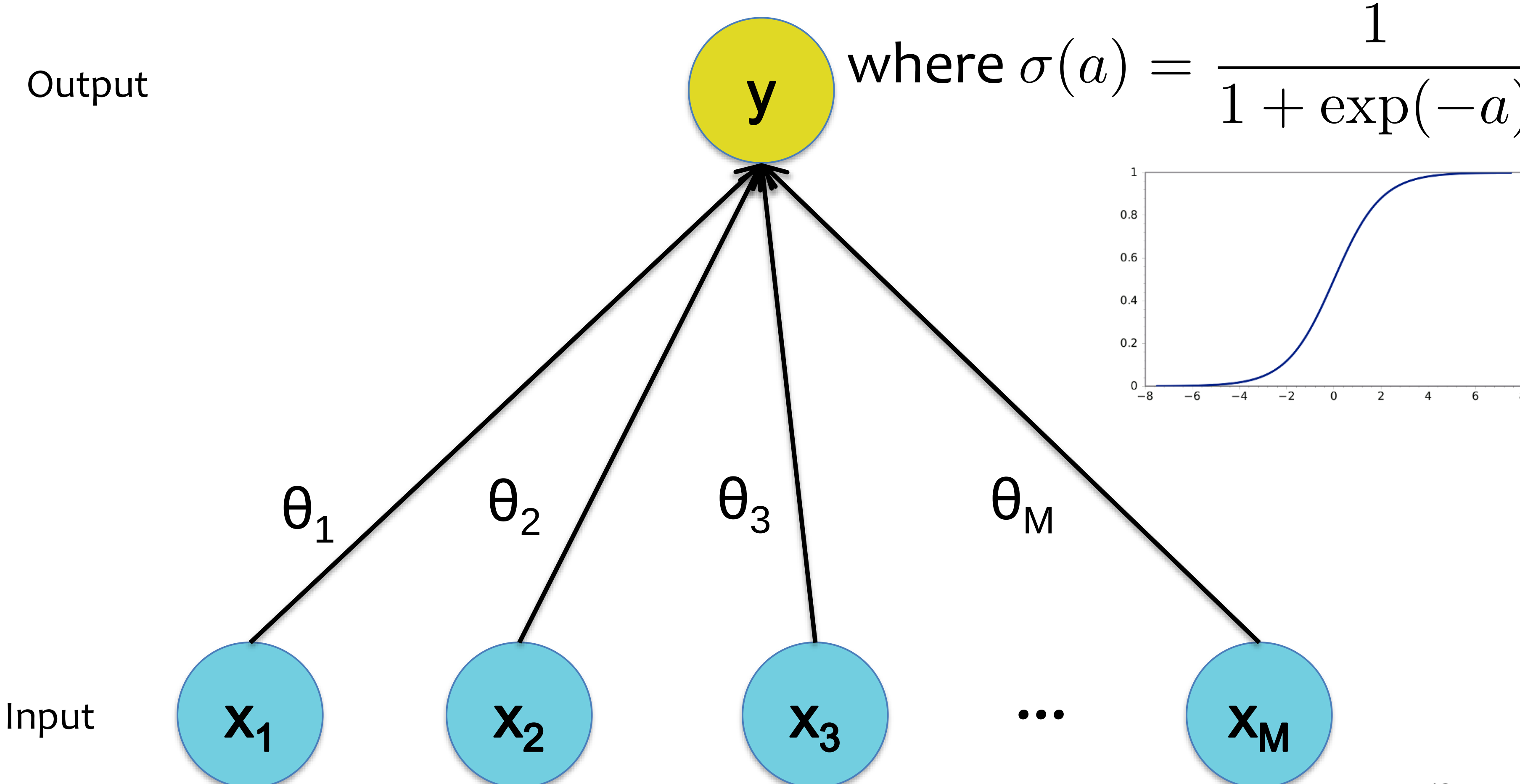
where $\sigma(a) = a$



Logistic Regression

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

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



Decision Functions

Logistic Regression

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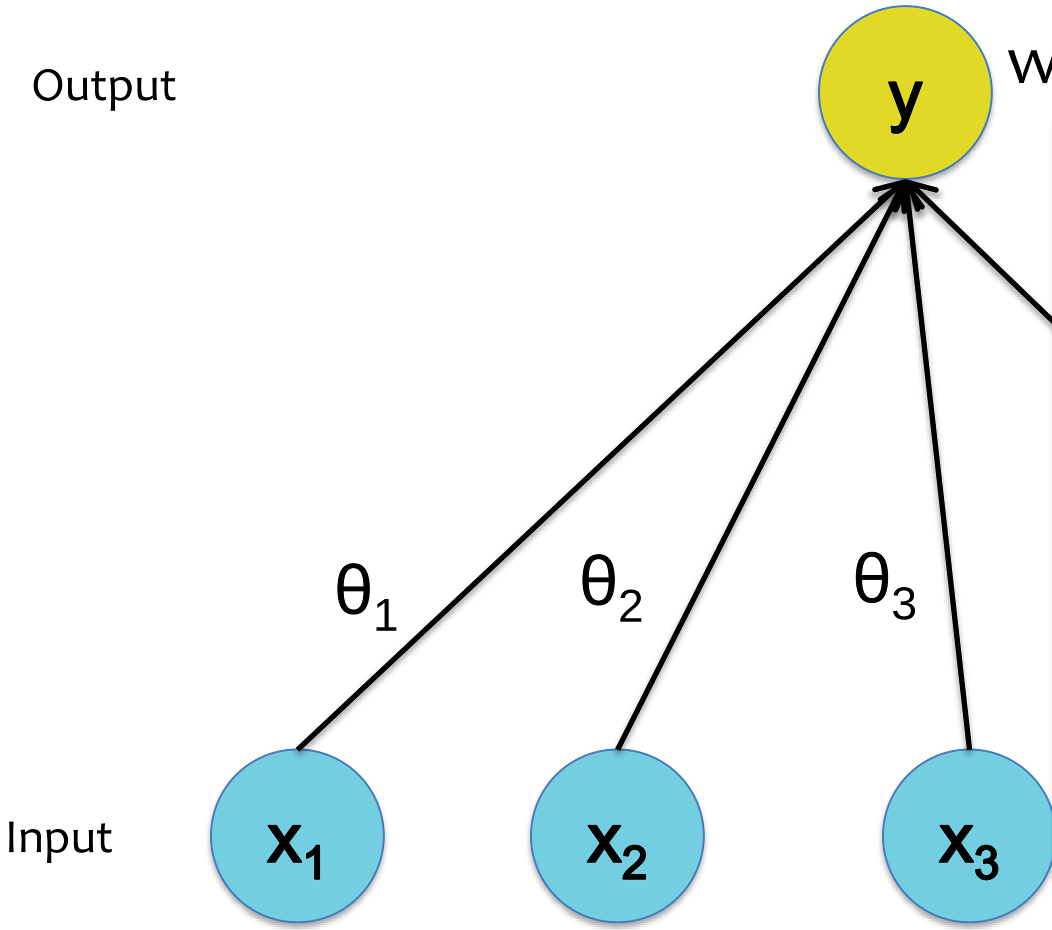

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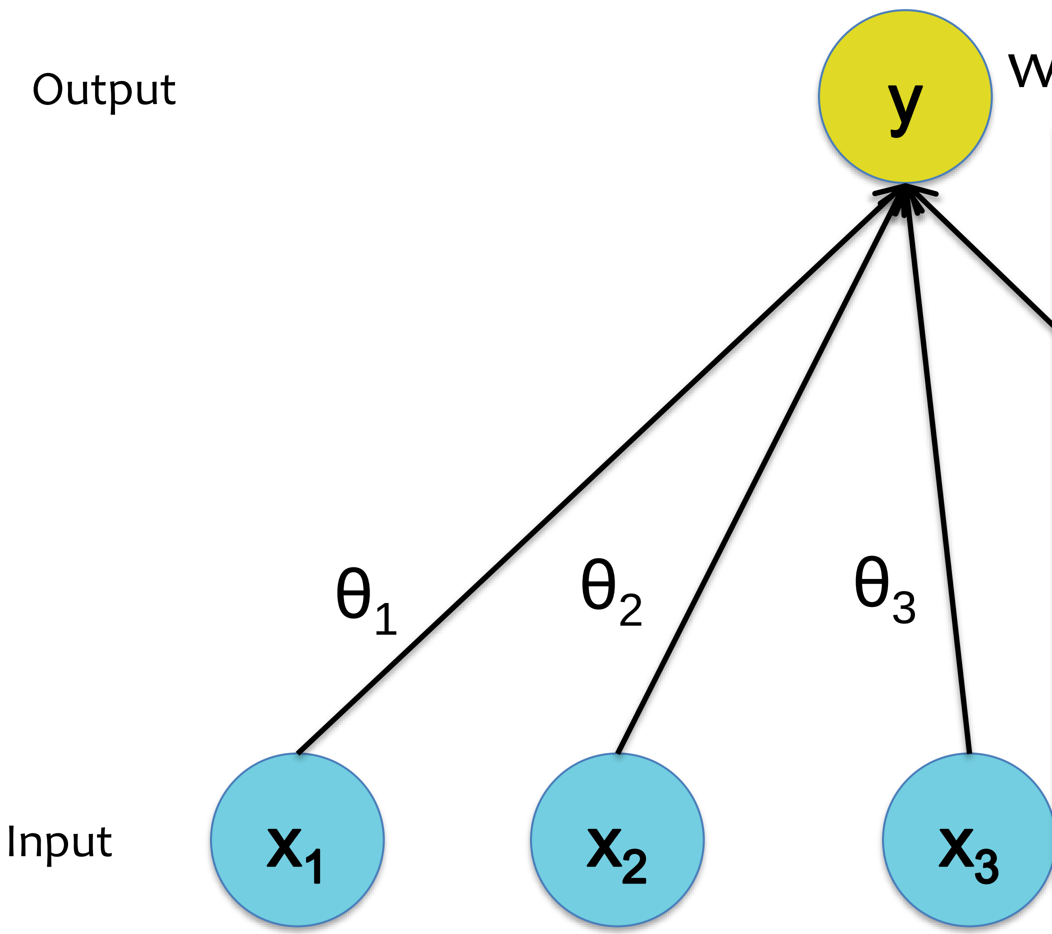

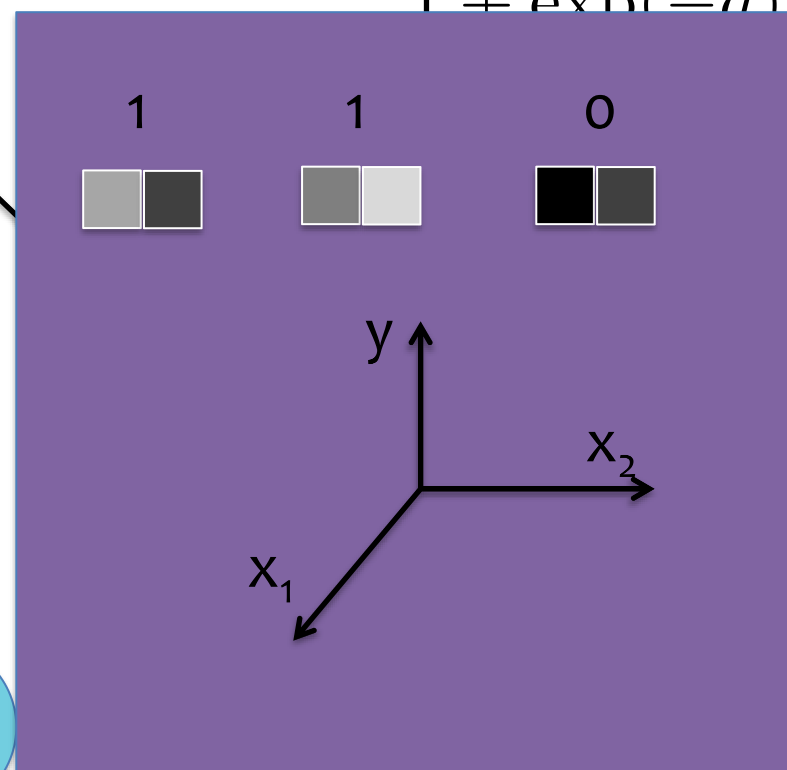

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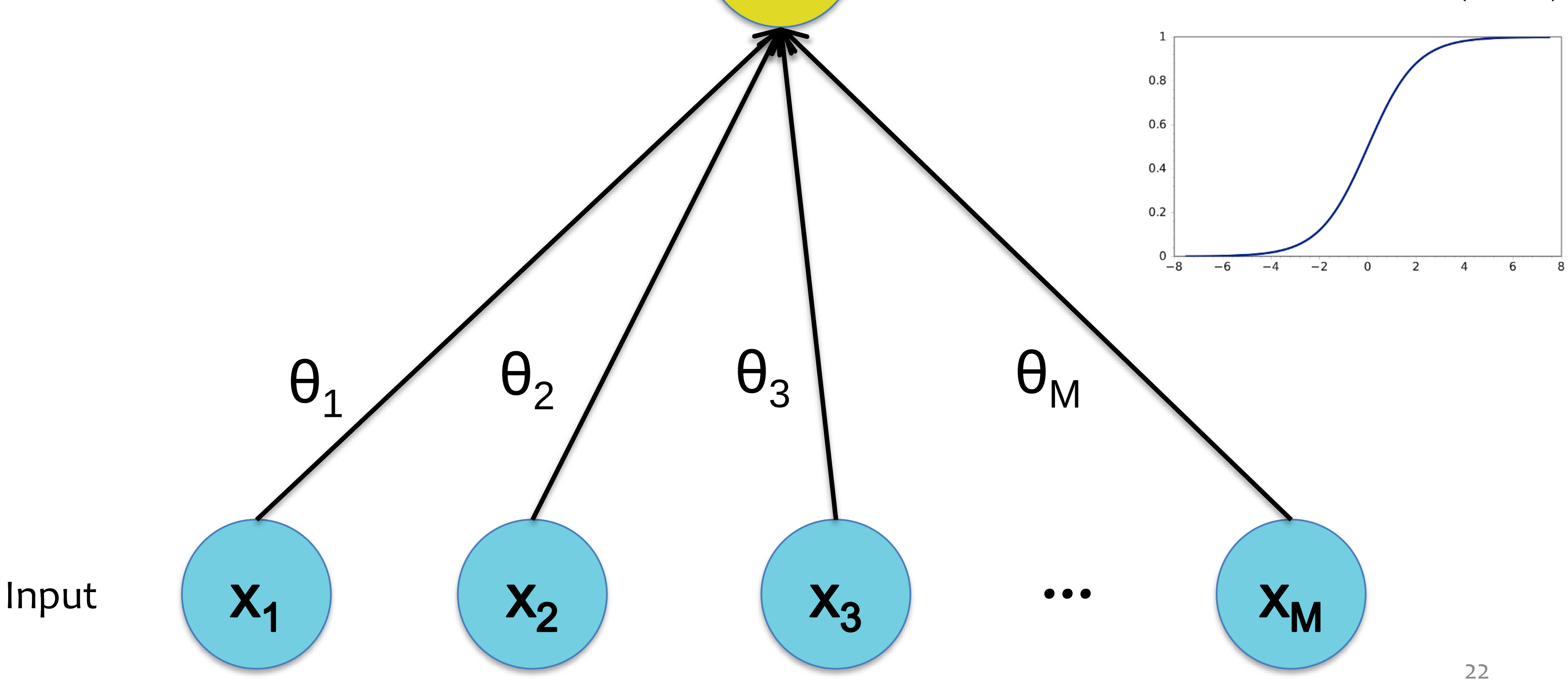
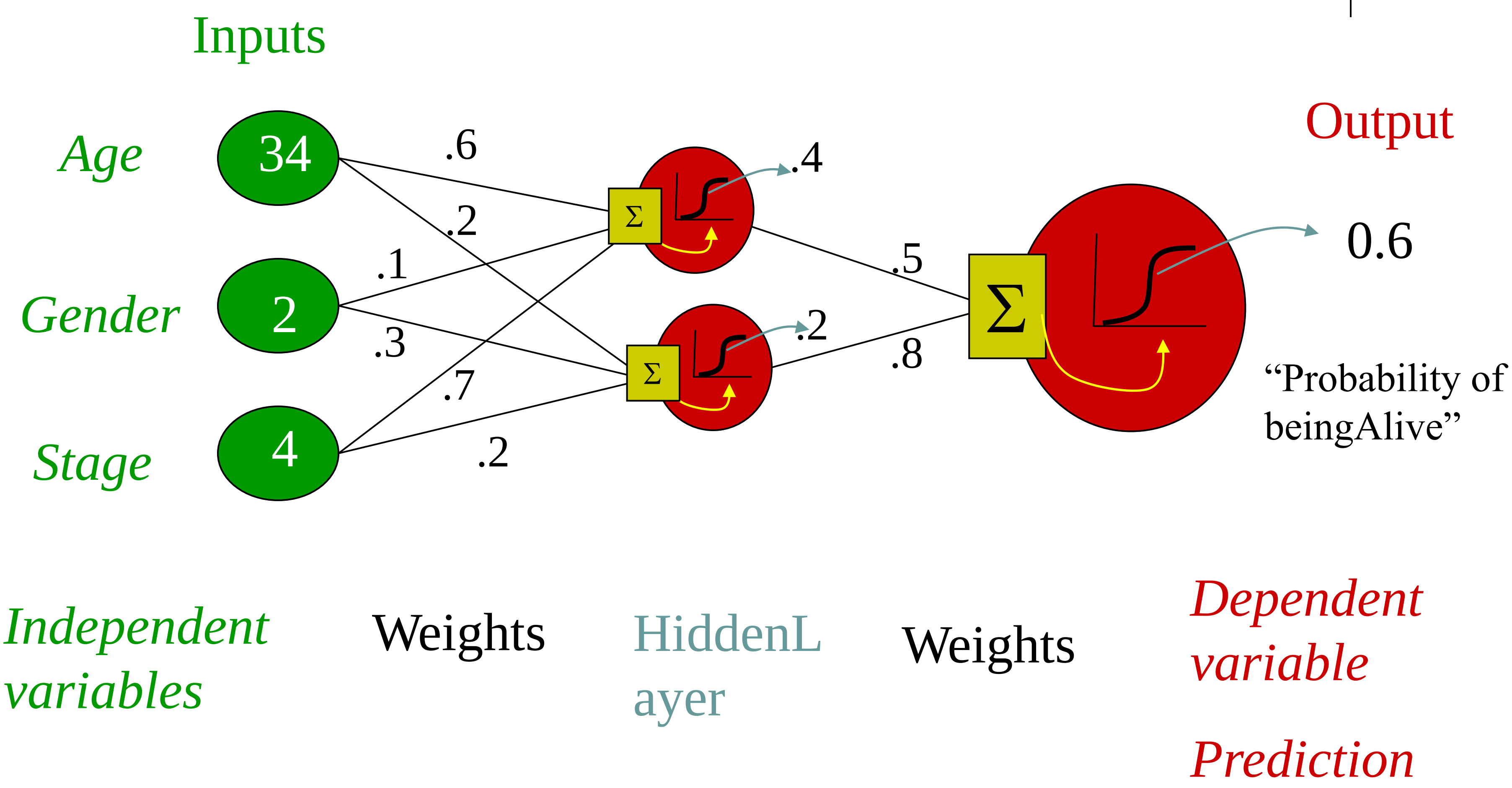
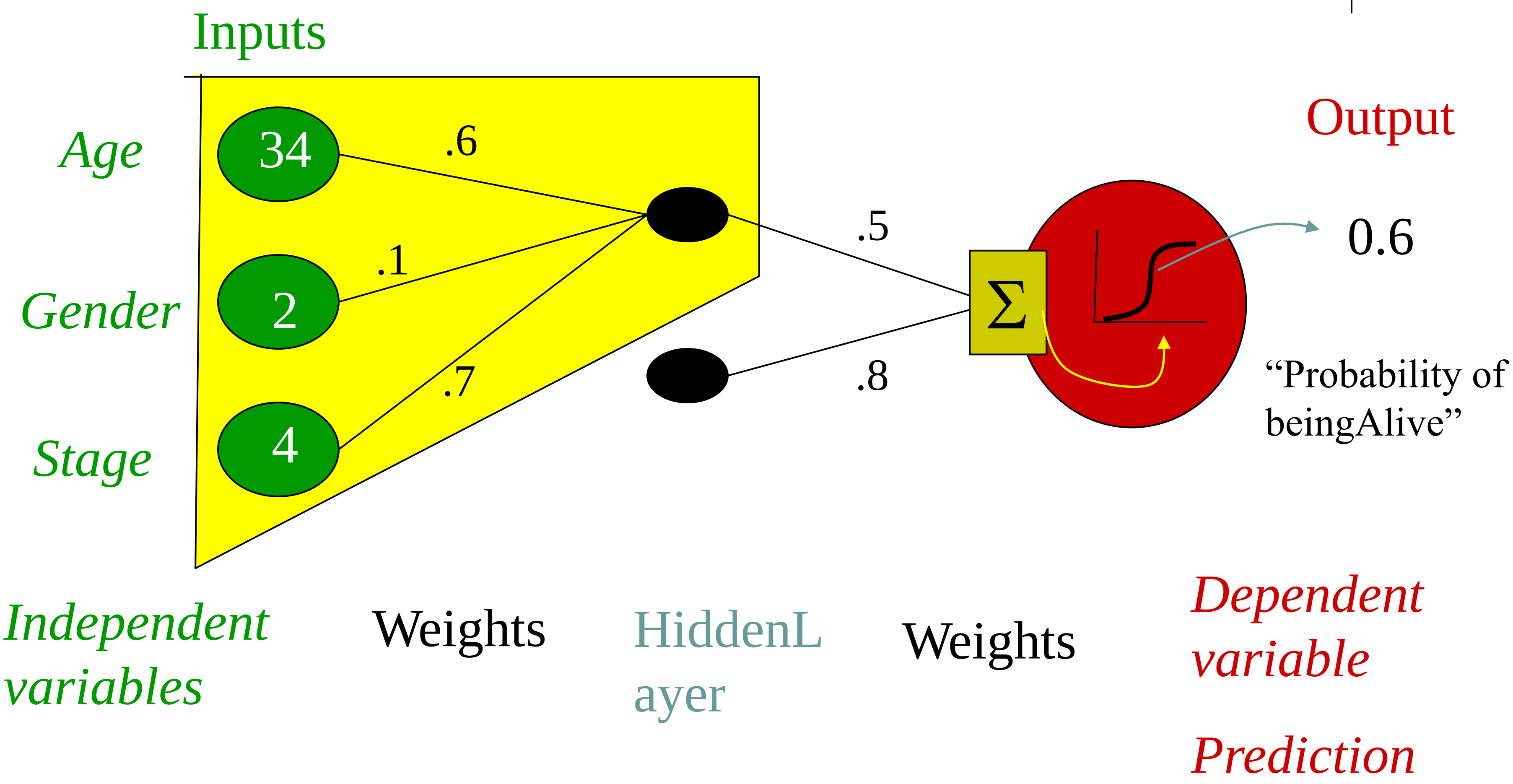
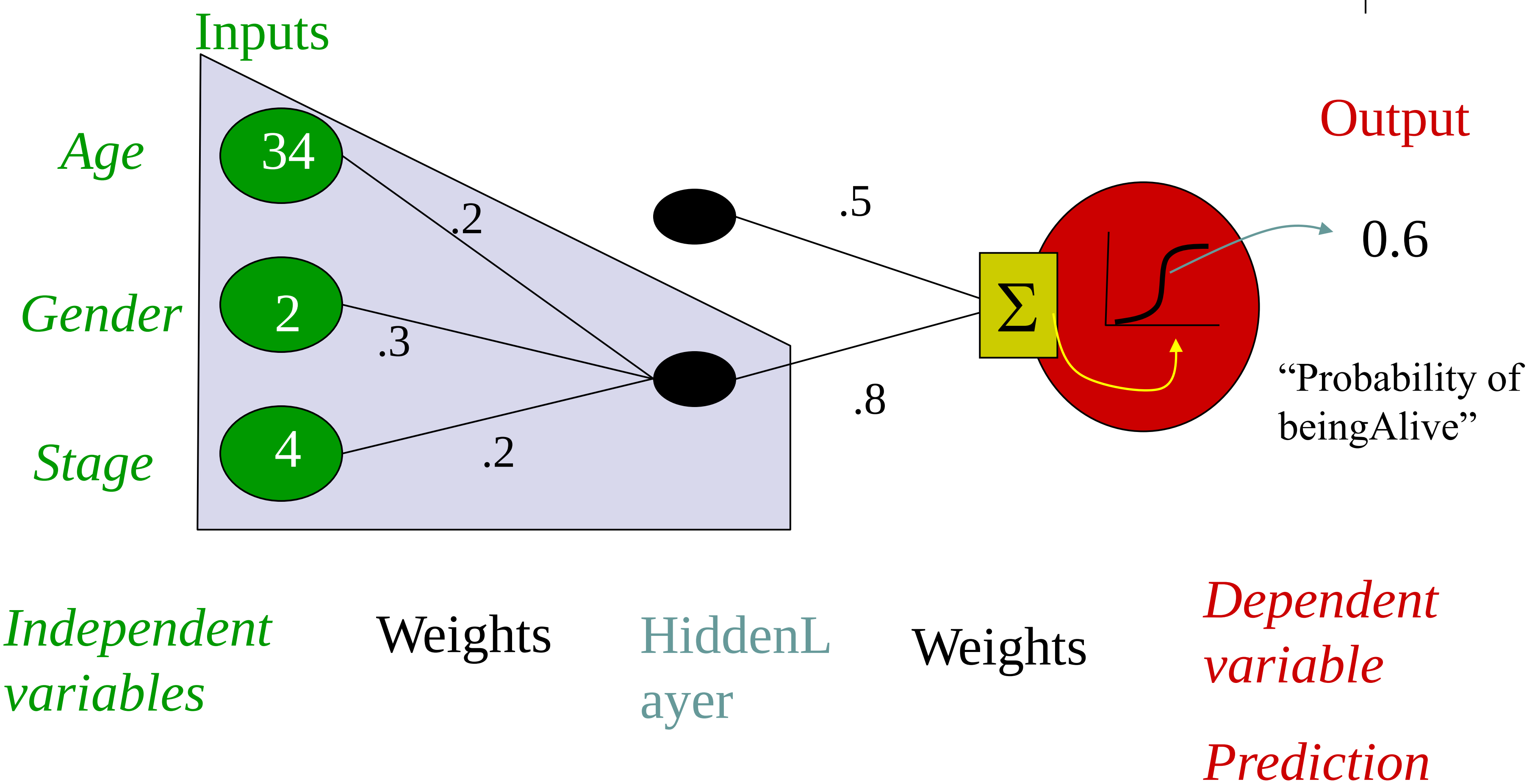


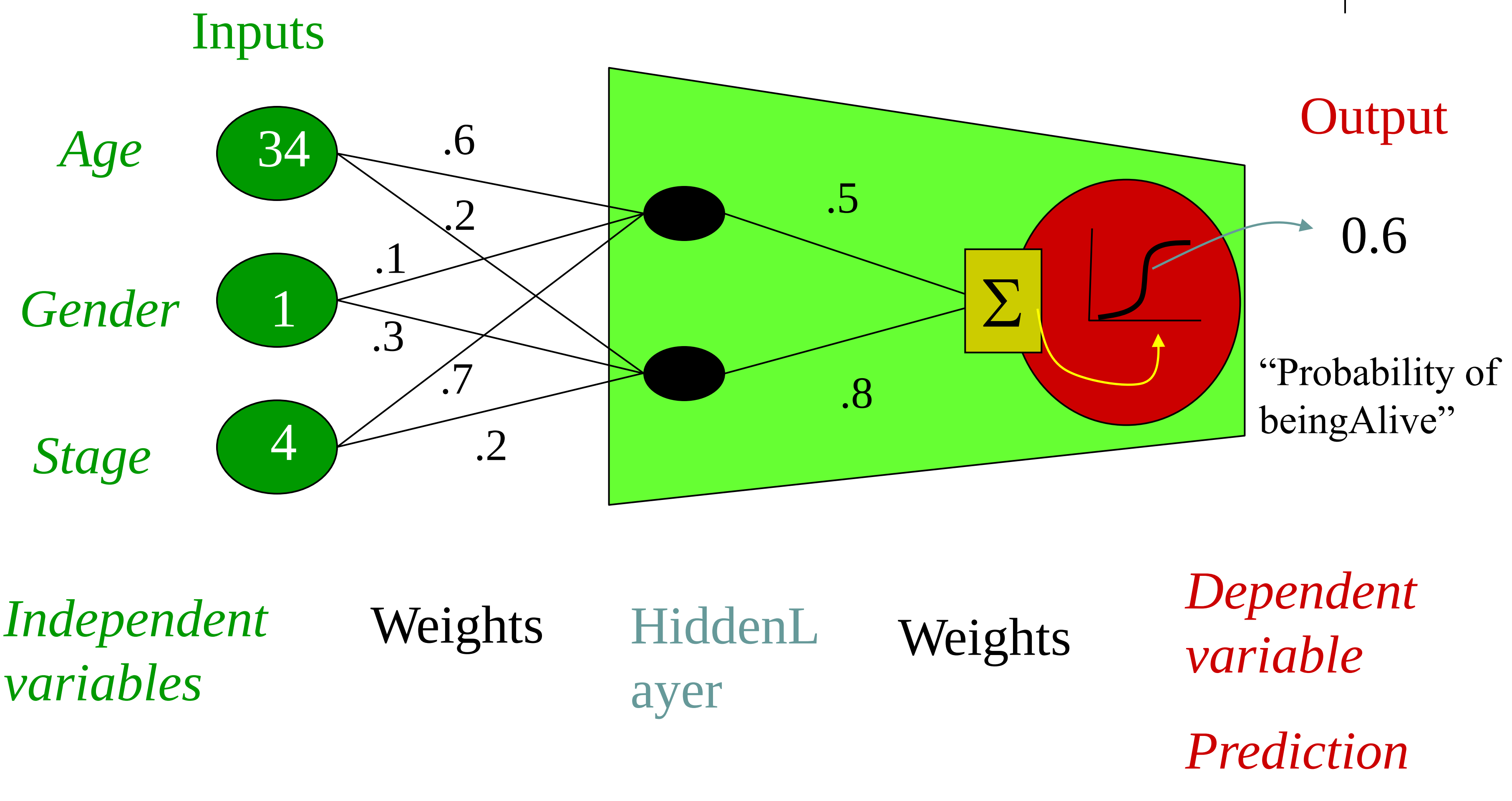
Neural Network Model



"Combined logistic models"




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


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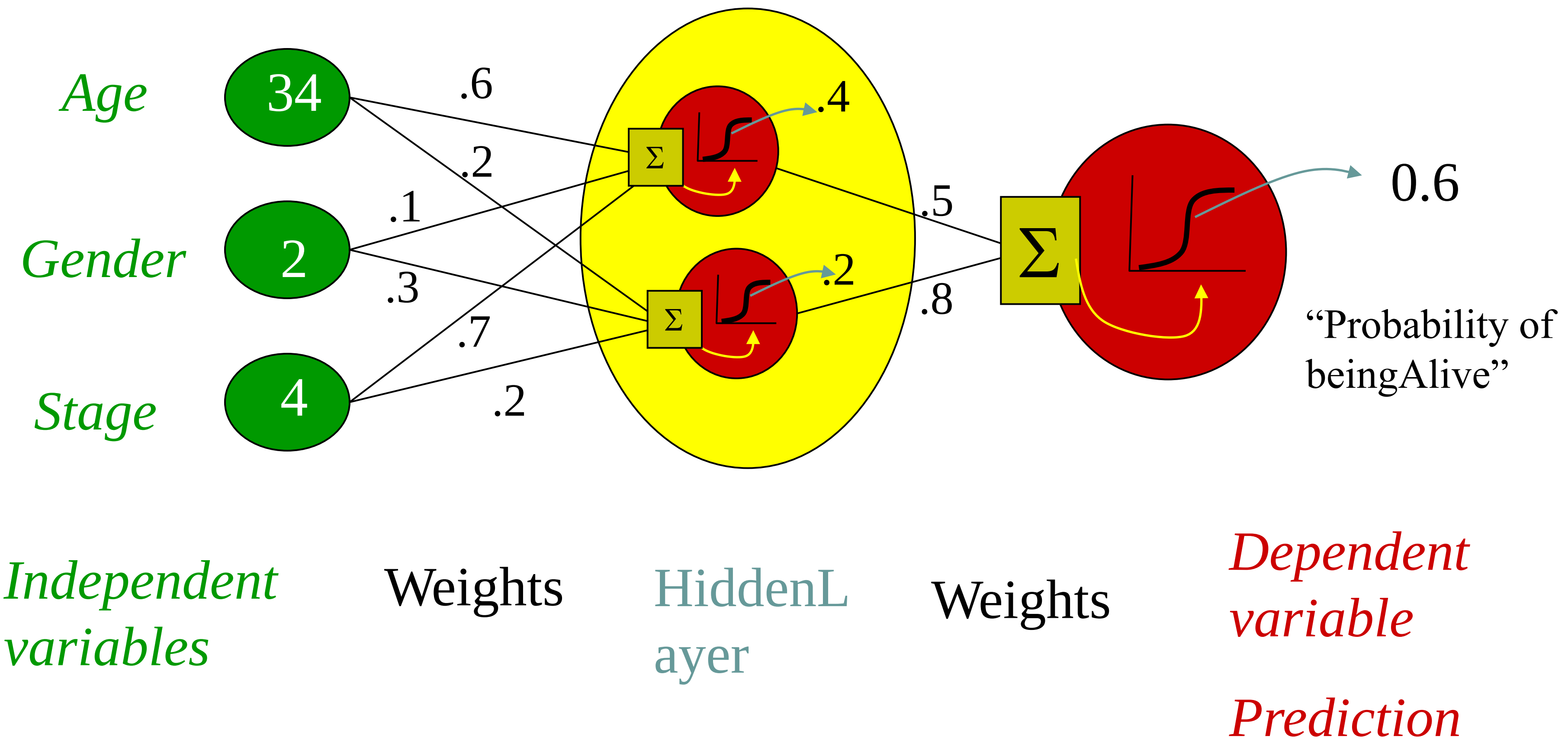
Prediction

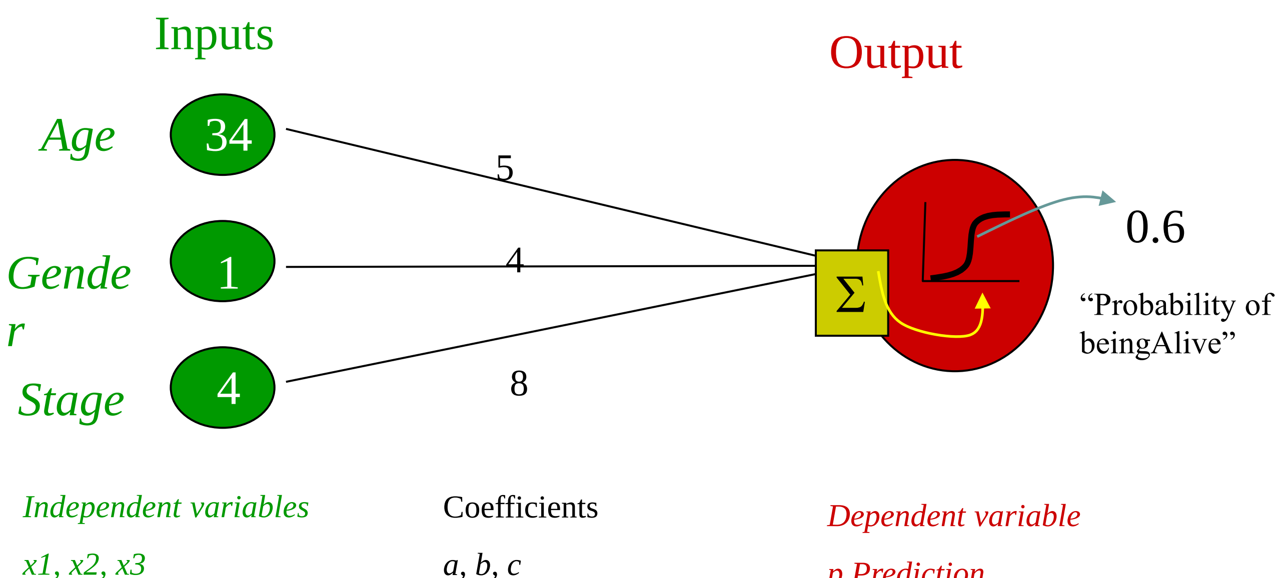
Not really, no target for hidden units...



Jargon Pseudo-Correspondence

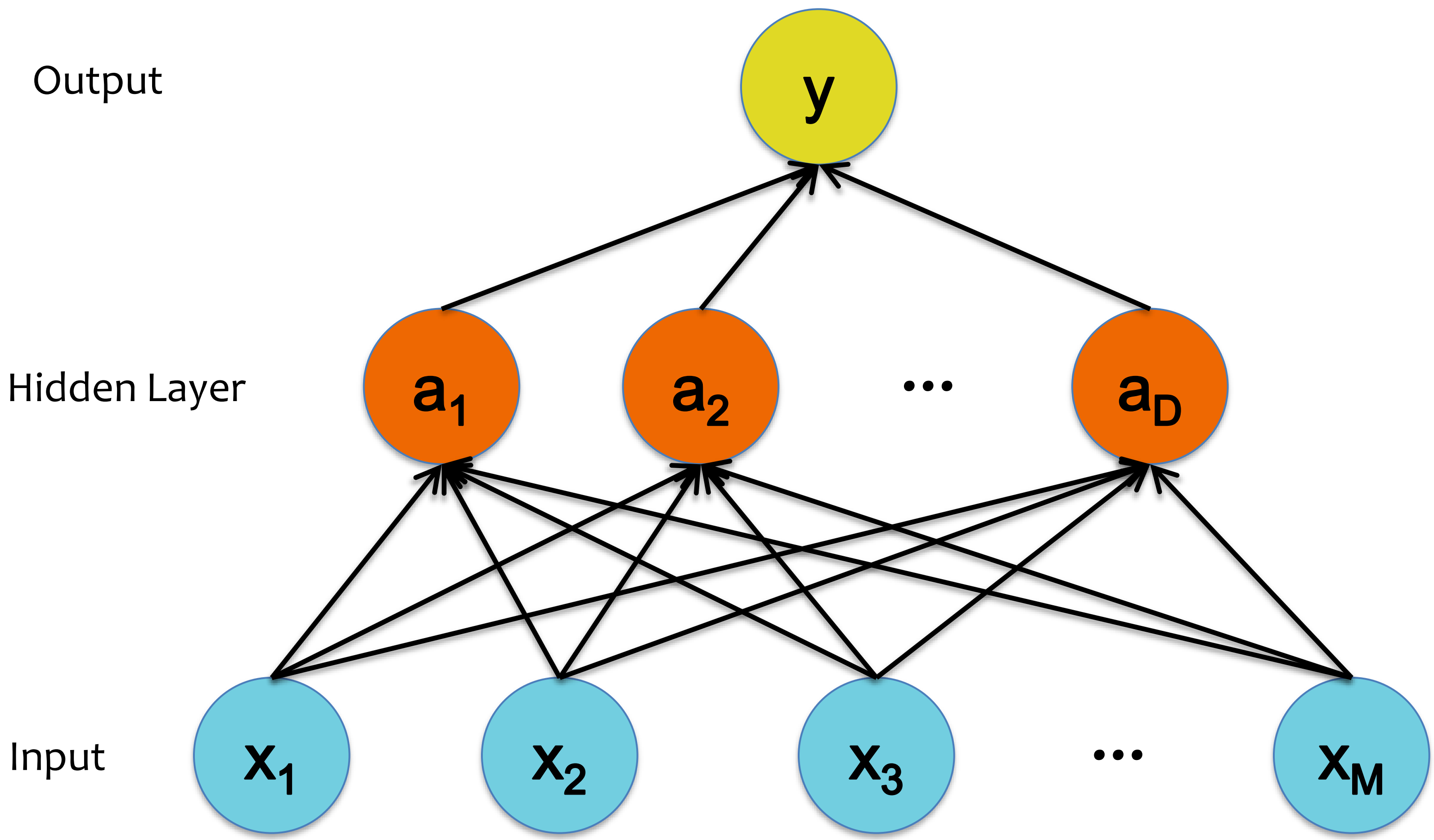
- Independent variable = input variable
- Dependent variable = output variable
- Coefficients = “weights”
- Estimates = “targets”

Logistic Regression Model (the sigmoid unit)



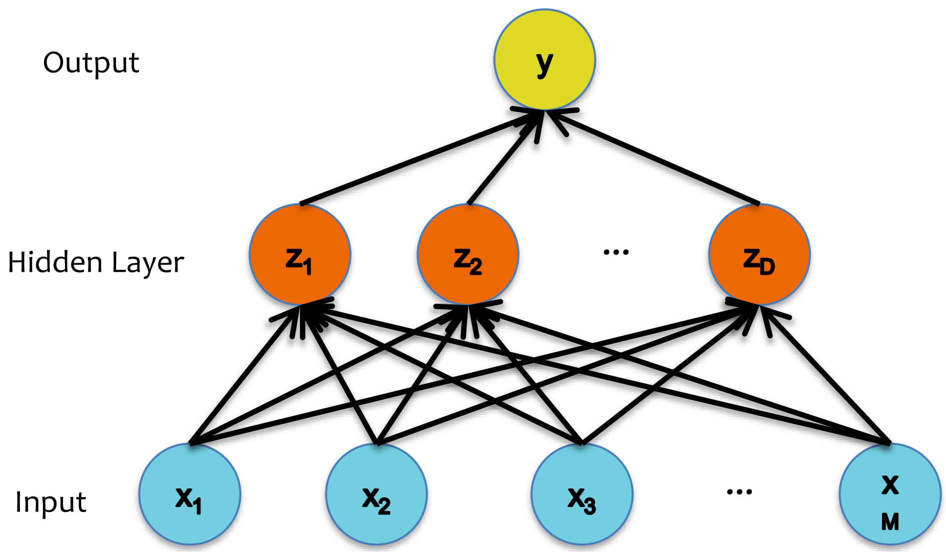
Decision Functions

Neural Network



Decision Functions

Neural Network



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

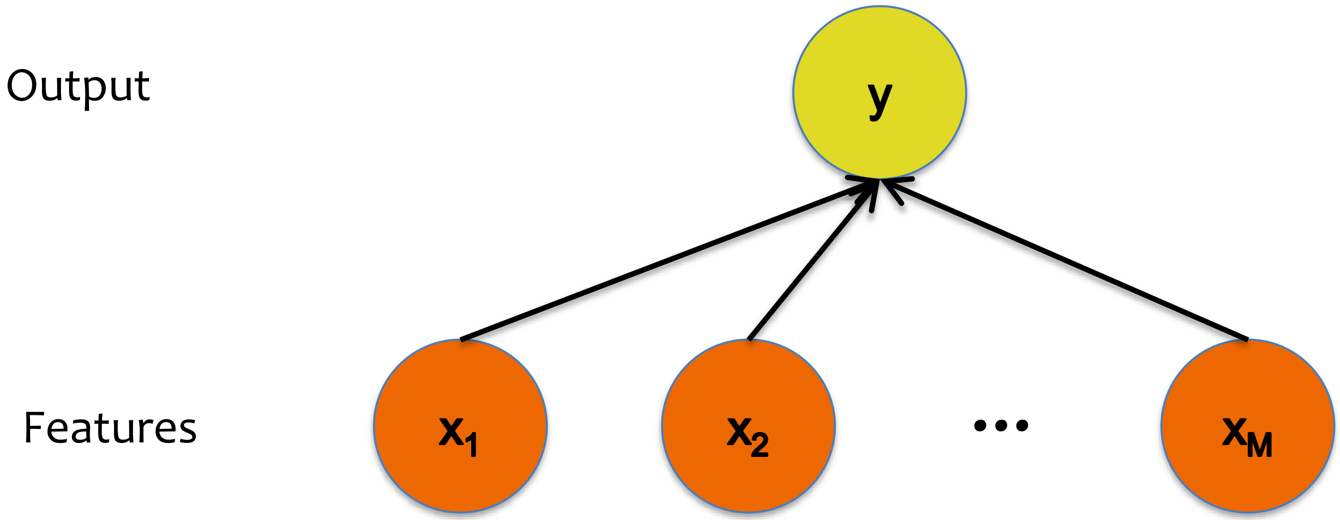
(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

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

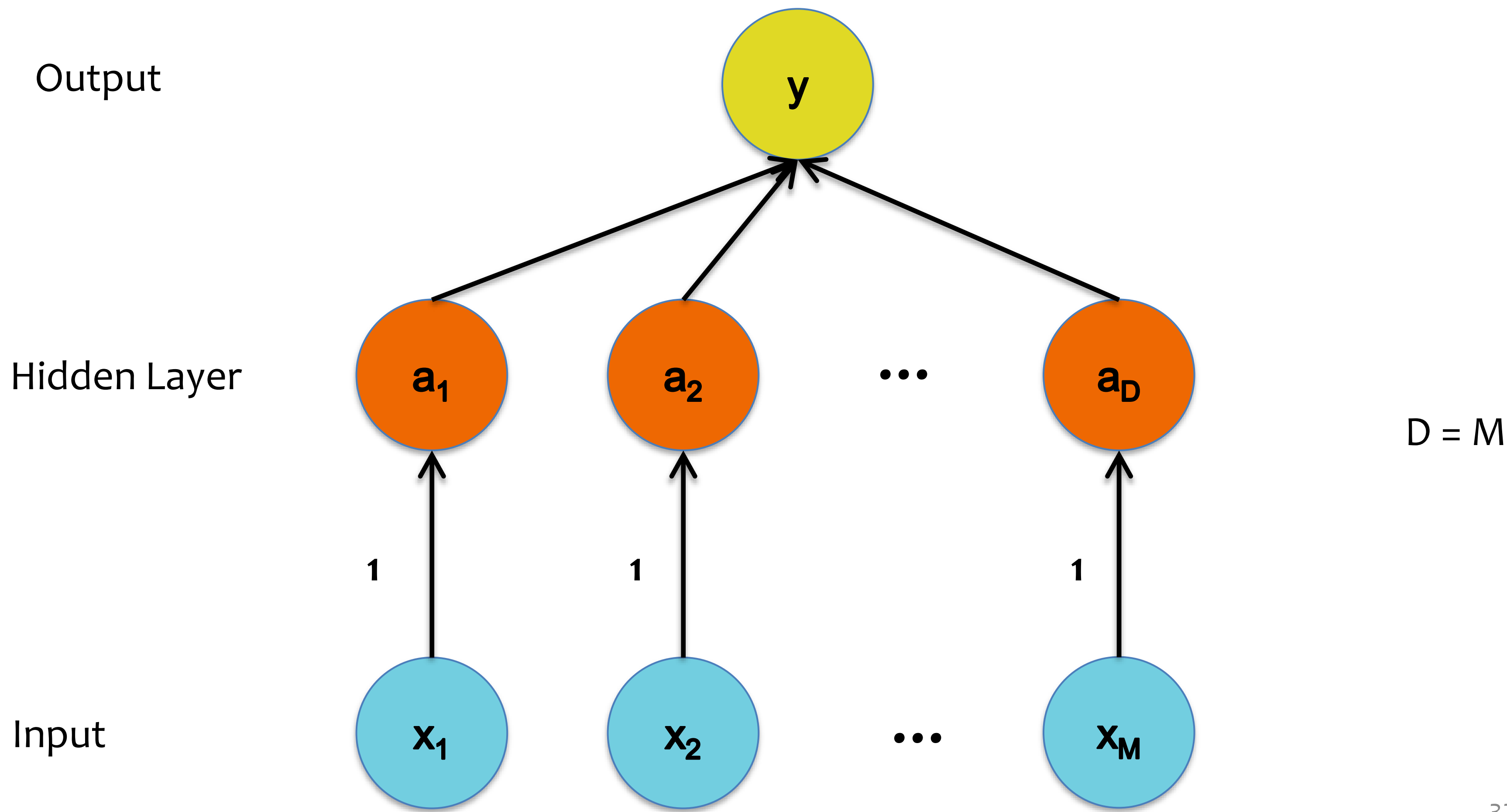
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \quad \forall j$

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

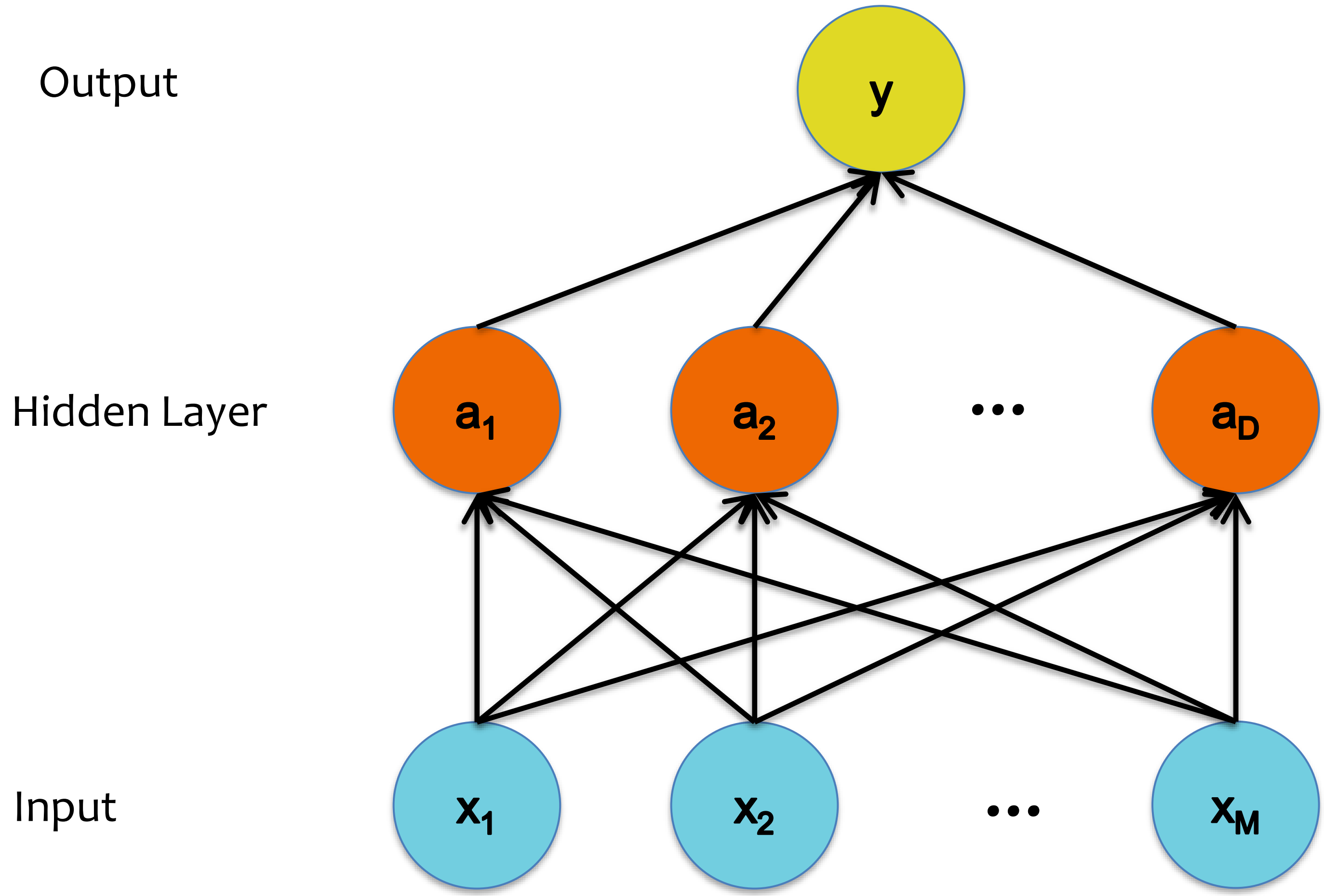
Building a Neural Net



Building a Neural Net

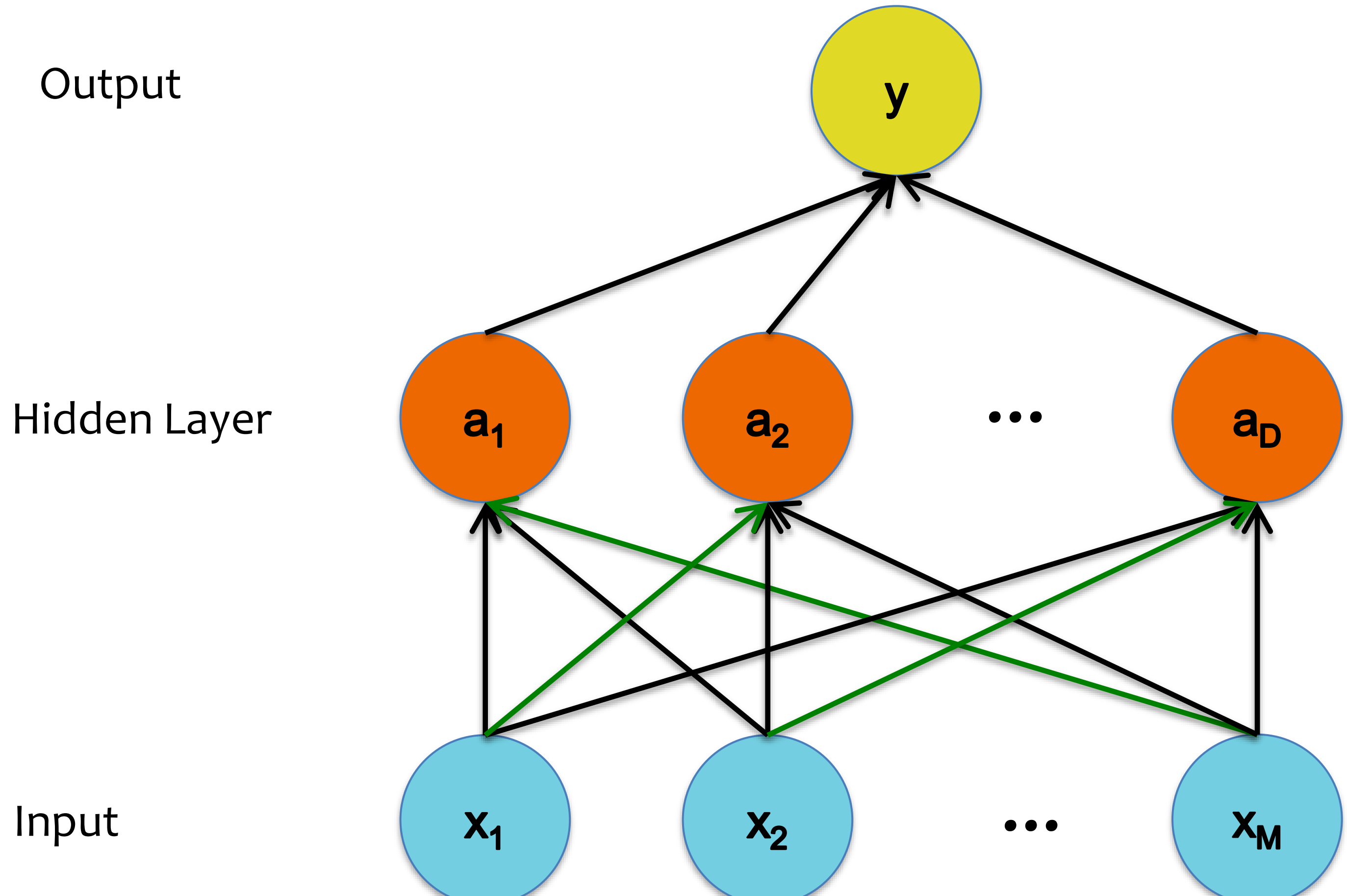


Building a Neural Net



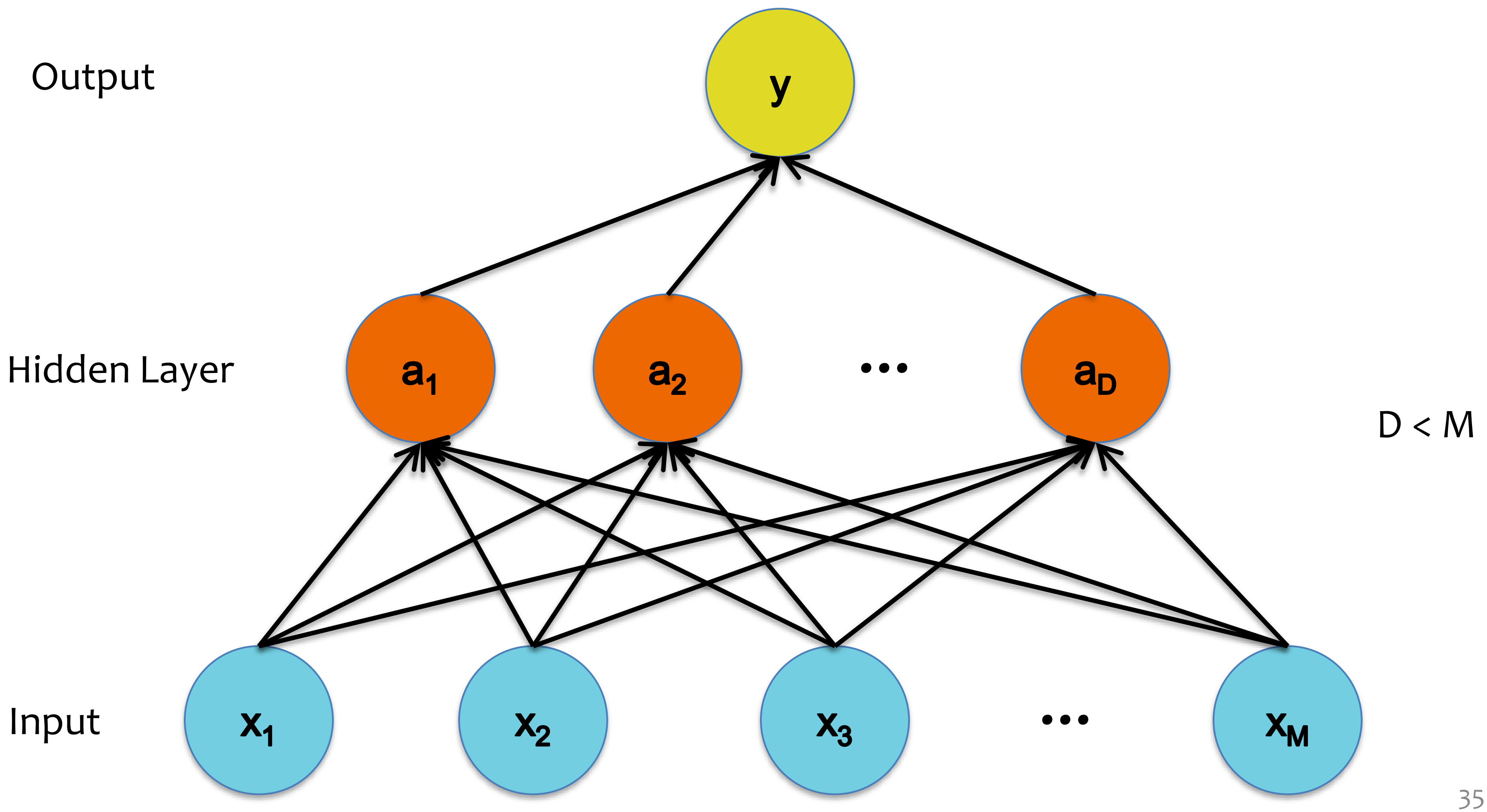
D = M

Building a Neural Net



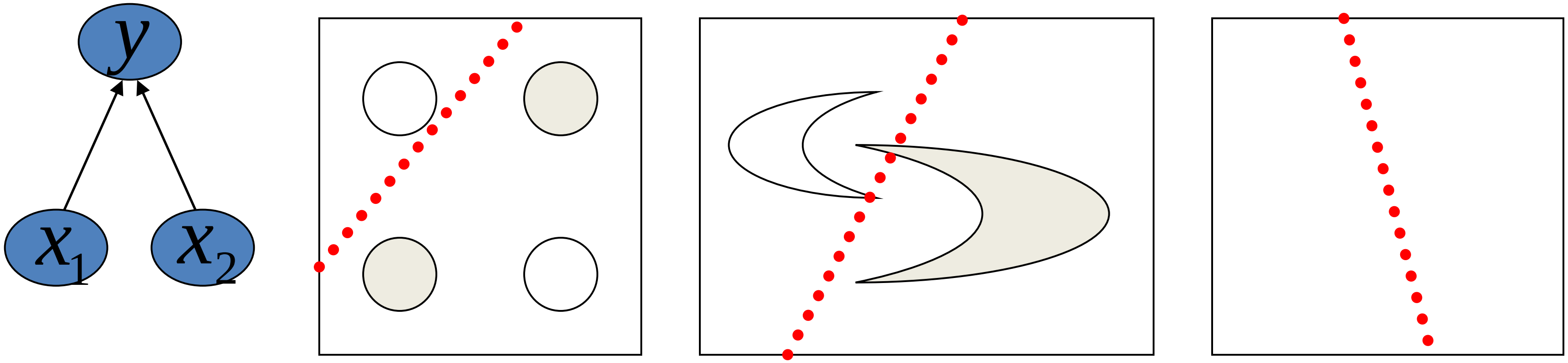
D = M

Building a Neural Net



Decision Boundary

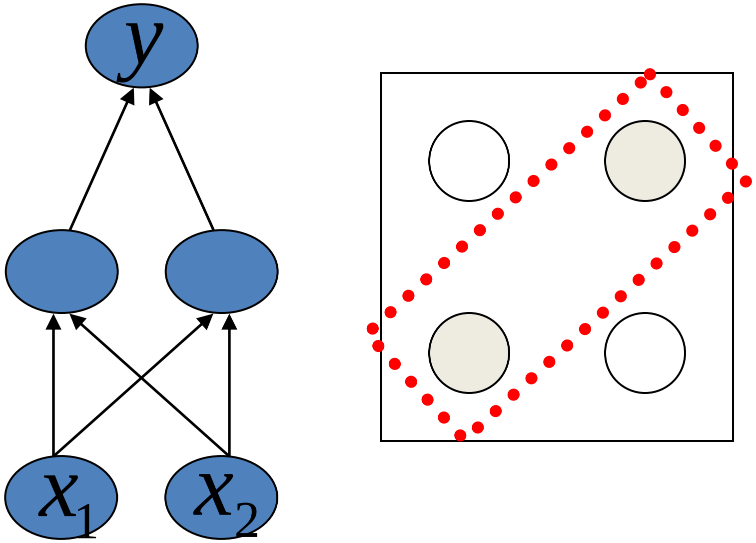
- 0 hidden layers: linear classifier
  - Hyperplanes



Example from to Eric Postma via Jason Eisner

Decision Boundary

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



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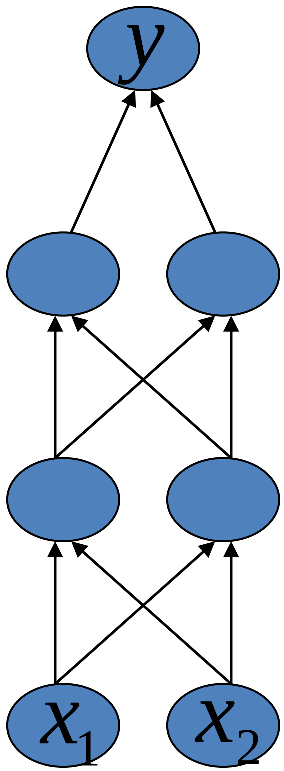
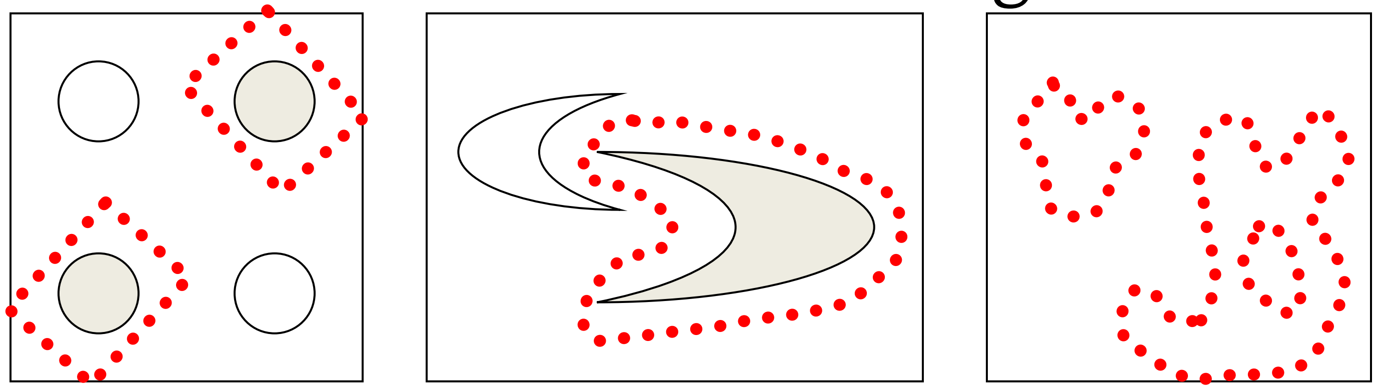
Decision Boundary



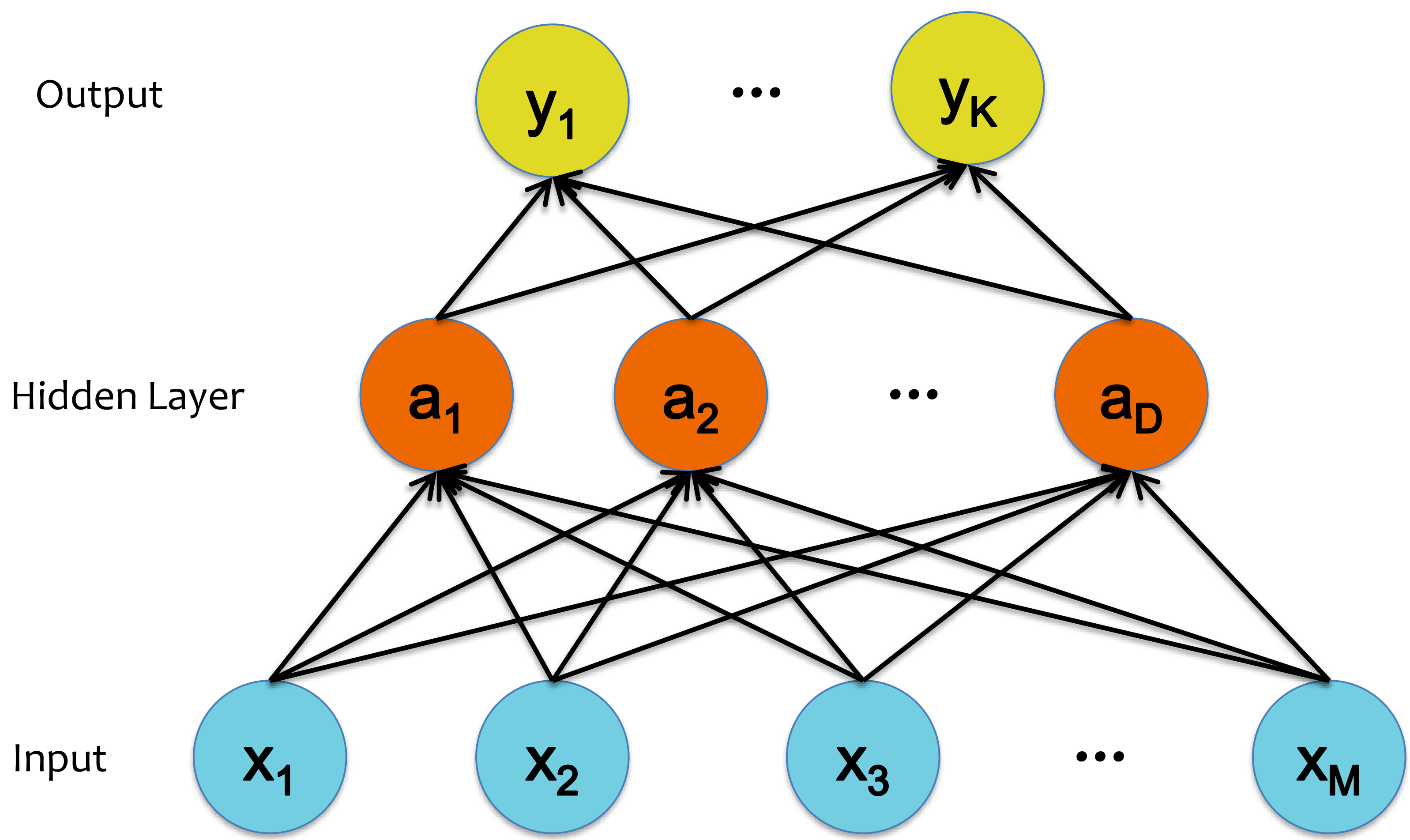
- 2 hidden layers
  - Combinations of convex regions



Example from to Eric Postma via Jason Eisner

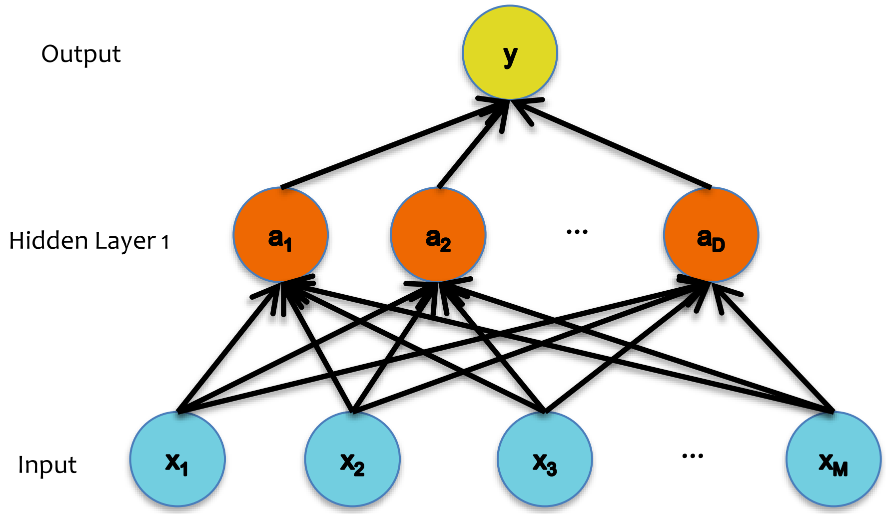
Decision Functions

Multi-Class Output



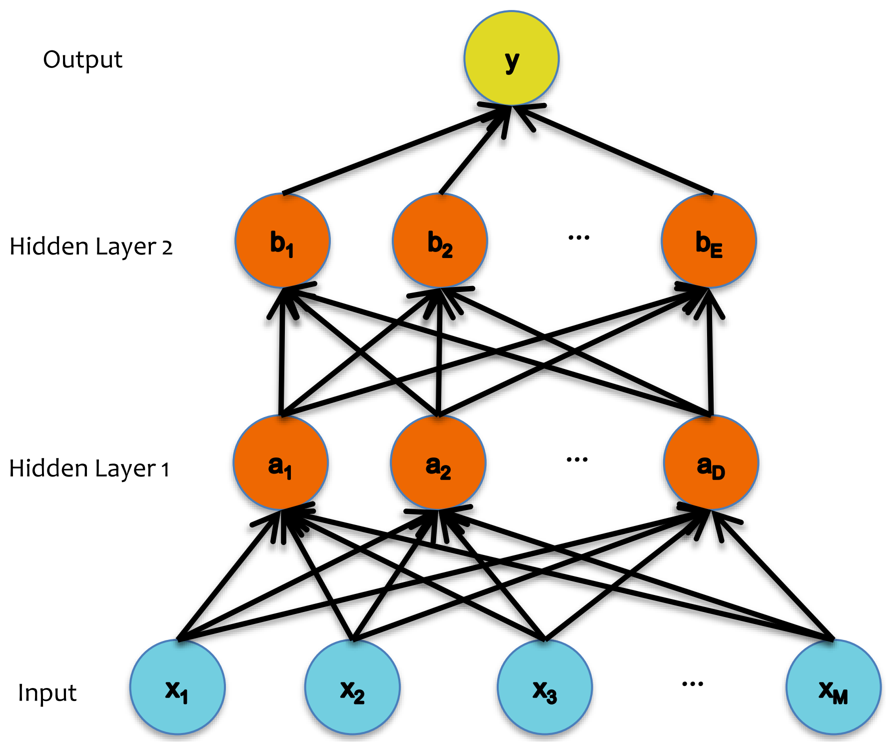
Deeper Networks

Next lecture:



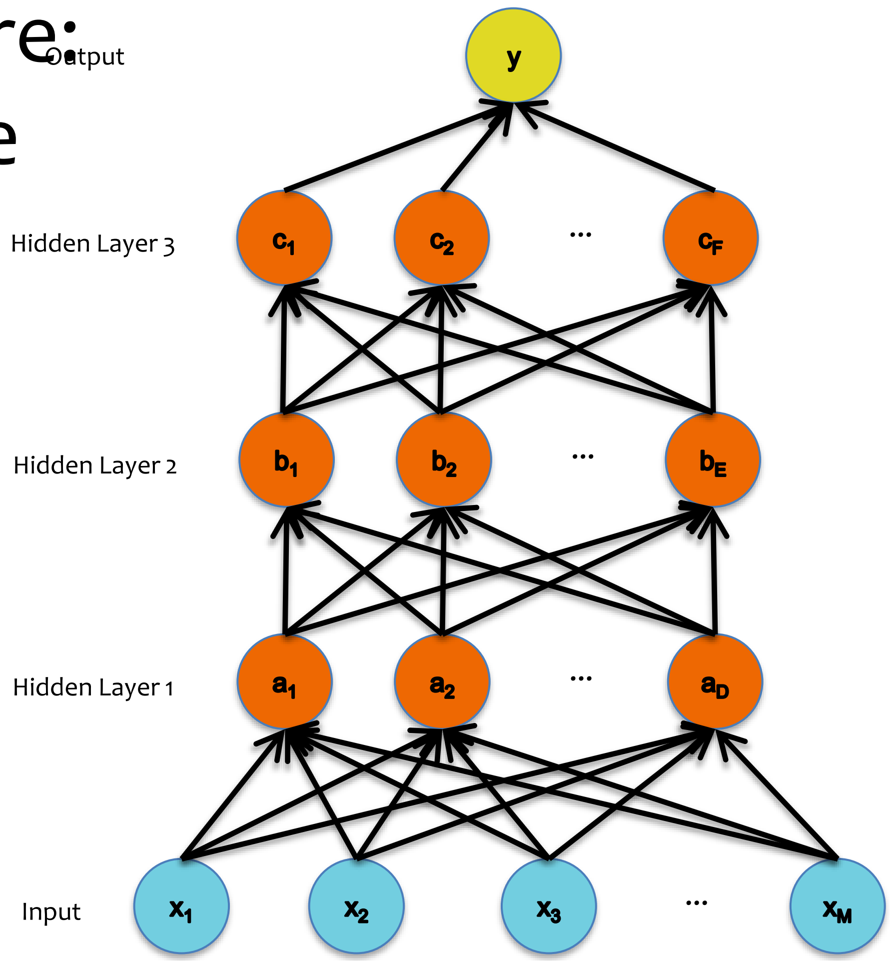
Deeper Networks

Next lecture:



Deeper Networks

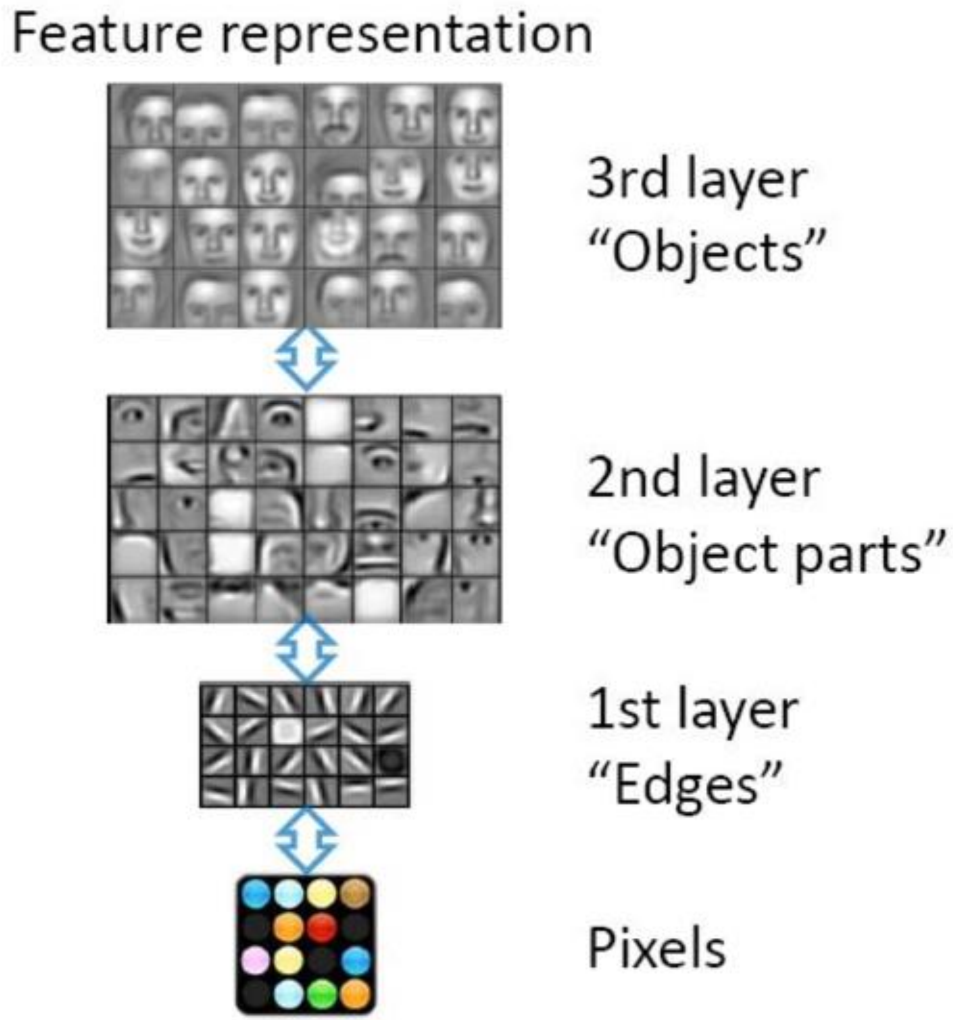
Next lecture: Making the neural networks deeper



Decision Functions

Different Levels of Abstraction

- We don’t know the “right” levels of abstraction
- So let the model figure it out!



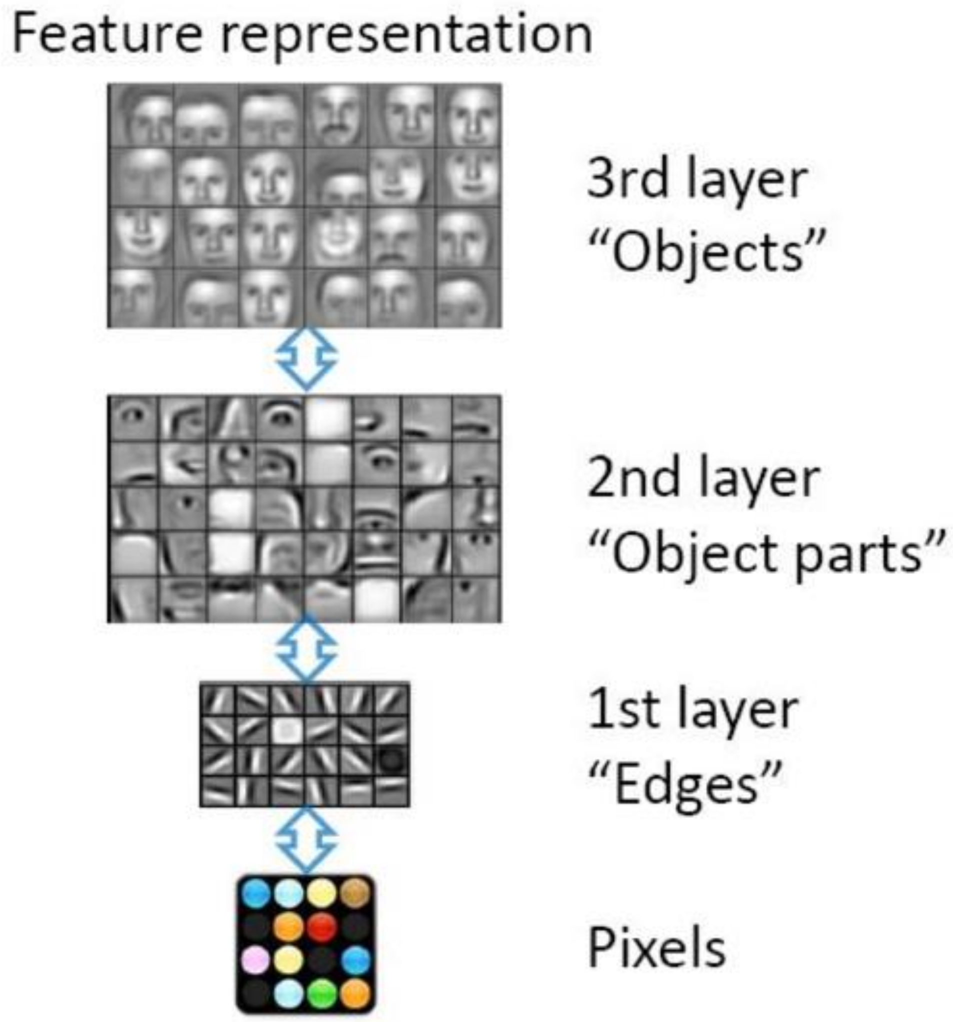
Example from Honglak Lee (NIPS 2010)

Decision Functions

Different Levels of Abstraction

Face Recognition:

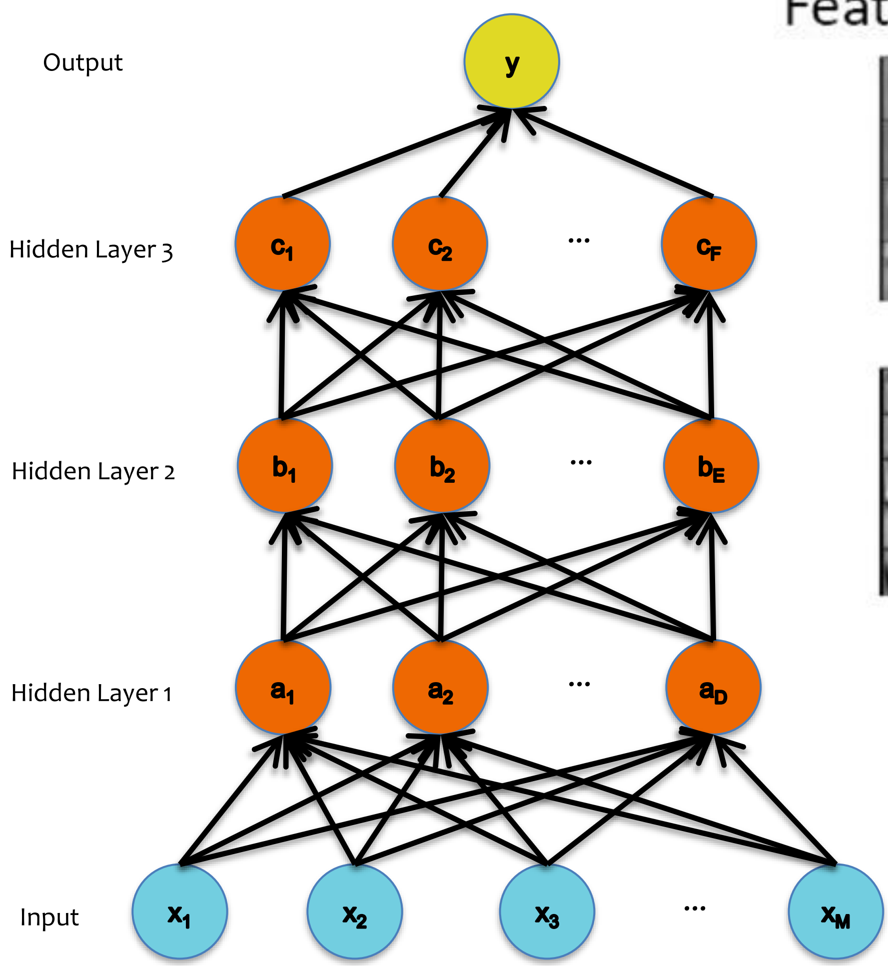
- Deep Network can build up increasingly higher levels of abstraction
- Lines, parts, regions

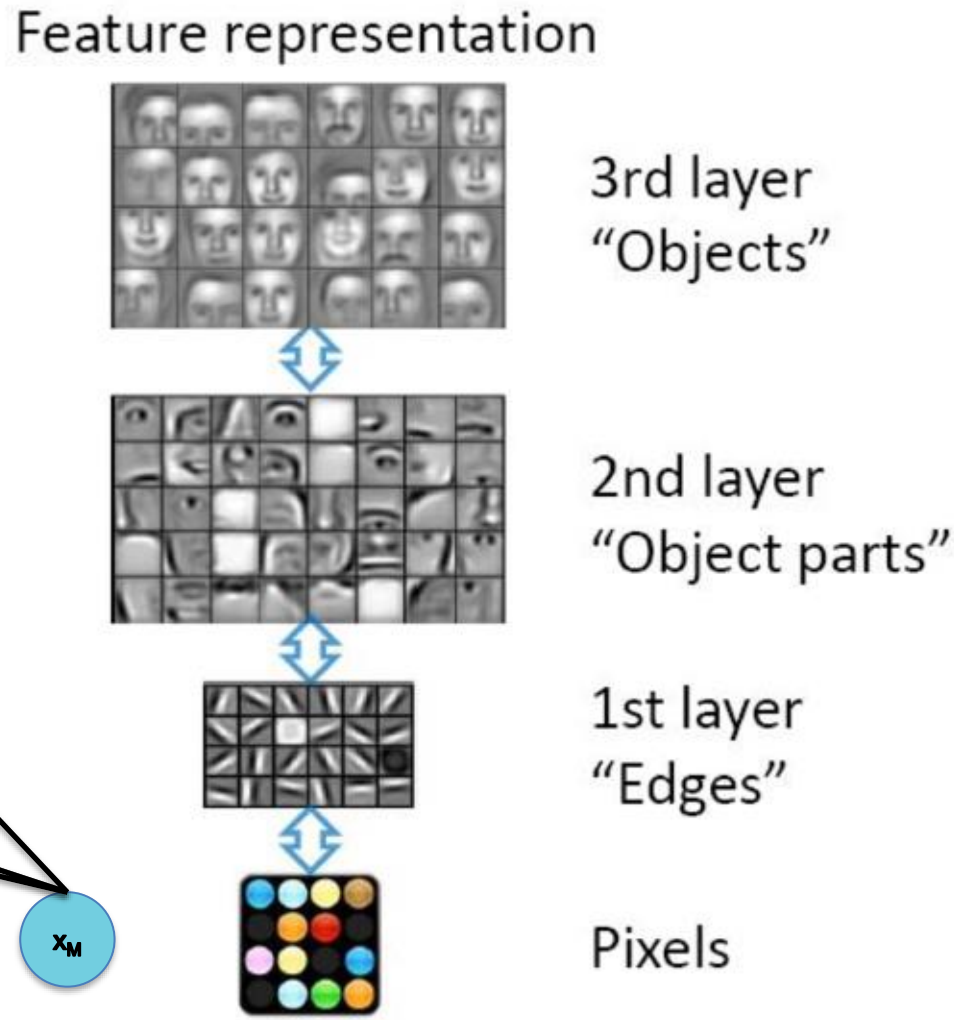


Example from Honglak Lee (NIPS 2010)

Decision Functions

Different Levels of Abstraction





Example from Honglak Lee (NIPS 2010)

ARCHITECTURES

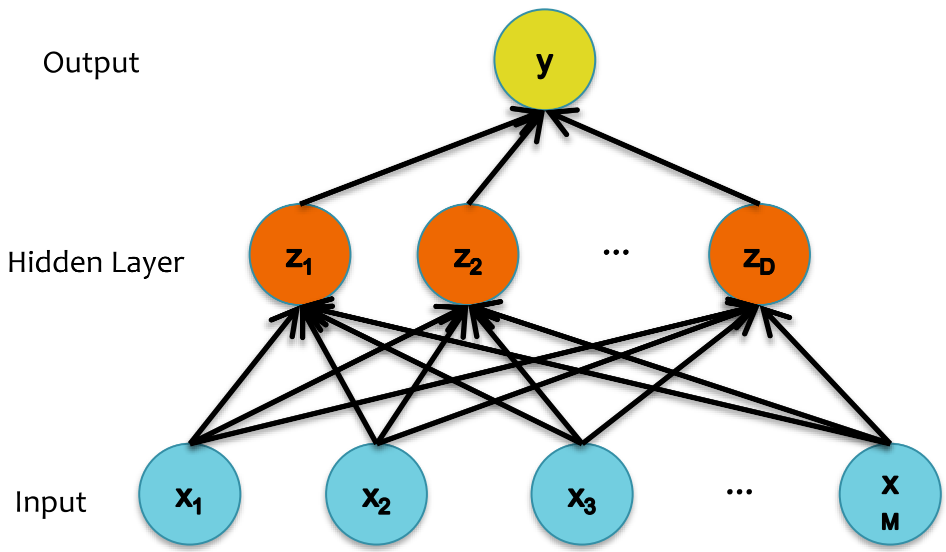
Neural Network Architectures

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

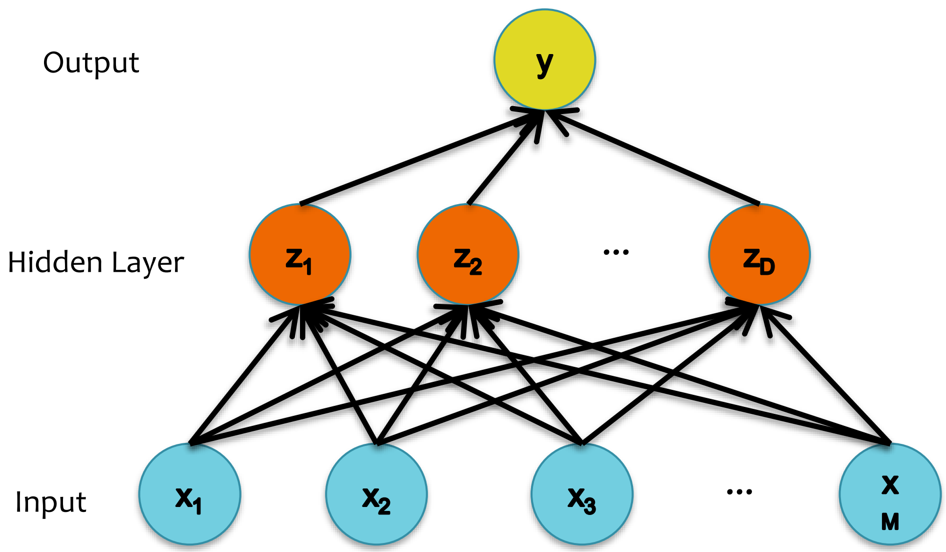
(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

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

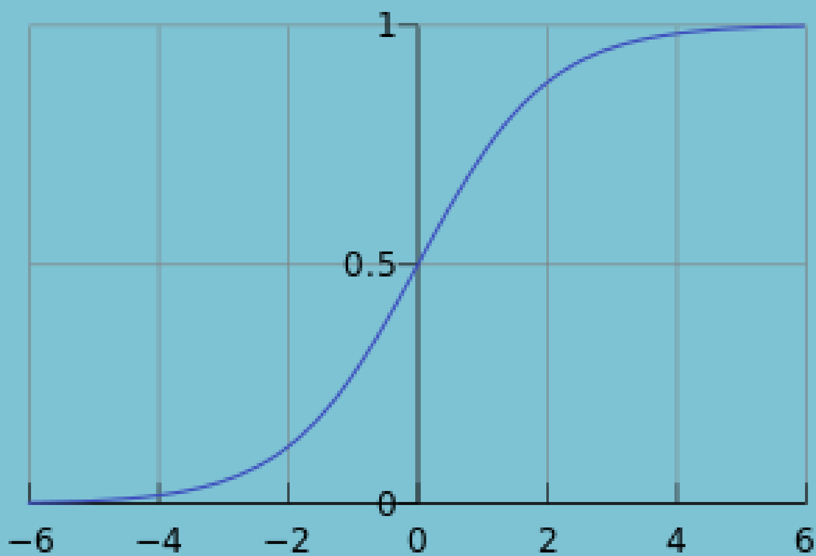
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

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

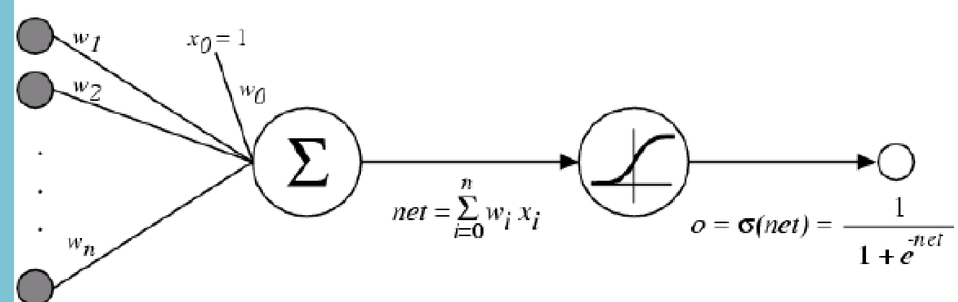
Activation Functions

Sigmoid / Logistic Function

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

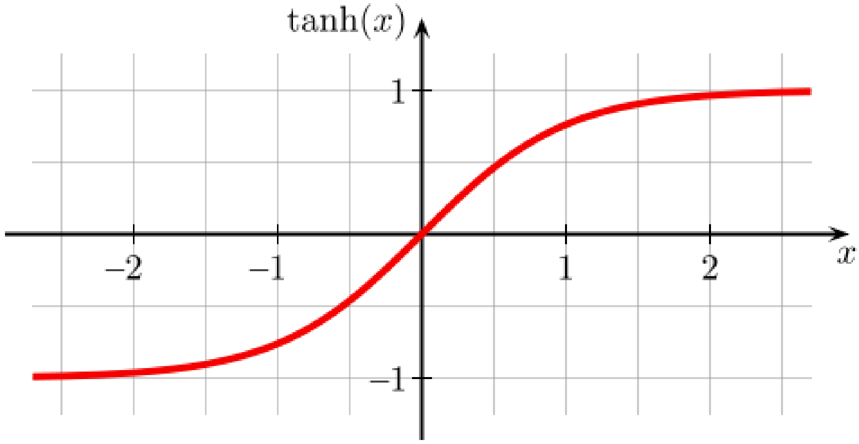


So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function…



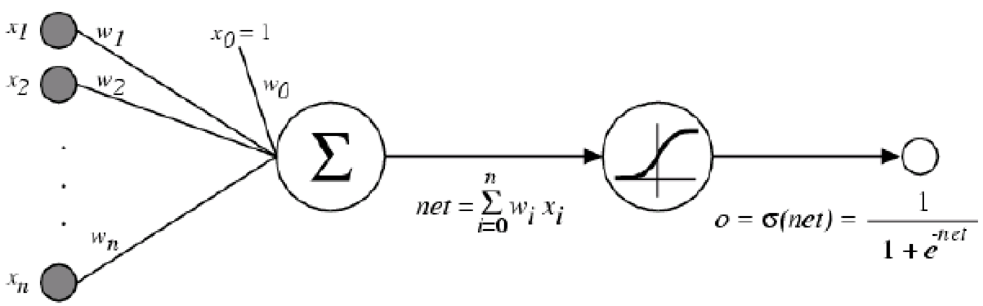
Activation Functions

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



Alternate 1:
tanh

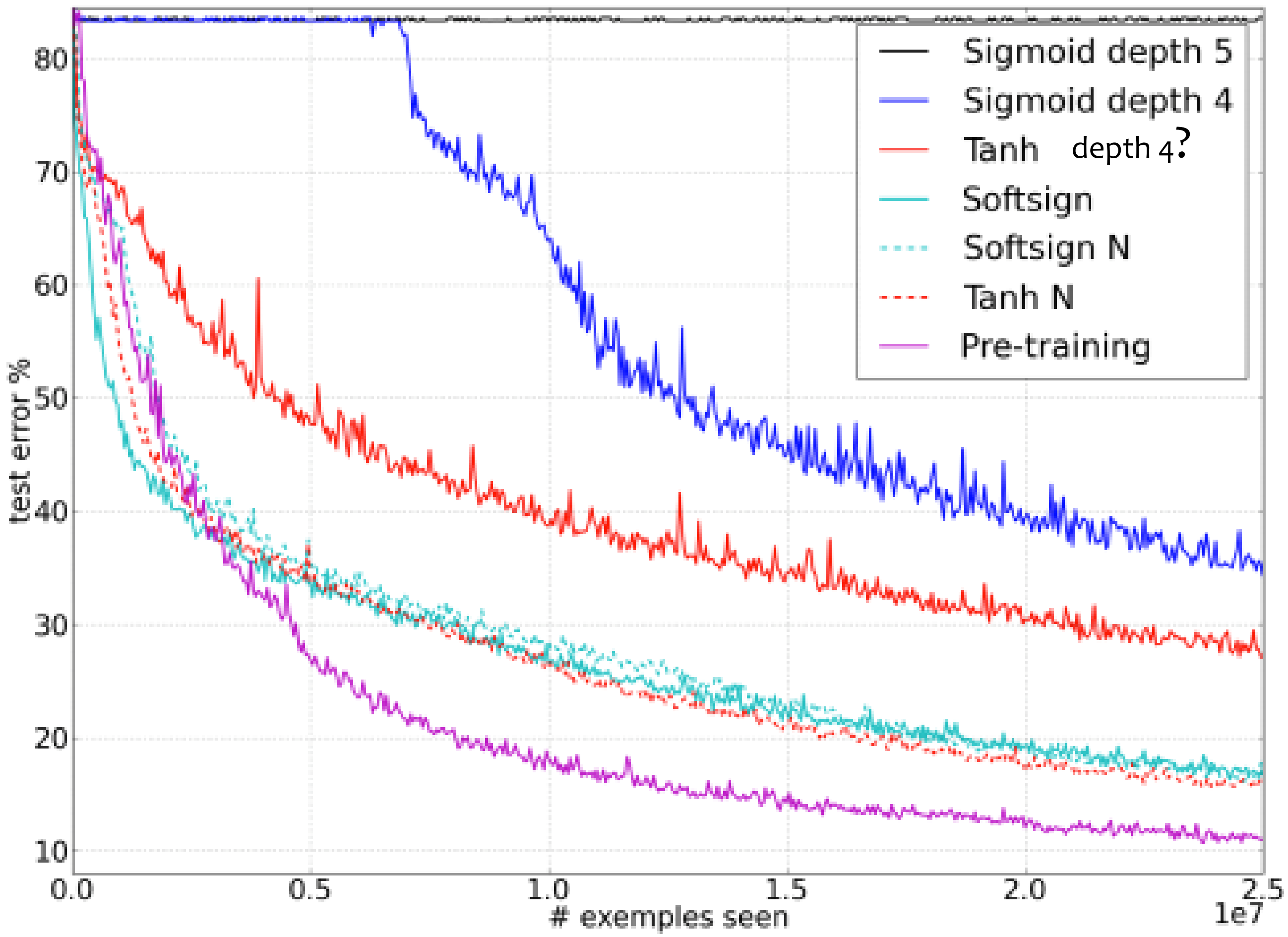
Like logistic function but shifted to range [-1, +1]



Slide from William Cohen

Understanding the difficulty of training deep feedforward neural networks

AI Stats 2010

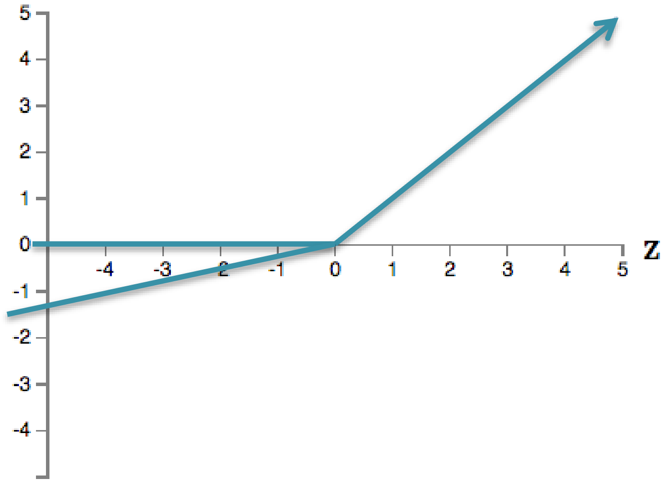


sigmoid
vs.
tanh

Figure from Glorot & Bentio (2010)

Activation Functions

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

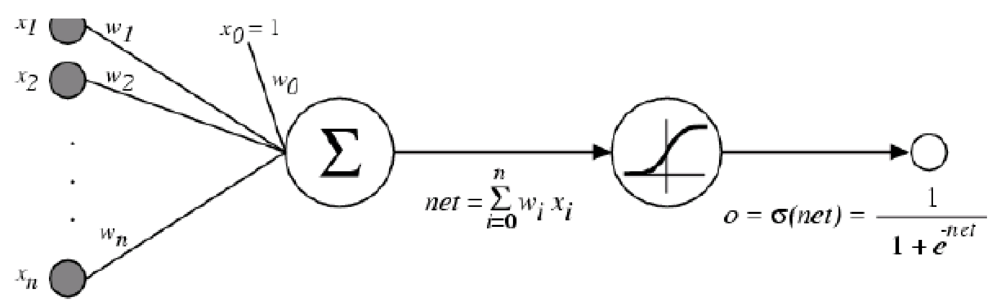


Alternate 2: rectified linear unit

Linear with a cutoff at zero

(Implementation: clip the gradient when you pass zero)

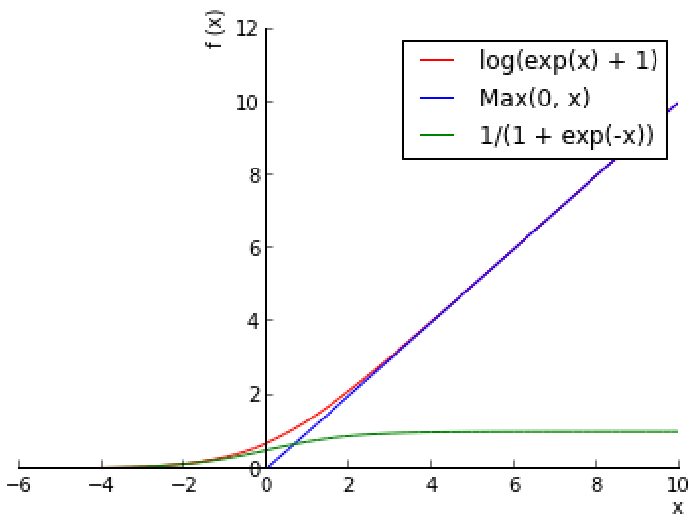
$$\max(0, w \cdot x + b).$$



Slide from William Cohen

Activation Functions

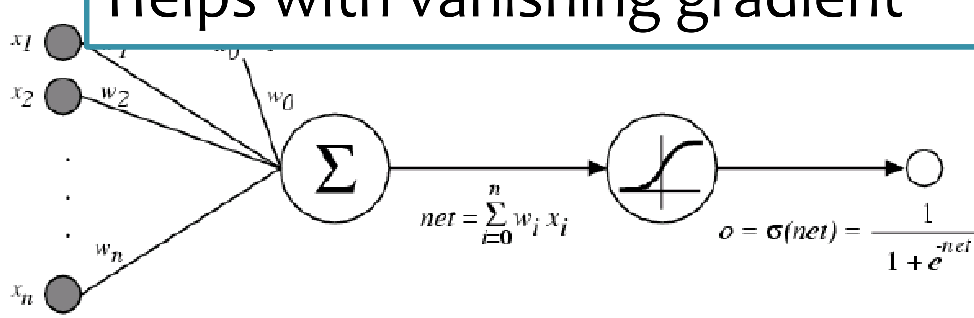
- A new change: modifying the nonlinearity
  - reLU often used in vision tasks



Alternate 2: rectified linear unit

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

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



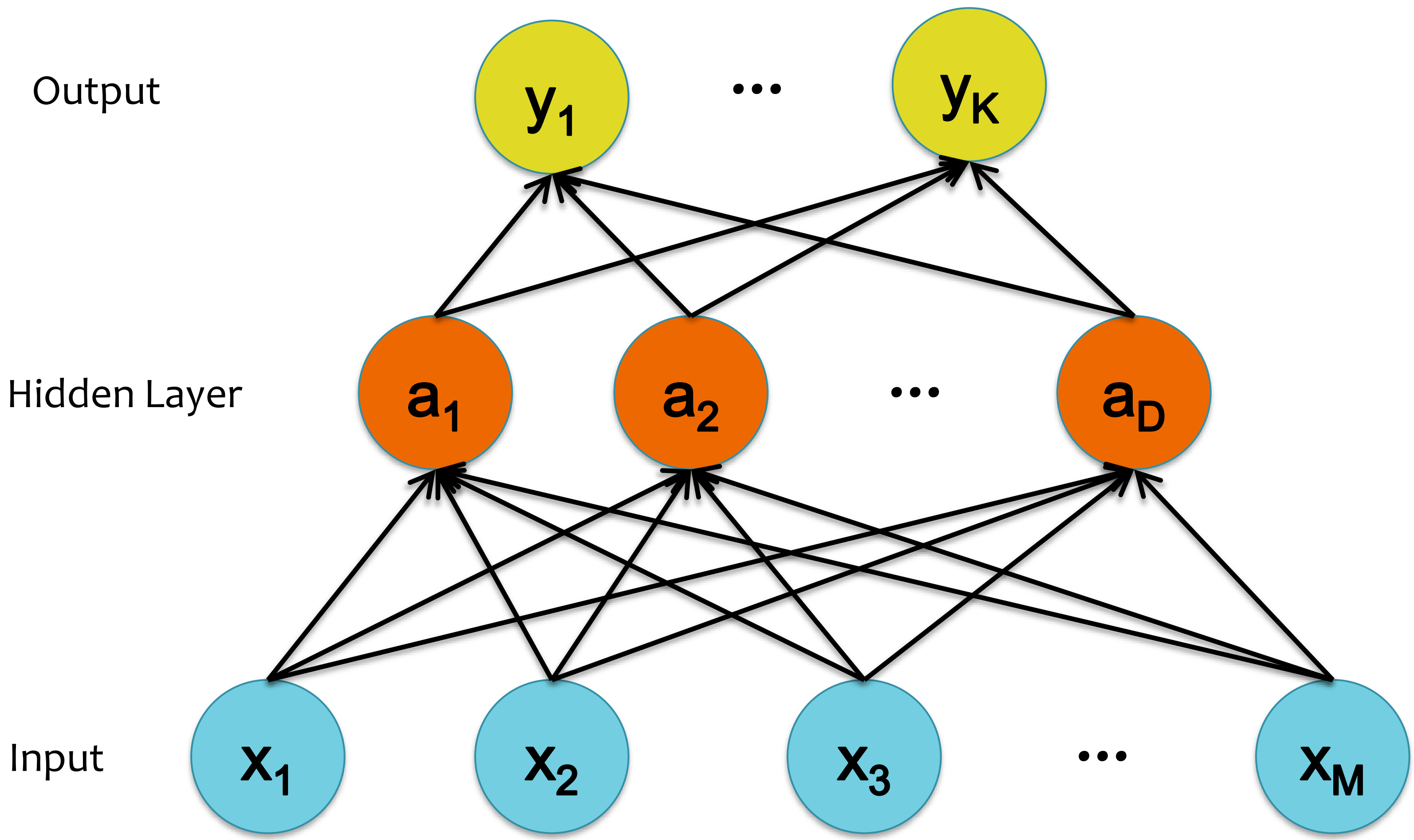
Slide from William Cohen

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

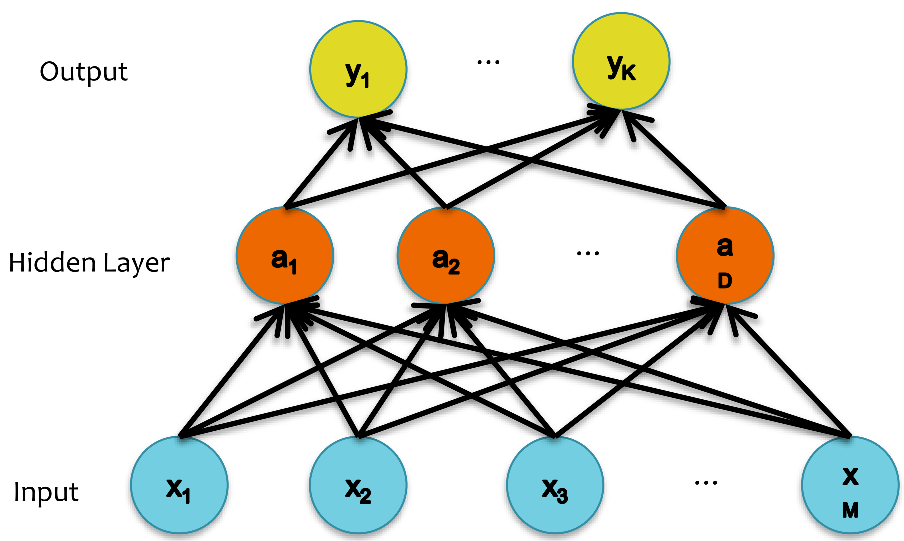
Multi-Class Output



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

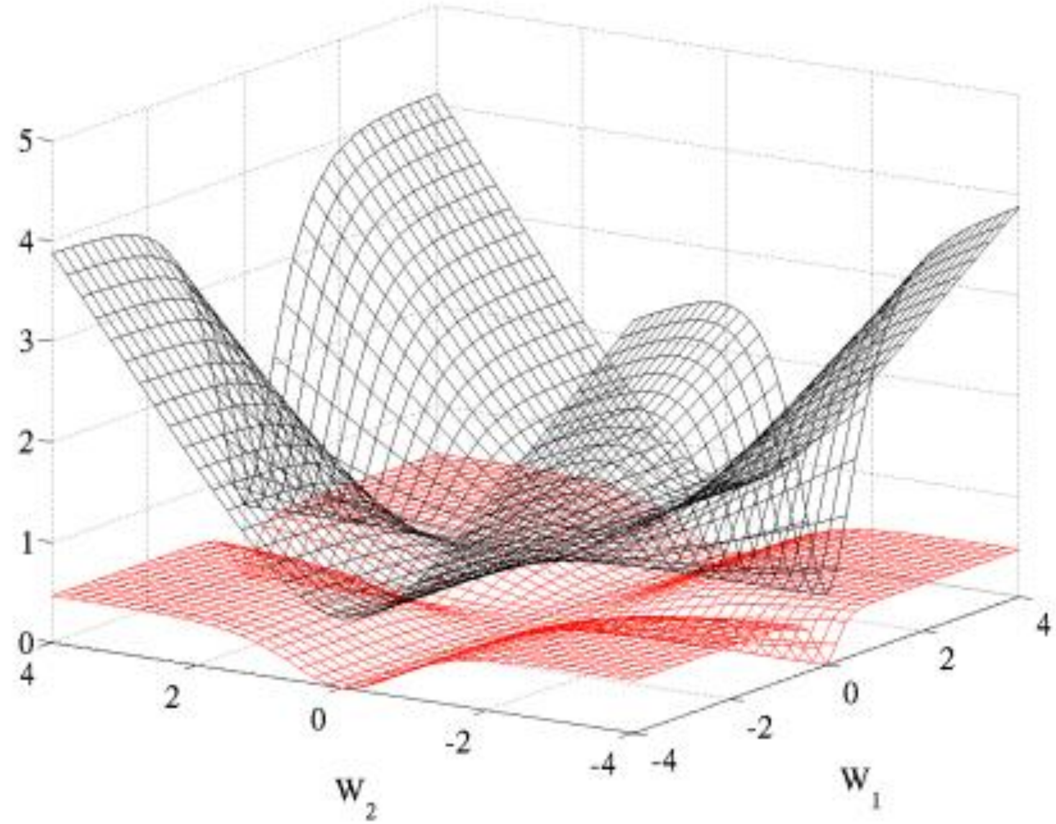


Figure 5: *Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, W_1 respectively on the first layer and W_2 on the second, output layer.*

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…

2) Minimizing sum of squared errors plus squared Euclidean norm of weights…

3) Minimizing cross-entropy…

4) Minimizing hinge loss…

…gives…

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

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

1. Given training data:

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

2. Choose each of these:

– Decision function

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

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?

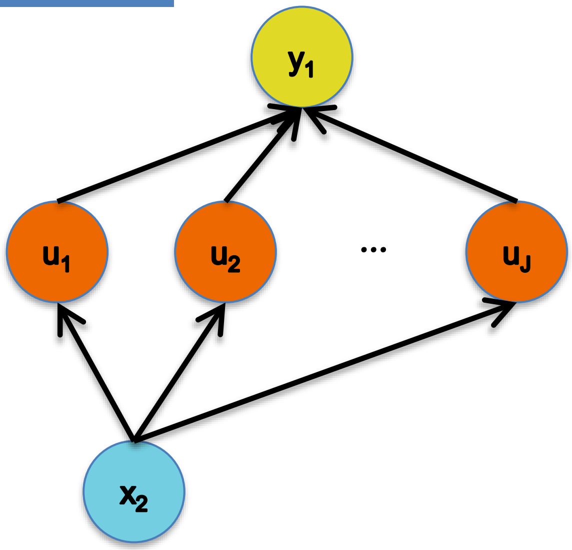
Training

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

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

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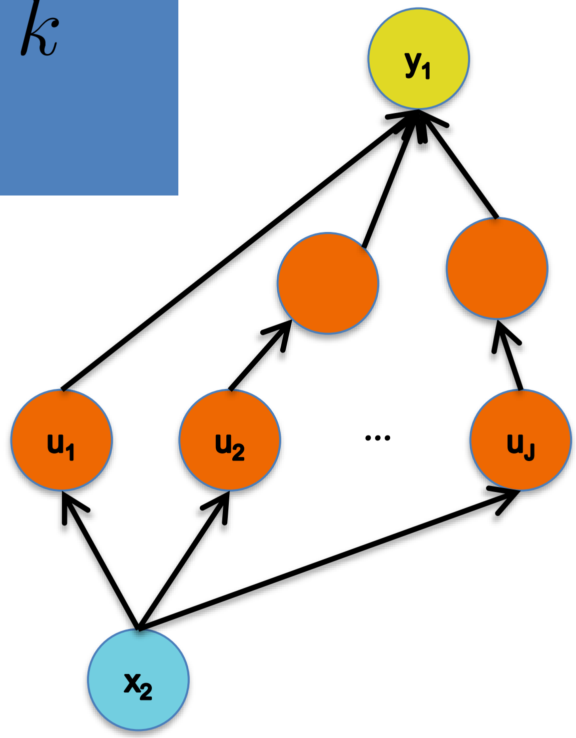


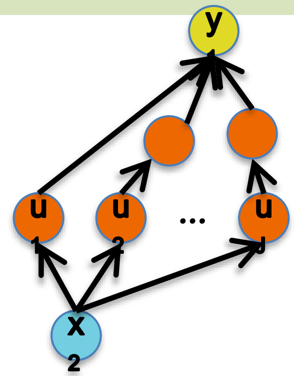
Backpropagation is just repeated application of the **chain rule** from Calculus 101.

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.
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

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

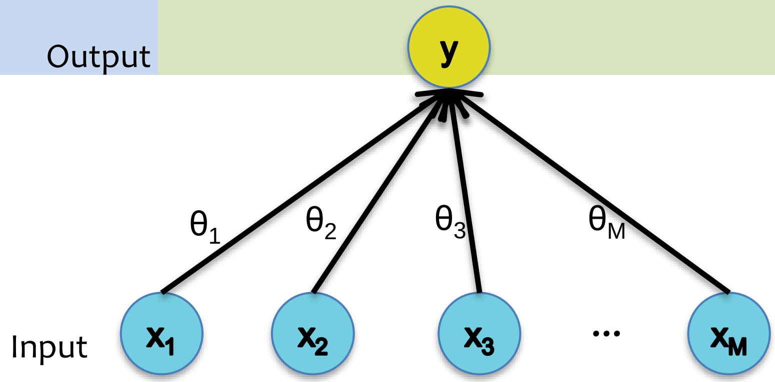
Backpropagation

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

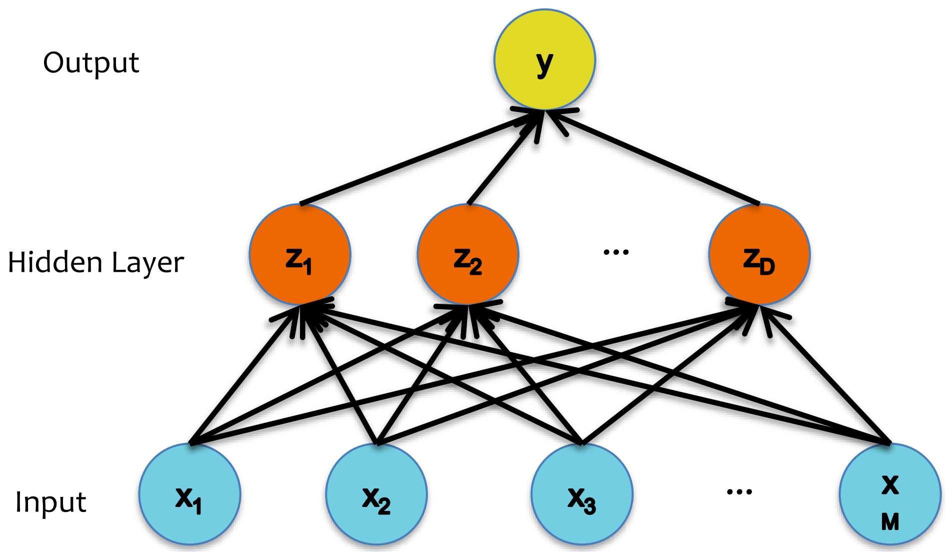
$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

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

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

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

Training Backpropagation



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

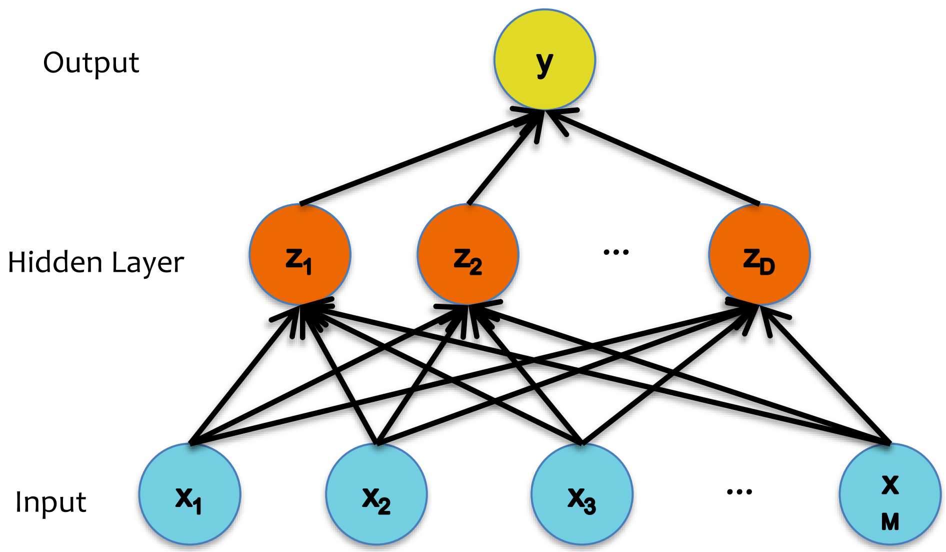
(D) Output (linear)
$b = \sum_{j=0}^{D} \beta_j z_j$

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

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

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

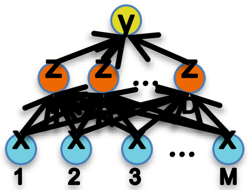
(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

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

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

Training | 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

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

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

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

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

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

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

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

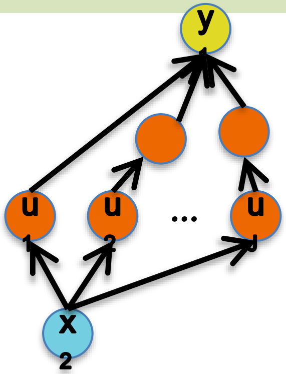
Training

Chain Rule

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

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.
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

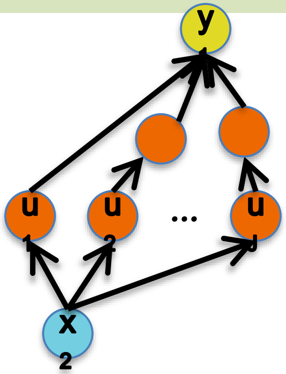
This algorithm is also called **automatic differentiation in the reverse-mode**

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 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	$y = \frac{1}{1 + \exp(-b)}$	$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \; \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Module 3	$b = \sum_{j=0}^{D} \beta_j z_j$	$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \; \frac{db}{d\beta_j} = z_j$ $\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \; \frac{db}{dz_j} = \beta_j$
Module 2	$z_j = \frac{1}{1 + \exp(-a_j)}$	$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \; \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Module 1	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \; \frac{da_j}{d\alpha_{ji}} = x_i$ $\frac{dJ}{dx_i} = \frac{dJ}{da_j}\frac{da_j}{dx_i}, \; \frac{da_j}{dx_i} = \sum_{j=0}^{D} \alpha_{ji}$

Background

A Recipe for

1. Given training dat

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

2. Choose each of th

– Decision functio

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

– Loss function

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

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)

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

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