# CSCE 496/896 Lecture 2: Basic Artificial Neural Networks

Stephen Scott

(Adapted from Vinod Variyam, Ethem Alpaydin, Tom Mitchell, Ian Goodfellow, and Aurélien Géron)

sscott@cse.unl.edu



## Introduction
### Supervised Learning

- **Supervised learning** is most fundamental, "classic" form of machine learning
- "Supervised" part comes from the part of *labels* for examples (instances)
- Many ways to do supervised learning; we'll focus on **artificial neural networks**, which are the basis for deep learning



## Introduction
### ANNs

Consider humans:

- Total number of neurons $\approx 10^{10}$
- Neuron switching time $\approx 10^{-3}$ second (vs. $10^{-10}$)
- Connections per neuron $\approx 10^4$–$10^5$
- Scene recognition time $\approx 0.1$ second
- 100 inference steps doesn't seem like enough

$\Rightarrow$ massive parallel computation



## Introduction
### Properties

Properties of artificial neural nets (ANNs):

- Many "neuron-like" switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically

Strong differences between ANNs for ML and ANNs for biological modeling



## When to Consider ANNs

- Input is high-dimensional discrete- or real-valued (e.g., raw sensor input)
- Output is discrete- or real-valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant
- Long training times acceptable



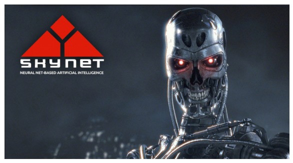
## Introduction
### History of ANNs

- **The Beginning:** Linear units and the Perceptron algorithm (1940s)
  - Spoiler Alert: stagnated because of inability to handle data not *linearly separable*
  - Aware of usefulness of multi-layer networks, but could not train
- **The Comeback:** Training of multi-layer networks with Backpropagation (1980s)
  - Many applications, but in 1990s replaced by large-margin approaches such as support vector machines and boosting

# Introduction

## History of ANNs (cont'd)

- **The Resurgence:** Deep architectures (2000s)
  - Better hardware[1] and software support allow for deep ($>$ 5–8 layers) networks
  - Still use Backpropagation, but
    - Larger datasets, algorithmic improvements (new loss and activation functions), and deeper networks improve performance considerably
  - Very impressive applications, e.g., captioning images
- **The Inevitable:** (TBD)
  - Oops




[1] Thank a gamer today.





# Outline

- Supervised learning
- Basic ANN units
  - Linear unit
  - Linear threshold units
  - Perceptron training rule
- Gradient Descent
- Nonlinearly separable problems and multilayer networks
- Backpropagation
- Types of activation functions
- Putting everything together





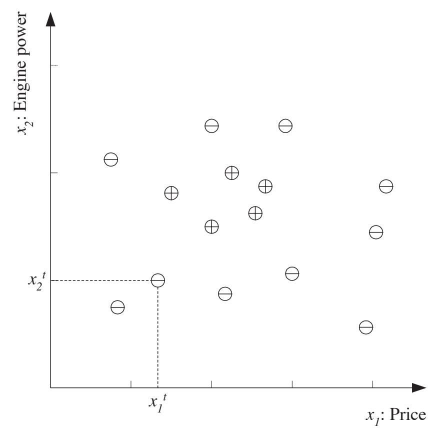
# Learning from Examples

- Let $C$ be the **target function** (or **target concept**) to be learned
  - Think of $C$ as a function that takes as input an **example** (or **instance**) and outputs a **label**
- **Goal:** Given **training set** $\mathcal{X} = \{(\boldsymbol{x}^t, y^t)\}_{t=1}^N$ where $y^t = C(\boldsymbol{x}^t)$, output **hypothesis** $h \in \mathcal{H}$ that approximates $C$ in its classifications of new instances
- Each instance $\boldsymbol{x}$ represented as a vector of **attributes** or **features**
  - E.g., let each $\boldsymbol{x} = (x_1, x_2)$ be a vector describing attributes of a car; $x_1 =$ price and $x_2 =$ engine power
  - In this example, label is binary (positive/negative, yes/no, 1/0, $+1/-1$) indicating whether instance $\boldsymbol{x}$ is a "family car"





# Learning from Examples (cont'd)







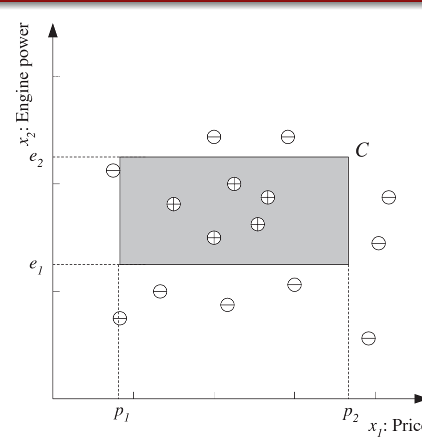

# Thinking about $C$

- Can think of target concept $C$ as a **function**
  - In example, $C$ is an axis-parallel box, equivalent to upper and lower bounds on each attribute
  - Might decide to set $\mathcal{H}$ (set of candidate hypotheses) to the same family that $C$ comes from
  - Not required to do so
- Can also think of target concept $C$ as a **set** of positive instances
  - In example, $C$ the continuous set of all positive points in the plane
- Use whichever is convenient at the time





# Thinking about $C$ (cont'd)



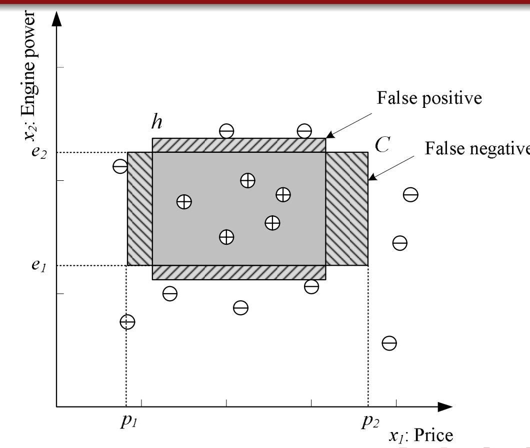
## Hypotheses and Error

- A learning algorithm uses training set $\mathcal{X}$ and finds a hypothesis $h \in \mathcal{H}$ that approximates $C$
- In example, $\mathcal{H}$ can be set of all axis-parallel boxes
- If $C$ guaranteed to come from $\mathcal{H}$, then we know that a perfect hypothesis exists
  - In this case, we choose $h$ from the **version space** = subset of $\mathcal{H}$ consistent with $\mathcal{X}$
  - What learning algorithm can you think of to learn $C$?
- Can think of two types of **error** (or **loss**) of $h$
  - **Empirical error** is fraction of $\mathcal{X}$ that $h$ gets wrong
  - **Generalization error** is probability that a new, randomly selected, instance is misclassified by $h$
    - Depends on the probability distribution over instances
  - Can further classify error as **false positive** and **false negative**



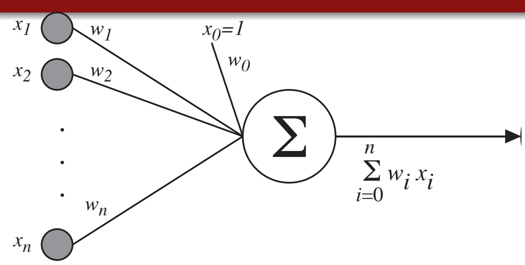
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott

## Hypotheses and Error (cont'd)






## Linear Unit (Regression)

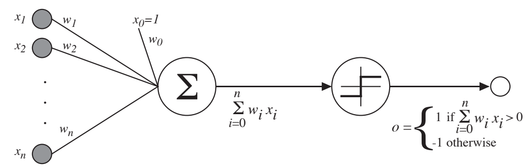



$$\hat{y} = f(\boldsymbol{x}; \boldsymbol{w}, b) = \boldsymbol{x}^\top \boldsymbol{w} + b = w_1 x_1 + \cdots + w_n x_n + b$$

- Each weight vector $\boldsymbol{w}$ is different $h$
- If set $w_0 = b$, can simplify above
- Forms the basis for many other activation functions



## Linear Threshold Unit (Binary Classification)

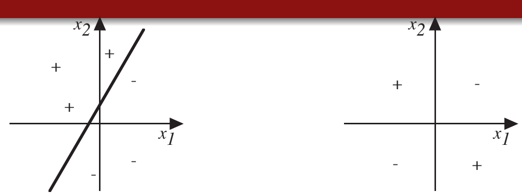



$$y = o(\boldsymbol{x}; \boldsymbol{w}, b) = \begin{cases} +1 & \text{if } f(\boldsymbol{x}; \boldsymbol{w}, b) > 0 \\ -1 & \text{otherwise} \end{cases}$$

(sometimes use $0$ instead of $-1$)



## Linear Threshold Unit
### Decision Surface




(a) (b)

Represents some useful functions

- What parameters $(\boldsymbol{w}, b)$ represent $g(x_1, x_2; \boldsymbol{w}, b) = AND(x_1, x_2)$?

But some functions not representable

- I.e., those not **linearly separable**
- Therefore, we'll want **networks** of units



## Linear Threshold Unit
### Non-Numeric Inputs

- What if attributes are not numeric?
- **Encode** them numerically
- E.g., if an attribute *Color* has values *Red*, *Green*, and *Blue*, can encode as **one-hot** vectors $[1, 0, 0]$, $[0, 1, 0]$, $[0, 0, 1]$
- Generally better than using a single integer, e.g., *Red* is 1, *Green* is 2, and *Blue* is 3, since there is no implicit ordering of the values of the attribute

# Perceptron Training Rule (Learning Algorithm)



$$w_j' \leftarrow w_j + \eta\,(y^t - \hat{y}^t)\,x_j^t$$

where

- $x_j^t$ is $j$th attribute of training instance $t$
- $y^t$ is label of training instance $t$
- $\hat{y}^t$ is Perceptron output on training instance $t$
- $\eta > 0$ is small constant (e.g., 0.1) called **learning rate**

I.e., if $(y - \hat{y}) > 0$ then increase $w_j$ w.r.t. $x_j$, else decrease

Can prove rule will converge if training data is linearly separable and $\eta$ sufficiently small



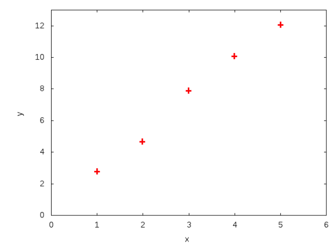


# Where Does the Training Rule Come From?
## Linear Regression



- Recall initial *linear unit* (no threshold)
- If only one feature, then this is a **regression** problem
- Find a straight line that best fits the training data
  - For simplicity, let it pass through the origin
  - Slope specified by parameter $w_1$

| $x^t$ | $y^t$ |
|---|---|
| 1 | 2.8 |
| 2 | 4.65 |
| 3 | 7.9 |
| 4 | 10.1 |
| 5 | 12.1 |








# Where Does the Training Rule Come From?
## Linear Regression



- Goal is to find a parameter $w_1$ to minimize **square loss**:

$$J(w_1) = \sum_{t=1}^{m} (\hat{y}^t - y^t)^2 = \sum_{t=1}^{m} (w_1 x^t - y^t)^2$$

$$= (1w_1 - 2.8)^2 + (2w_1 - 4.65)^2 + (3w_1 - 7.9)^2$$
$$+ (4w_1 - 10.1)^2 + (5w_1 - 12.1)^2$$
$$= 55w_1^2 - 273.4w_1 + 340.293$$

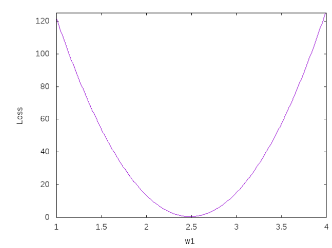




# Where Does the Training Rule Come From?
## Convex Quadratic Optimization



$$J(w_1) = 55w_1^2 - 273.4w_1 + 340.293$$




- Minimum is at $w_1 \approx 2.485$, with loss $\approx 0.53$
- What's special about that point?





# Where Does the Training Rule Come From?
## Gradient Descent



- Recall that a function has a (local) minimum or maximum where the derivative is $0$

$$\frac{d}{dw_1} J(w_1) = 110w_1 - 273.4$$

- Setting this $= 0$ and solving for $w_1$ yields $w_1 \approx 2.485$
- Motivates the use of **gradient descent** to solve in high-dimensional spaces with nonconvex functions:

$$\mathbf{w}' = \mathbf{w} - \eta \nabla J(\mathbf{w})$$

- $\eta$ is **learning rate** to moderate updates
- Gradient is a vector of partial derivatives: $\left[\frac{\partial J}{\partial w_i}\right]_{i=1}^{n}$





# Where Does the Training Rule Come From?
## Gradient Descent Example



- In our example, initialize $w_1$, then repeatedly update

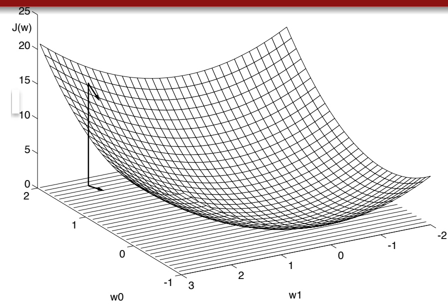
$$w_1' = w_1 - \eta(110\,w_1 - 273.4)$$

| eta | 0.01 | | | |
|---|---|---|---|---|
| round | w | J | grad | update |
| 0 | 1 | 121.893 | -163.4 | 1.634 |
| 1 | 2.634 | 1.74498 | 16.34 | -0.1634 |
| 2 | 2.4706 | 0.5434998 | -1.634 | 0.01634 |
| 3 | 2.48694 | 0.531485 | 0.1634 | -0.001634 |
| 4 | 2.485306 | 0.53136485 | -0.01634 | 0.0001634 |
| 5 | 2.4854694 | 0.53136365 | 0.001634 | -1.634E-05 |
| 6 | 2.48545306 | 0.53136364 | -0.0001634 | 1.634E-06 |
| 7 | 2.48545469 | 0.53136364 | 1.634E-05 | -1.634E-07 |
| 8 | 2.48545453 | 0.53136364 | -1.634E-06 | 1.634E-08 |
| 9 | 2.48545455 | 0.53136364 | 1.634E-07 | -1.634E-09 |
| 10 | 2.48545455 | 0.53136364 | -1.634E-08 | 1.634E-10 |
| 11 | 2.48545455 | 0.53136364 | 1.634E-09 | -1.634E-11 |
| 12 | 2.48545455 | 0.53136364 | -1.634E-10 | 1.6337E-12 |
| 13 | 2.48545455 | 0.53136364 | 1.6314E-11 | -1.631E-13 |
| 14 | 2.48545455 | 0.53136364 | -1.592E-12 | 1.5916E-14 |
| 15 | 2.48545455 | 0.53136364 | 0 | 0 |

- Could also update one at a time: $\frac{\partial J}{\partial w_1} = 2w_1\,(x^t)^2 - 2x^t y^t$

## Where Does the Training Rule Come From?
### Gradient Descent






$$\frac{\partial J}{\partial \boldsymbol{w}} = \left[\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}, \cdots, \frac{\partial J}{\partial w_n}\right]$$

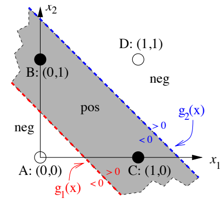
In general, define loss function $J$, compute gradient of $J$ w.r.t. $J$'s parameters, then apply gradient descent



## Handling Nonlinearly Separable Problems
### The XOR Problem



Using linear threshold units




Represent with **intersection** of two linear separators

$$g_1(\boldsymbol{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 1/2$$

$$g_2(\boldsymbol{x}) = 1 \cdot x_1 + 1 \cdot x_2 - 3/2$$

pos $= \{\boldsymbol{x} \in \mathbb{R}^2 : g_1(\boldsymbol{x}) > 0$ AND $g_2(\boldsymbol{x}) < 0\}$

neg $= \{\boldsymbol{x} \in \mathbb{R}^2 : g_1(\boldsymbol{x}), g_2(\boldsymbol{x}) < 0$ OR $g_1(\boldsymbol{x}), g_2(\boldsymbol{x}) > 0\}$



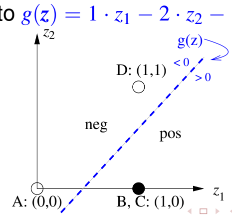
## Handling Nonlinearly Separable Problems
### The XOR Problem (cont'd)



Let $z_i = \begin{cases} 0 & \text{if } g_i(\boldsymbol{x}) < 0 \\ 1 & \text{otherwise} \end{cases}$

| Class | $(x_1, x_2)$ | $g_1(\boldsymbol{x})$ | $z_1$ | $g_2(\boldsymbol{x})$ | $z_2$ |
|---|---|---|---|---|---|
| pos | B: $(0,1)$ | $1/2$ | 1 | $-1/2$ | 0 |
| pos | C: $(1,0)$ | $1/2$ | 1 | $-1/2$ | 0 |
| neg | A: $(0,0)$ | $-1/2$ | 0 | $-3/2$ | 0 |
| neg | D: $(1,1)$ | $3/2$ | 1 | $1/2$ | 1 |

Now feed $z_1, z_2$ into $g(\boldsymbol{z}) = 1 \cdot z_1 - 2 \cdot z_2 - 1/2$

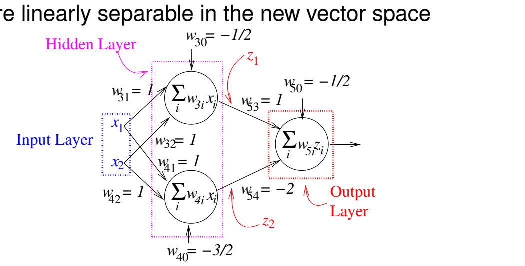





## Handling Nonlinearly Separable Problems
### The XOR Problem (cont'd)



In other words, we **remapped** all vectors $\boldsymbol{x}$ to $\boldsymbol{z}$ such that the classes are linearly separable in the new vector space




This is a **two-layer perceptron** or **two-layer feedforward neural network**

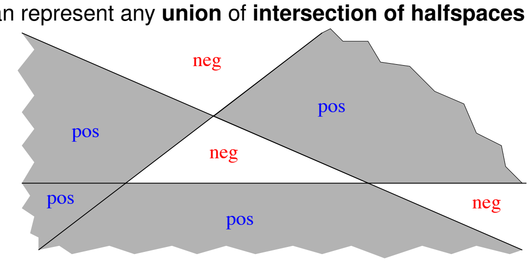
Can use many **nonlinear** activation functions in hidden layer



## Handling Nonlinearly Separable Problems
### General Nonlinearly Separable Problems



By adding up to 2 **hidden layers** of linear threshold units, can represent any **union** of **intersection of halfspaces**




First hidden layer defines halfspaces, second hidden layer takes intersection (AND), output layer takes union (OR)



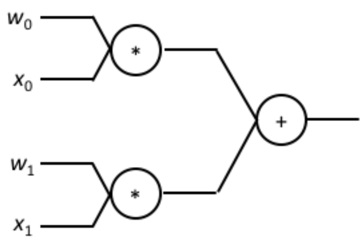
## Training Multiple Layers



- In a multi-layer network, have to tune parameters in all layers
- In order to train, need to know the gradient of the loss function w.r.t. each parameter
- The **Backpropagation** algorithm first **feeds forward** the network's inputs to its outputs, then **propagates back** error via repeated application of **chain rule** for derivatives
- Can be decomposed in a simple, modular way

## Computation Graphs

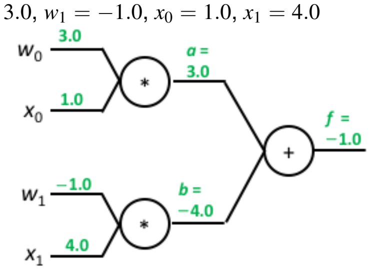
- Given a complicated function $f(\cdot)$, want to know its partial derivatives w.r.t. its parameters
- Will represent $f$ in a modular fashion via a **computation graph**
- E.g., let $f(\mathbf{w}, \mathbf{x}) = w_0 x_0 + w_1 x_1$






## Computation Graphs

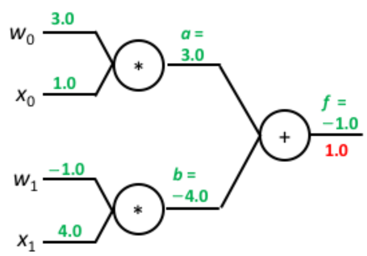
E.g., $w_0 = 3.0$, $w_1 = -1.0$, $x_0 = 1.0$, $x_1 = 4.0$






## Computation Graphs

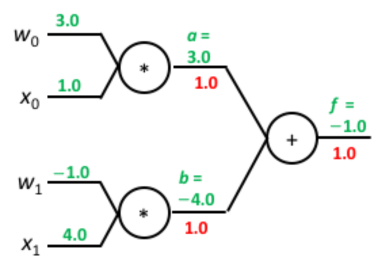
- So what?
- Can now decompose gradient calculation into basic operations
- $\frac{\partial f}{\partial f} = 1$






## Computation Graphs

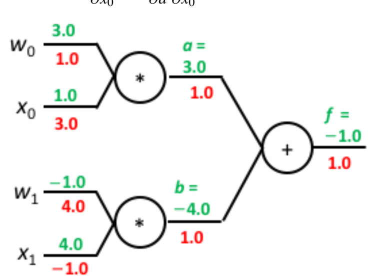
- If $g(y, z) = y + z$ then $\frac{\partial g}{\partial y} = \frac{\partial g}{\partial z} = 1$
- Via chain rule, $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial a} = (1.0)(1.0) = 1.0$
- Same with $\frac{\partial f}{\partial b}$






## Computation Graphs

- If $h(y, z) = yz$ then $\frac{\partial h}{\partial y} = z$
- Via chain rule, $\frac{\partial f}{\partial x_0} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial x_0} = 1.0 w_0 = 3.0$

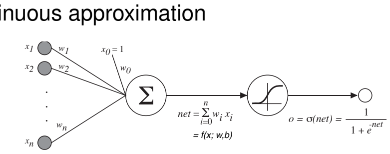



So for $\mathbf{x} = [1.0, 4.0]^\top$, $\nabla f(\mathbf{w}) = [1.0, 4.0]^\top$



## The Sigmoid Unit
### Basics

- How does this help us with multi-layer ANNs?
- First, let's replace the threshold function with a continuous approximation




$\sigma(net)$ is the **logistic function**

$$\sigma(net) = \frac{1}{1 + e^{-net}}$$

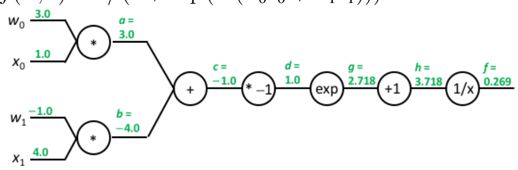
(a type of **sigmoid** function)

**Squashes** $net$ into $[0, 1]$ range

## The Sigmoid Unit
### Computation Graph



Let $f(\mathbf{w},\mathbf{x}) = 1/\left(1+\exp\left(-\left(w_0x_0+w_1x_1\right)\right)\right)$

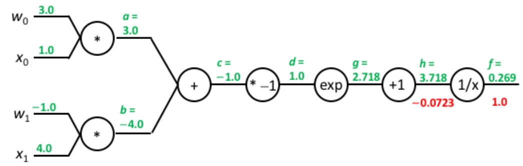





## The Sigmoid Unit



$\frac{\partial f}{\partial h} = 1.0(-1/h^2) = -0.0723$

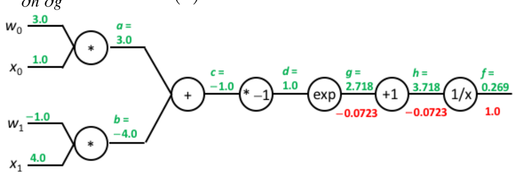





## The Sigmoid Unit
### Gradient



$\frac{\partial f}{\partial g} = \frac{\partial f}{\partial h}\frac{\partial h}{\partial g} = -0.0723(1) = -0.0723$

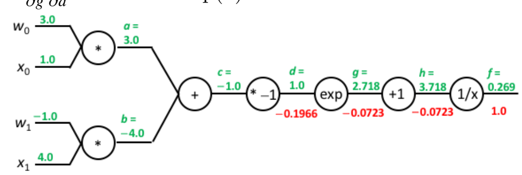





## The Sigmoid Unit
### Gradient



$\frac{\partial f}{\partial d} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial d} = -0.0723\exp(d) = -0.1966$

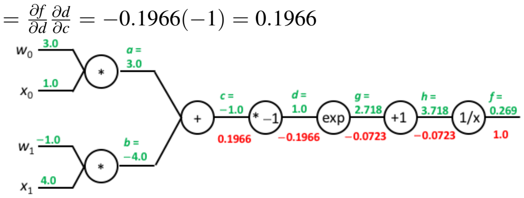




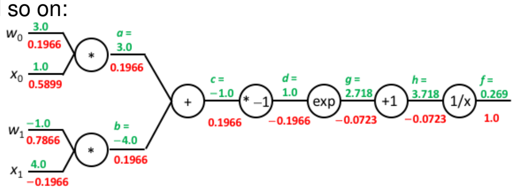

## The Sigmoid Unit
### Gradient



$\frac{\partial f}{\partial c} = \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = -0.1966(-1) = 0.1966$




and so on:

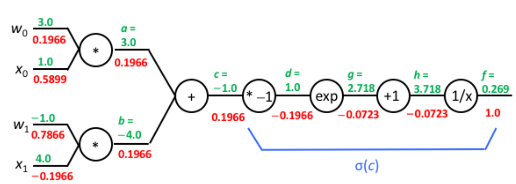



So for $\mathbf{x} = [1.0, 4.0]^\top$, $\nabla f(\mathbf{w}) = [0.1966, 0.7866]^\top$



## The Sigmoid Unit
### Gradient






Note that $\frac{\partial f}{\partial c} = \sigma(c)(1-\sigma(c))$, so

$$\frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial w_1} = \sigma(c)(1-\sigma(c))(1)x_1$$

# Sigmoid Unit
## Weight Update

- If $\hat{y}^t = \sigma(\mathbf{w} \cdot \mathbf{x}^t)$ is prediction on training instance $\mathbf{x}^t$ with label $y^t$, let loss be $J(\mathbf{w}) = \frac{1}{2}\left(\hat{y}^t - y^t\right)^2$, so

$$\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial w_1} &= \left(\hat{y}^t - y^t\right)\left(\frac{\partial}{\partial w_1}\left(\hat{y}^t - y^t\right)\right) \\
&= \left(\hat{y}^t - y^t\right)\left(\frac{\partial}{\partial w_1}\hat{y}^t\right) \\
&= \left(\hat{y}^t - y^t\right)\left(\hat{y}^t\left(1 - \hat{y}^t\right)x_1^t\right)
\end{aligned}$$

- So update rule is

$$w_1' = w_1 - \eta\, \hat{y}^t\left(1 - \hat{y}^t\right)\left(\hat{y}^t - y^t\right)x_1^t$$

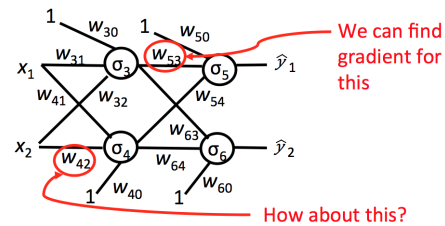
- In general,

$$\boxed{\mathbf{w}' = \mathbf{w} - \eta\, \hat{y}^t\left(1 - \hat{y}^t\right)\left(\hat{y}^t - y^t\right)\mathbf{x}^t}$$



# Multilayer Networks

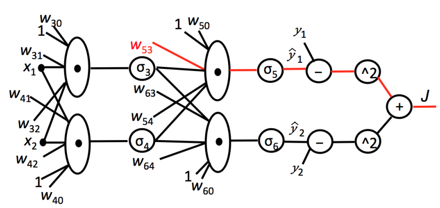
- That update formula works for **output units** when we know the target labels $\mathbf{y}^t$ (here, a vector to encode **multi-class** labels)
- But for a **hidden unit**, we don't know its target output!




$w_{ji}$ = weight from node $i$ to node $j$



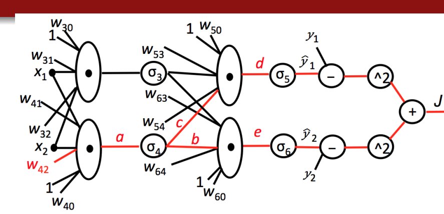
# Training Multilayer Networks
## Output Units



- Let loss on instance $(\mathbf{x}^t, \mathbf{y}^t)$ be $J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n}\left(\hat{y}_i^t - y_i^t\right)^2$
- Weights $w_{5*}$ and $w_{6*}$ tie to output units
- Gradients and weight updates done as before
- E.g., $w_{53}' = w_{53} - \eta\frac{\partial J}{\partial w_{53}} = w_{53} - \eta\hat{y}_1(1 - \hat{y}_1)(\hat{y}_1 - y_1)\sigma_3$



# Training Multilayer Networks
## Hidden Units



Multivariate chain rule says we sum paths from $J$ to $w_{42}$:

$$\begin{aligned}
\frac{\partial J}{\partial w_{42}} &= \frac{\partial J}{\partial a}\frac{\partial a}{\partial w_{42}} = \left(\frac{\partial J}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial J}{\partial b}\frac{\partial b}{\partial a}\right)\frac{\partial a}{\partial w_{42}} \\
&= \left(\frac{\partial J}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial J}{\partial e}\frac{\partial e}{\partial b}\frac{\partial b}{\partial a}\right)\frac{\partial a}{\partial w_{42}} \\
&= \left([\hat{y}_1(1 - \hat{y}_1)(\hat{y}_1 - y_1)]\,[w_{54}]\,[\sigma_4(a)(1 - \sigma_4(a))]\right. \\
&+ \left.[\hat{y}_2(1 - \hat{y}_2)(\hat{y}_2 - y_2)]\,[w_{64}]\,[\sigma_4(a)(1 - \sigma_4(a))]\right)x_2
\end{aligned}$$



# Training Multilayer Networks
## Hidden Units

- Analytical solution is messy, but we don't need the formula; only need to **compute** gradient
- The modular form of a computation graph means that once we've computed $\frac{\partial J}{\partial d}$ and $\frac{\partial J}{\partial e}$, we can plug those values in and compute gradients for earlier layers
  - Doesn't matter if layer is output, or farther back; can run indefinitely backward
- **Backpropagation** of error from outputs to inputs
- Define **error term** of hidden node $h$ as

$$\delta_h \leftarrow \hat{y}_h\left(1 - \hat{y}_h\right)\sum_{k \in down(h)} w_{k,h}\,\delta_k\ ,$$

where $\hat{y}_k$ is output of node $k$ and $down(h)$ is set of nodes immediately downstream of $h$
- Note that this formula is specific to sigmoid units



# Training Multilayer Networks
## Hidden Units

- We are **propagating back** error terms $\delta$ from output layer toward input layers, scaling with the weights
- Scaling with the weights characterizes how much of the error term each hidden unit is "responsible for"
- Process:
  1. Submit inputs $\mathbf{x}$
  2. **Feed forward** signal to outputs
  3. Comptue network loss
  4. Propagate error back to compute loss gradient w.r.t. each weight
  5. Update weights

## Backpropagation Algorithm
### Sigmoid Activation Units and Square Loss

Initialize weights

Until termination condition satisfied do

- For each training example $(\boldsymbol{x}^t, \boldsymbol{y}^t)$ do
  1. Input $\boldsymbol{x}^t$ to the network and compute the outputs $\hat{\boldsymbol{y}}^t$
  2. For each output unit $k$
  $$\delta_k^t \leftarrow \hat{y}_k^t\,(1-\hat{y}_k^t)\,(y_k^t-\hat{y}_k^t)$$
  3. For each hidden unit $h$
  $$\delta_h^t \leftarrow \hat{y}_h^t\,(1-\hat{y}_h^t)\sum_{k \in down(h)} w_{k,h}^t\,\delta_k^t$$
  4. Update each network weight $w_{j,i}^t$
  $$w_{j,i}^t \leftarrow w_{j,i}^t + \Delta w_{j,i}^t$$
  where $\Delta w_{j,i}^t = \eta\,\delta_j^t\,x_{j,i}^t$ and $x_{j,i}^t$ is signal sent from node $i$ to node $j$



## Backpropagation Algorithm
### Notes

- Formula for $\delta$ assumes sigmoid activation function
  - Straightforward to change to new activation function via computation graph
- Initialization used to be via random numbers near zero, e.g., from $\mathcal{N}(0,1)$
  - More refined methods available (later)
- Algorithm as presented updates weights after each instance
  - Can also accumulate $\Delta w_{j,i}^t$ across multiple training instances in the same **mini-batch** and do a single update per mini-batch
    - $\Rightarrow$ **Stochastic gradient descent** (SGD)
  - Extreme case: Entire training set is a single batch (**batch gradient descent**)



## Types of Output Units

Given hidden layer outputs $\boldsymbol{h}$

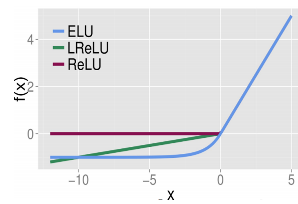
- Linear unit: $\hat{y} = \boldsymbol{w}^\top \boldsymbol{h} + b$
  - Minimizing square loss with this output unit maximizes **log likelihood** when labels from normal distribution
    - I.e., find a set of parameters $\boldsymbol{\theta}$ that is most likely to generate the labels of the training data
  - Works well with GD training
- Sigmoid: $\hat{y} = \sigma(\boldsymbol{w}^\top \boldsymbol{h} + b)$
  - Approximates non-differentiable threshold function
  - More common in older, shallower networks
  - Can be used to predict probabilities
- Softmax unit: Start with $\boldsymbol{z} = W^\top \boldsymbol{h} + \boldsymbol{b}$
  - Predict probability of label $i$ to be softmax$(\boldsymbol{z})_i = \exp(z_i) / \left(\sum_j \exp(z_j)\right)$
  - Continuous, differentiable approximation to argmax



## Types of Hidden Units

Rectified linear unit (ReLU): $\max\{0, W^\top \boldsymbol{x} + \boldsymbol{b}\}$

- Good default choice
- In general, GD works well when functions nearly linear
- Variations: **leaky ReLU** and **exponential ReLU** replace $z < 0$ side with $0.01z$ and $\alpha(\exp(z) - 1)$, respectively




Logistic sigmoid (done already) and $\tanh$

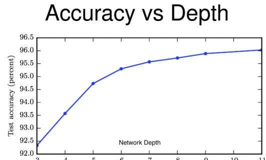
- Nice approximation to threshold, but don't train well in deep networks since they saturate



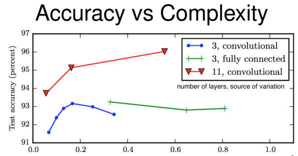
## Putting Everything Together
### Hidden Layers

- How many layers to use?
  - Deep networks build potentially useful representations of data via composition of simple functions
  - Performance improvement not simply from more complex network (number of parameters)
  - Increasing number of layers still increases chances of overfitting, so need significant amount of training data with deep network; training time increases as well

Accuracy vs Depth




Accuracy vs Complexity






## Putting Everything Together
### Universal Approximation Theorem

- Any boolean function can be represented with two layers
- Any bounded, continuous function can be represented with arbitrarily small error with two layers
- Any function can be represented with arbitrarily small error with three layers

Only an **EXISTENCE PROOF**

- Could need exponentially many nodes in a layer
- May not be able to find the right weights
- Highlights risk of overfitting and need for **regularization**

## Putting Everything Together
### Initialization

- Previously, initialized weights to random numbers near 0 (from $\mathcal{N}(0,1)$)
  - Sigmoid nearly linear there, so GD expected to work better
  - But in deep networks, this increases variance per layer, resulting in **vanishing gradients** and poor optimization
- **Glorot initialization** controls variance per layer: If layer has $n_{in}$ inputs and $n_{out}$ outputs, initialize via uniform over $[-r, r]$ or $\mathcal{N}(0, \sigma)$
  - $r = a\sqrt{\frac{6}{n_{in}+n_{out}}}$ and $\sigma = a\sqrt{\frac{2}{n_{in}+n_{out}}}$

| Activation | $a$ |
|---|---|
| Logistic | 1 |
| tanh | 4 |
| ReLU | $\sqrt{2}$ |



Nebraska Lincoln
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott
Introduction | Supervised Learning | Basic Units | Gradient Descent | Nonlinearly Separable Problems | Backprop | Types of Units | Putting Things Together

## Putting Everything Together
### Optimizers

Variations on gradient descent optimization:

- Momentum optimization
- AdaGrad
- RMSProp
- Adam



Nebraska Lincoln
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott
Introduction | Supervised Learning | Basic Units | Gradient Descent | Nonlinearly Separable Problems | Backprop | Types of Units | Putting Things Together

## Putting Everything Together
### Momentum Optimization

- Use a **momentum** term $\beta$ to keep updates moving in same direction as previous trials
- Replace original GD update $\mathbf{w}' = \mathbf{w} - \eta\nabla J(\mathbf{w})$ with

$$\mathbf{w}' = \mathbf{w} - \mathbf{m} \ ,$$

where

$$\mathbf{m} = \beta\mathbf{m} + \eta\nabla J(\mathbf{w})$$

- Using sigmoid activation and square loss, replace $\Delta w_{ji}^t = \eta\,\delta_j^t\,x_{ji}^t$ with

$$\Delta w_{ji}^t = \eta\,\delta_j^t\,x_{ji}^t + \beta\,\Delta w_{ji}^{t-1}$$

- Can help move through small local minima to better ones & move along flat surfaces

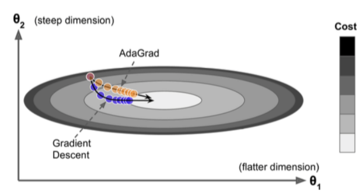


Nebraska Lincoln
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott
Introduction | Supervised Learning | Basic Units | Gradient Descent | Nonlinearly Separable Problems | Backprop | Types of Units | Putting Things Together

## Putting Everything Together
### AdaGrad

- Standard GD can too quickly descend steepest slope, then slowly crawl through a valley
- **AdaGrad** adapts learning rate by scaling it down in steepest dimensions:
  $\mathbf{w}' = \mathbf{w} - \eta\nabla J(\mathbf{w}) \oslash \sqrt{\mathbf{s}+\epsilon}$, where
  $\mathbf{s} = \mathbf{s} + \nabla J(\mathbf{w}) \otimes \nabla J(\mathbf{w})$ ,
  $\otimes$ and $\oslash$ are element-wise multiplication and division and $\epsilon = 10^{-10}$ prevents division by 0

$\mathbf{s}$ accumulates squares of gradient, and learning rate for each dimension scaled down






Nebraska Lincoln
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott
Introduction | Supervised Learning | Basic Units | Gradient Descent | Nonlinearly Separable Problems | Backprop | Types of Units | Putting Things Together

## Putting Everything Together
### RMSProp

- AdaGrad tends to stop too early for neural networks due to over-aggressive downscaling
- **RMSProp** exponentially decays old gradients to address this

$$\mathbf{w}' = \mathbf{w} - \eta\nabla J(\mathbf{w}) \oslash \sqrt{\mathbf{s}+\epsilon} \ ,$$

where

$$\mathbf{s} = \beta\mathbf{s} + (1-\beta)\nabla J(\mathbf{w}) \otimes \nabla J(\mathbf{w})$$



Nebraska Lincoln
CSCE 496/896 Lecture 2: Basic Artificial Neural Networks
Stephen Scott
Introduction | Supervised Learning | Basic Units | Gradient Descent | Nonlinearly Separable Problems | Backprop | Types of Units | Putting Things Together

## Putting Everything Together
### Adam

**Adam** (adaptive moment estimation) combines Momentum optimization and RMSProp

1. $\mathbf{m} = \beta_1\mathbf{m} + (1-\beta_1)\nabla J(\mathbf{w})$
2. $\mathbf{s} = \beta_2\mathbf{s} + (1-\beta_2)\nabla J(\mathbf{w}) \otimes \nabla J(\mathbf{w})$
3. $\mathbf{m} = \mathbf{m}/(1-\beta_1^t)$
4. $\mathbf{s} = \mathbf{s}/(1-\beta_2^t)$
5. $\mathbf{w}' = \mathbf{w} - \eta\mathbf{m} \oslash \sqrt{\mathbf{s}+\epsilon}$

- Iteration counter $t$ used in 3 and 4 to prevent $\mathbf{m}$ and $\mathbf{s}$ from vanishing
- Can set $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$