CSCE 479/879 Lecture 2: Basic Artificial Neural Networks

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

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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

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 ≈ 0.1 second
- 100 inference steps doesn't seem like enough

$\Rightarrow$ massive parallel computation

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

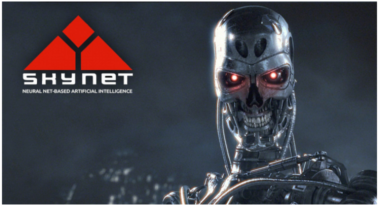
- Input is high-dimensional discrete- or real-valued (e.g., raw sensor input)
- Output is discrete- or real-valued
- Output is a vector of values
- Possibly noisy data
- Form of target function is unknown
- Human readability of result is unimportant
- Long training times acceptable

- **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

Brief 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

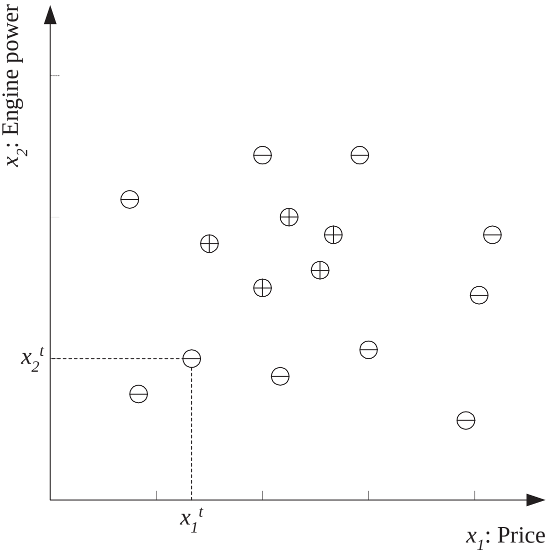
- Supervised learning
- Basic ANN units
  - Linear unit
  - Linear threshold units
  - Perceptron training rule
- Gradient Descent
- Nonlinearly separable problems and multilayer networks
- Backpropagation
- Types of activation functions
- Putting everything together

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)

Alpaydin (2014)

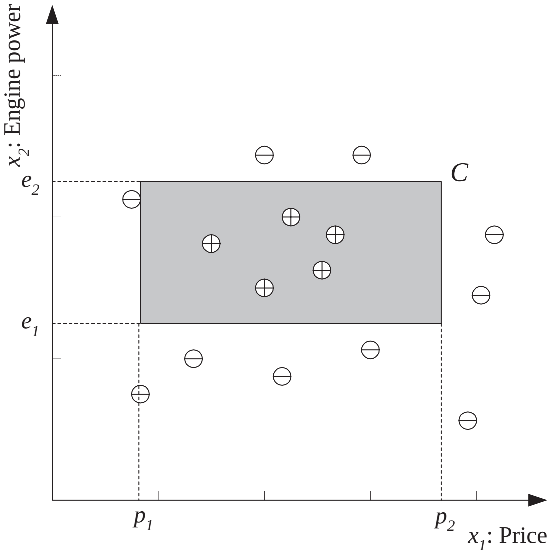


Thinking about C

- 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)

Alpaydin (2014)

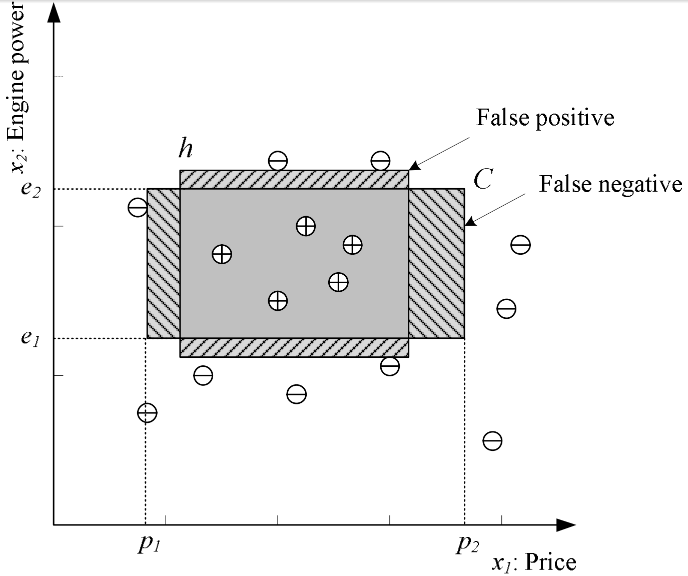


Hypotheses and Error

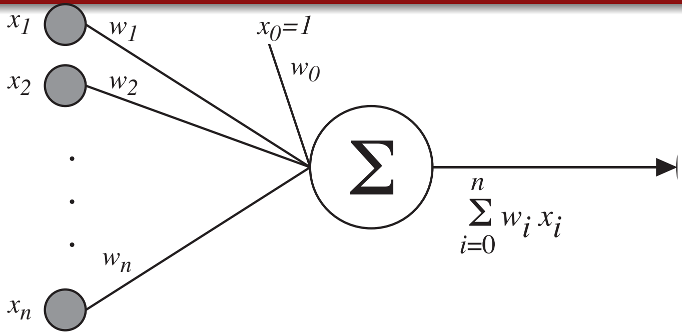
- A learning algorithm uses training set $\mathcal{X}$ and finds a hypothesis $h \in \mathcal{H}$ that approximates C
- In example, $\mathcal{H}$ can be set of all axis-parallel boxes
- If C guaranteed to come from $\mathcal{H}$, then we know that a perfect hypothesis exists
  - In this case, we choose 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**

Hypotheses and Error (cont'd)

Alpaydin (2014)



Linear Unit (Regression)
Mitchell (1997)



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

- 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)

Mitchell (1997)

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Introduction

Supervised Learning

Basic Units

Linear Unit

Linear Threshold Unit

Perceptron Training Rule

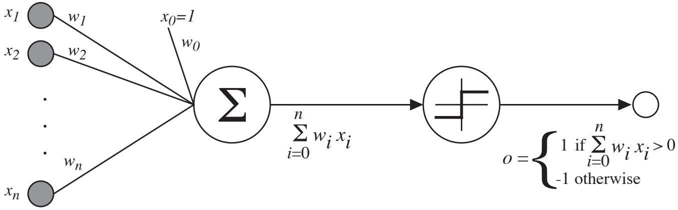
Gradient Descent

Nonlinearly Separable Problems

Backprop

Types of Units

Putting Things

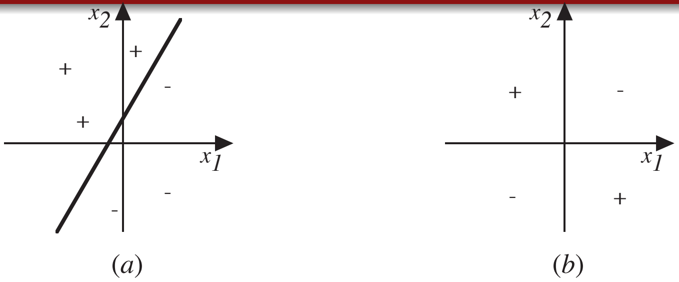


$$y = o(\boldsymbol{x}; \boldsymbol{w}, b) = \begin{cases} +1 & \text{if } f(\boldsymbol{x}; \boldsymbol{w}, b) > 0 \\ -1 & \text{otherwise} \end{cases}$$

(sometimes use 0 instead of -1)

Linear Threshold Unit

Decision Surface (Mitchell 1997)



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)

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

where

- x_j^t is jth 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

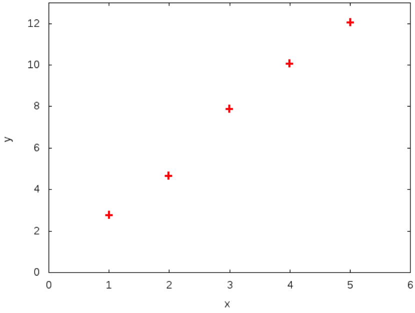
Can prove rule will converge if training data is linearly separable and η sufficiently small

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

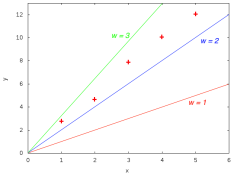
x^t	y^t
1	2.8
2	4.65
3	7.9
4	10.1
5	12.1



Where Does the Training Rule Come From?

Linear Regression

- If we use hypothesis $w_1 = 1$, then **square loss** is



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

$$= \sum_{t=1}^{m} \left(1x^t - y^t\right)^2 = (1 - 2.8)^2 + (2 - 4.65)^2 + (3 - 7.9)^2$$

$$+(4 - 10.1)^2 + (5 - 12.1)^2 = 121.8925$$

- If we use $w_2 = 2$, then we get $J(2) = 13.4925$
- Can plot $J(w_1)$ versus w_1
- Goal is to find w_1 to minimize $J(w_1)$

- Can write $J(w_1)$ in general:

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

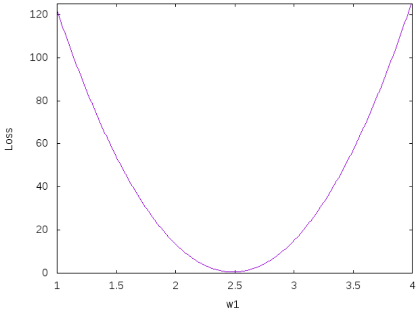
$$= (1w_1 - 2.8)^2 + (2w_1 - 4.65)^2 + (3w_1 - 7.9)^2$$

$$+(4w_1 - 10.1)^2 + (5w_1 - 12.1)^2$$

$$= 55w_1^2 - 273.4w_1 + 340.293$$

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 ≈ 0.53
- What's special about that point?

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

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

- 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:

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

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

Where Does the Training Rule Come From?
Gradient Descent Example

- In our example, initialize w_1, then repeatedly update

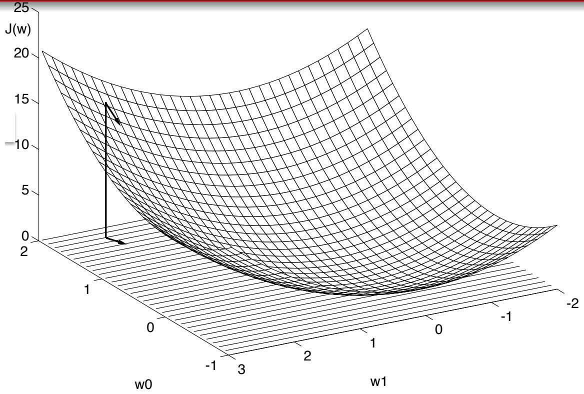
$$w_1' = w_1 - \eta(110\, w_1 - 273.4)$$

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: $\frac{\partial J}{\partial w_1} = 2w_1\,(x^t)^2 - 2x^t y^t$
  - $\Rightarrow$ **Stochastic gradient descent** (SGD)

Where Does the Training Rule Come From?

Gradient Descent (Mitchell 1997)

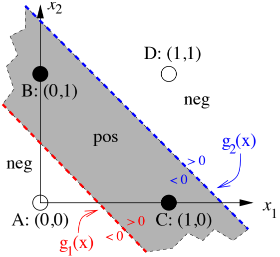


$$\frac{\partial J}{\partial \mathbf{w}} = \left[\frac{\partial J}{\partial w_0}, \frac{\partial J}{\partial w_1}, \cdots, \frac{\partial J}{\partial w_n} \right]$$

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

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

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

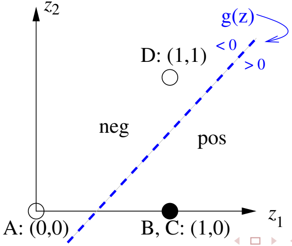
pos $= \{\boldsymbol{x} \in \mathbb{R}^2 : g_1(\boldsymbol{x}) > 0$ AND $g_2(\boldsymbol{x}) < 0\}$

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

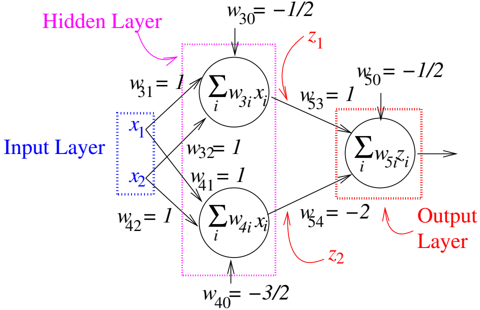
Let $z_i = \begin{cases} 0 & \text{if } g_i(\mathbf{x}) < 0 \\ 1 & \text{otherwise} \end{cases}$

Class	(x_1, x_2)	$g_1(\mathbf{x})$	z_1	$g_2(\mathbf{x})$	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 $g(\mathbf{z}) = 1 \cdot z_1 - 2 \cdot z_2 - 1/2$



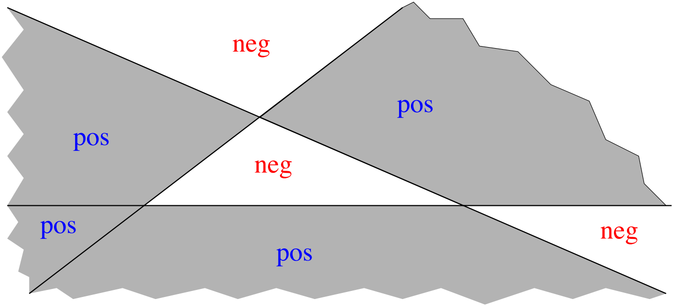
In other words, we **remapped** all vectors $\mathbf{x}$ to $\mathbf{z}$ such that the classes are linearly separable in the new vector space



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

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

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



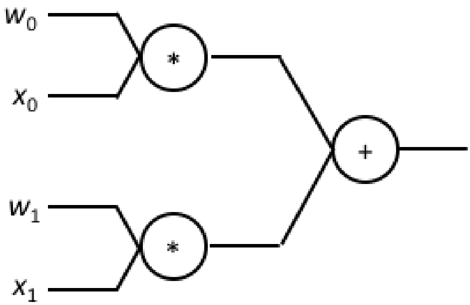
First hidden layer defines halfspaces, second hidden layer takes intersection (AND), output layer takes union (OR)

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

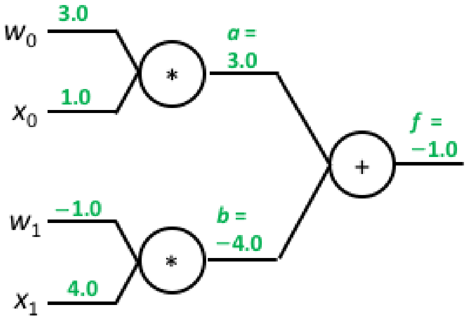
Computation Graphs

- 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** (like what we do in TensorFlow)
- E.g., let $f(\mathbf{w}, \mathbf{x}) = w_0x_0 + w_1x_1$



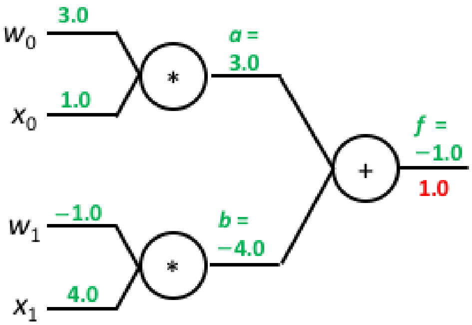
Computation Graphs

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



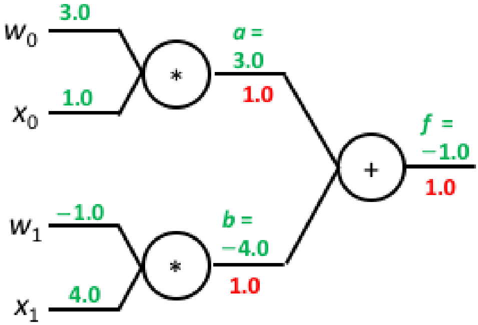
Computation Graphs

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



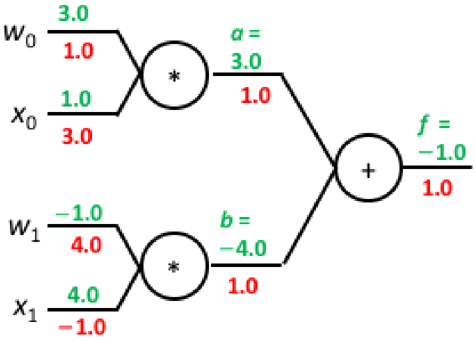
Computation Graphs

- 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

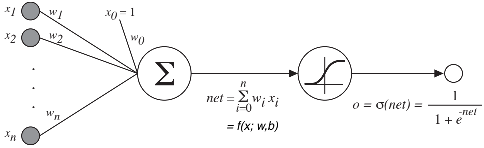
- If $h(y,z) = yz$ then $\frac{\partial h}{\partial y} = z$
- Via chain rule, $\frac{\partial f}{\partial x_0} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial x_0} = 1.0 w_0 = 3.0$



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**

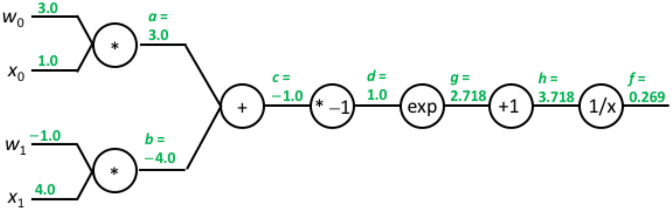
$$\sigma(net) = \frac{1}{1 + e^{-net}}$$

(a type of **sigmoid** function)

Squashes net into $[0, 1]$ range

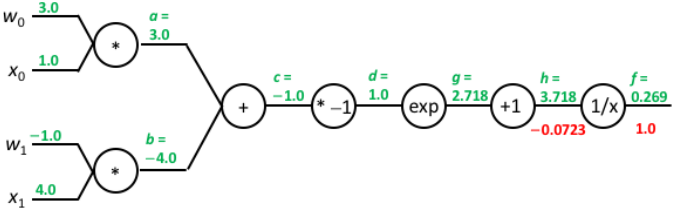
The Sigmoid Unit
Computation Graph

Let $f(\mathbf{w}, \mathbf{x}) = 1/\left(1 + \exp\left(-\left(w_0 x_0 + w_1 x_1\right)\right)\right)$



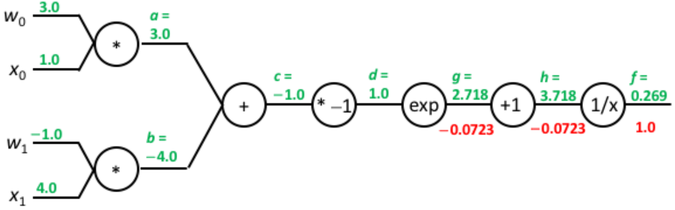
The Sigmoid Unit

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



The Sigmoid Unit
Gradient

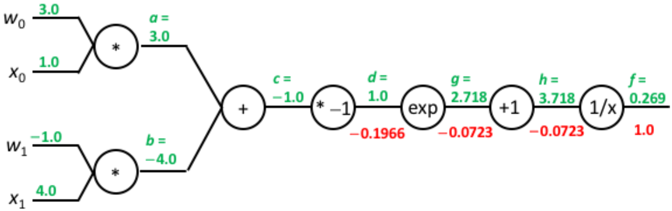
$$\frac{\partial f}{\partial g} = \frac{\partial f}{\partial h}\frac{\partial h}{\partial g} = -0.0723(1) = -0.0723$$



The Sigmoid Unit

Gradient

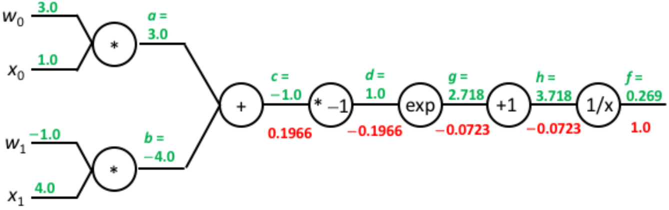
$$\frac{\partial f}{\partial d} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial d} = -0.0723\exp(d) = -0.1966$$



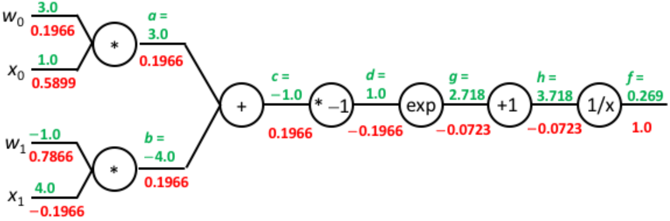
The Sigmoid Unit

Gradient

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



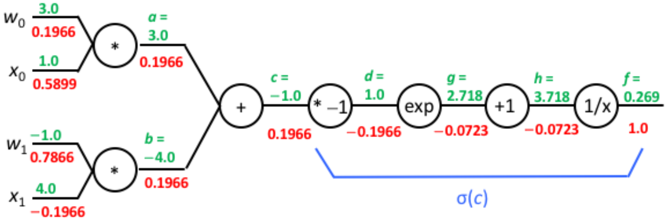
and so on:



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

The Sigmoid Unit

Gradient

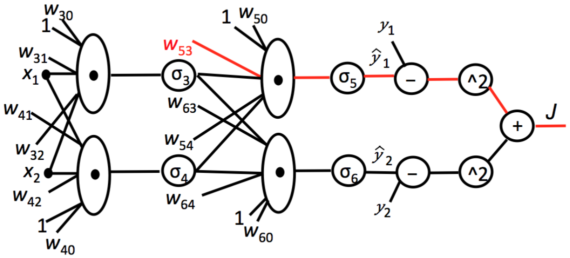


Note that $\frac{\partial f}{\partial c} = \sigma(c)(1 - \sigma(c))$, so

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

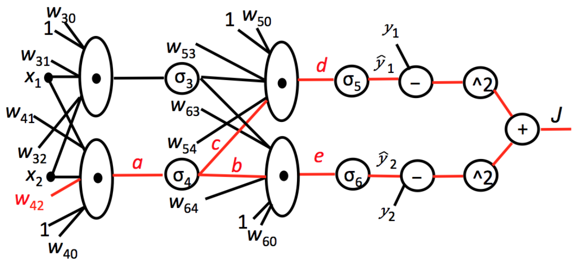
This is **modular**, so once we have a formula for the gradient for this unit, we can apply it anywhere in a larger graph

Training Multilayer Networks
Output Units



- Let loss on instance $(\mathbf{x}^t, \mathbf{y}^t)$ be $J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n} (\hat{y}_i^t - y_i^t)^2$
- 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}:

$$\frac{\partial J}{\partial w_{42}} = \frac{\partial J}{\partial a}\frac{\partial a}{\partial w_{42}} = \left(\frac{\partial J}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial J}{\partial b}\frac{\partial b}{\partial a}\right)\frac{\partial a}{\partial w_{42}}$$

$$= \left(\frac{\partial J}{\partial d}\frac{\partial d}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial J}{\partial e}\frac{\partial e}{\partial b}\frac{\partial b}{\partial a}\right)\frac{\partial a}{\partial w_{42}}$$

$$= \left([\hat{y}_1(1-\hat{y}_1)(\hat{y}_1 - y_1)]\,[w_{54}]\,[\sigma_4(a)(1-\sigma_4(a))]\right.$$

$$\left. + \; [\hat{y}_2(1-\hat{y}_2)(\hat{y}_2 - y_2)]\,[w_{64}]\,[\sigma_4(a)(1-\sigma_4(a))]\right) x_2$$

- Analytical solution is messy, but we don't need the formula; only need to **compute** gradient for specific input(s)
- 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

- We are **propagating back** error from output layer toward input layers
- 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
- All done automatically in TensorFlow, etc.: **Automatic differentiation** based on computation graph

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 δ 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

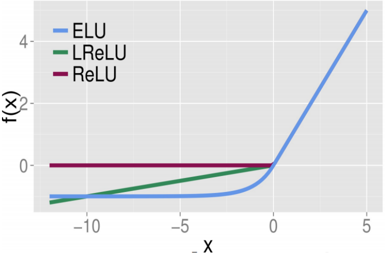
Given hidden layer outputs $\boldsymbol{h}$

- 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): $\max\{0, \boldsymbol{w}^\top \boldsymbol{x} + \boldsymbol{b}\}$

- 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

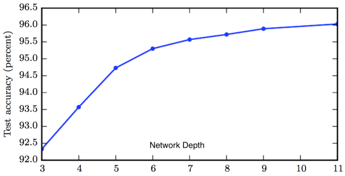


Logistic sigmoid (done already) and $\tanh$

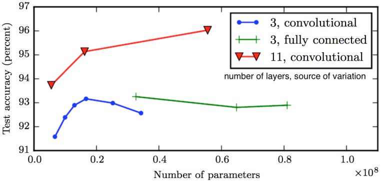
- Nice approximation to threshold, but don't train well in deep networks since they saturate

- 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



- 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	$\sqrt{2}$

Putting Everything Together

Optimizers

Variations on gradient descent optimization:

- Momentum optimization
- AdaGrad
- RMSProp
- Adam

Putting Everything Together

Momentum Optimization

- Use a **momentum** term β 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

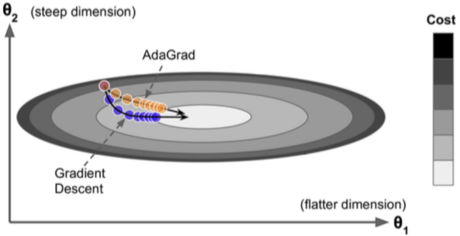
$$\Delta w_{ji}^t = \eta\, \delta_j^t\, x_{ji}^t + \beta\, \Delta w_{ji}^{t-1}$$

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

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



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

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

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 $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$