Northeastern University
College *of* Engineering

IE6600-Workshop

Introduction to Neural Networks

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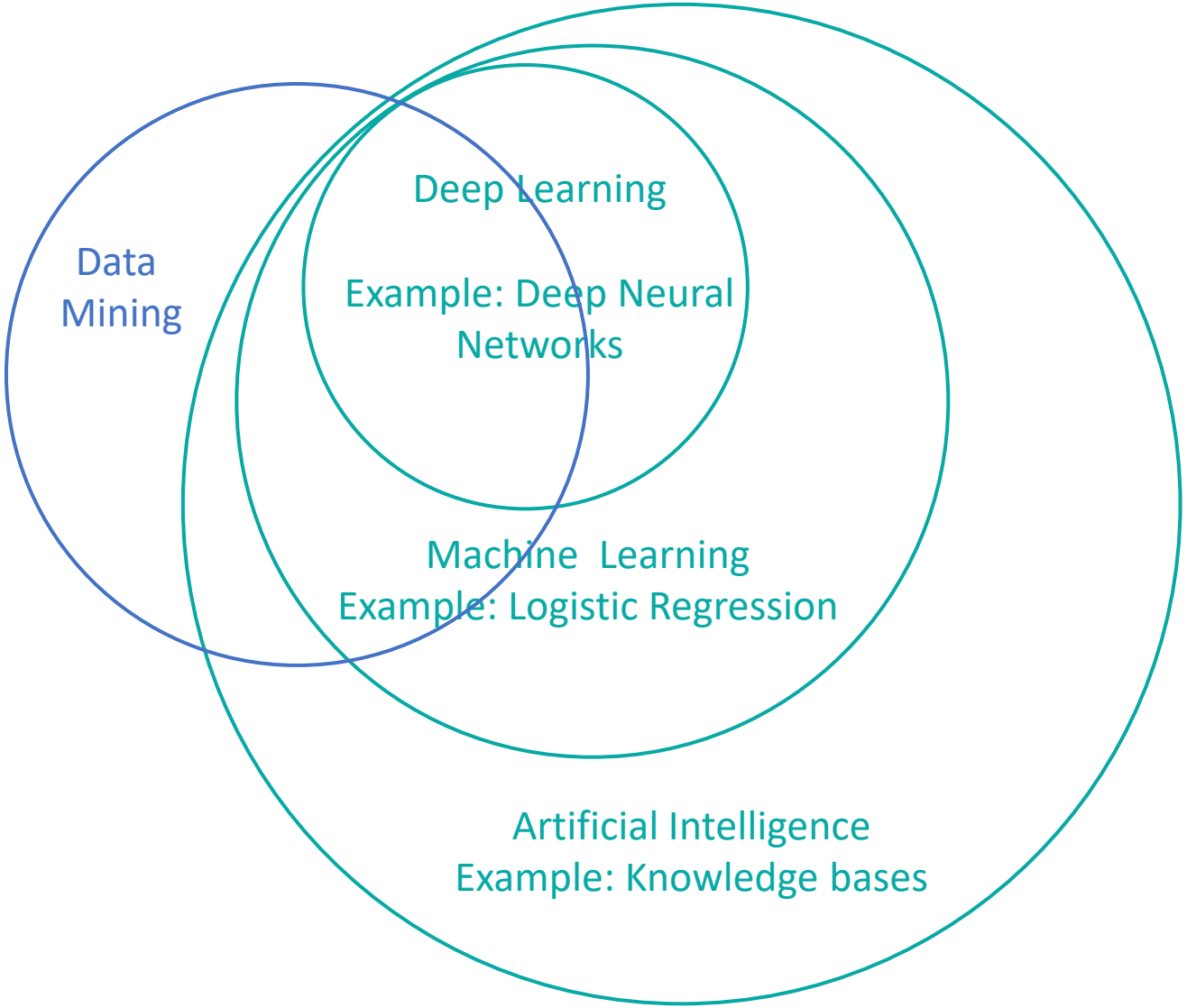
0.Introduction

Introduction



Introduction

Neural networks are a fundamental computational tool, and a very old one. They are called neural because their origins lie in the *McCulloch-Pitts neuron* (McCulloch and Pitts, 1943), But the modern no longer draws on these early biological inspirations.

Introduction *Some Denotations in Machine Learning*

A set of n×1 dimension $D(X,Y) = \{(x_i, y_i)\}_{i=1}^{n}, (x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}^n$

Statistics:

$$Y = \beta_0 + \beta_1 X * + \epsilon$$

Machine Learning:

$$Y = f(\mathrm{x}) = w_0 + w_1 x + \mathrm{b}$$

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Introduction

1-line summary of Machine Learning: $y = f(w^T x + b)$

Introduction *Generative and Discriminative Classifier*

1. Generative classifiers (e.g., Naïve Bayes):
   Imagine we're trying to distinguish dog images from cat images. A generative model would have the goal of understanding what dogs look like and what cats look like. You might literally ask such a model to 'generate', i.e. draw, a dog. Given a test image, the system then asks whether it's the cat model or the dog model that better fits (is less surprised by) the image, and chooses that as its label.

2. Discriminative classifiers (e.g., Logistic regression) :
   A discriminative model, by contrast, is only trying to learn to distinguish the classes (perhaps without learning much about them).

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Introduction *Generative and Discriminative Classifier*

A set of n points X_i in a d- dimension space, y_i denote the class for each point, with $y_i \in \{y_1, y_2, \dots, y_k\}$. Training classifiers estimates: $P(y_i|X)$

1. Generative classifiers (e.g., Naïve Bayes):
   a) Assumptions on: $P(X|y_i)P(y_i)$ $\hat{y} = arg\max_i\{P(X|y_i)P(y_i)\}$
   b) Estimate parameters of $P(X|y_i)P(y_i)$ directly from training data
   c) Use Bayes theorem to calculate $P(y_i|X)$

2. Discriminative classifiers (e.g., Logistic regression) :
   a) Assumptions on: $P(y_i|X)$
   b) Estimate parameters of $P(y_i|X)$ directly from training data

Introduction *Components of a probabilistic machine learning classifier*

Like naive Bayes, logistic regression is a probabilistic classifier that makes use of supervised machine learning.

1. A feature representation of the input. For each input observation $x_i = \{x_1, \ldots, x_d\}$
2. A classification function that computes $\hat{y}$, the estimated class, via $P(y_i|X)$, we will introduce the **sigmoid**
3. An objective function for learning, usually involving minimizing error on training examples. We will introduce **the cross-entropy loss function**
4. An algorithm for optimizing the objective function. We introduce the **stochastic gradient descent algorithm.**

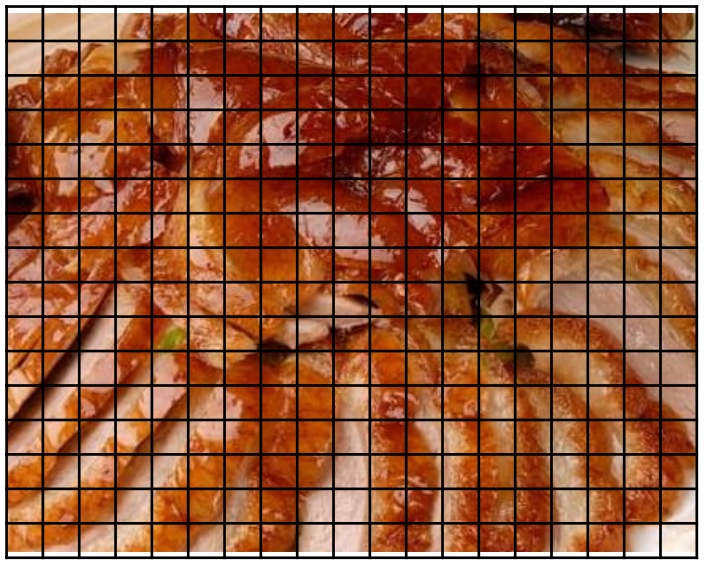
Logistic regression has two phases:

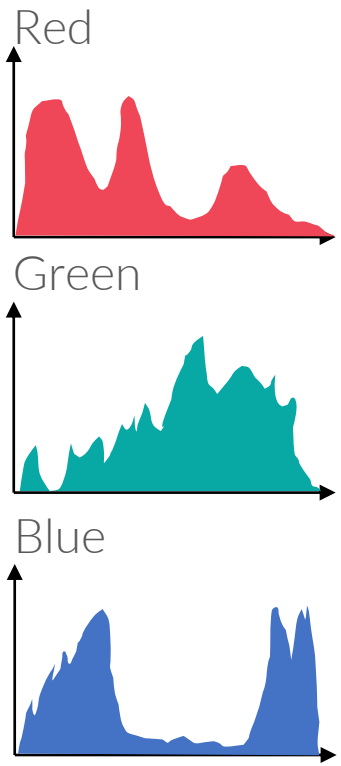
Training: we train the system (specifically the weights w and b) using stochastic gradient descent and the cross-entropy loss.

Test: Given a test example X we compute $P(y_i|X)$ and return the higher probability label $y = 1$ or $y = 0$.

Introduction

1-line summary of Machine Learning: $y = f(w^T x + b)$

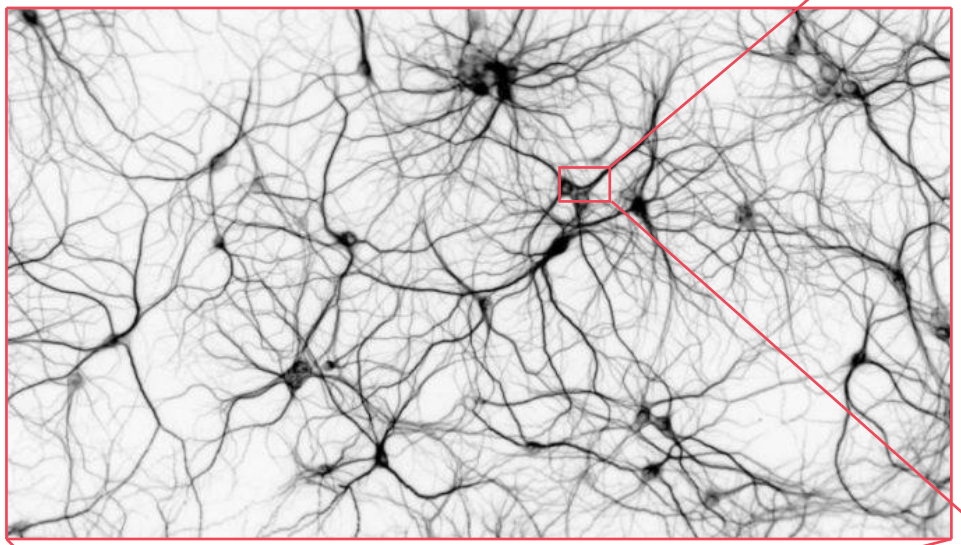


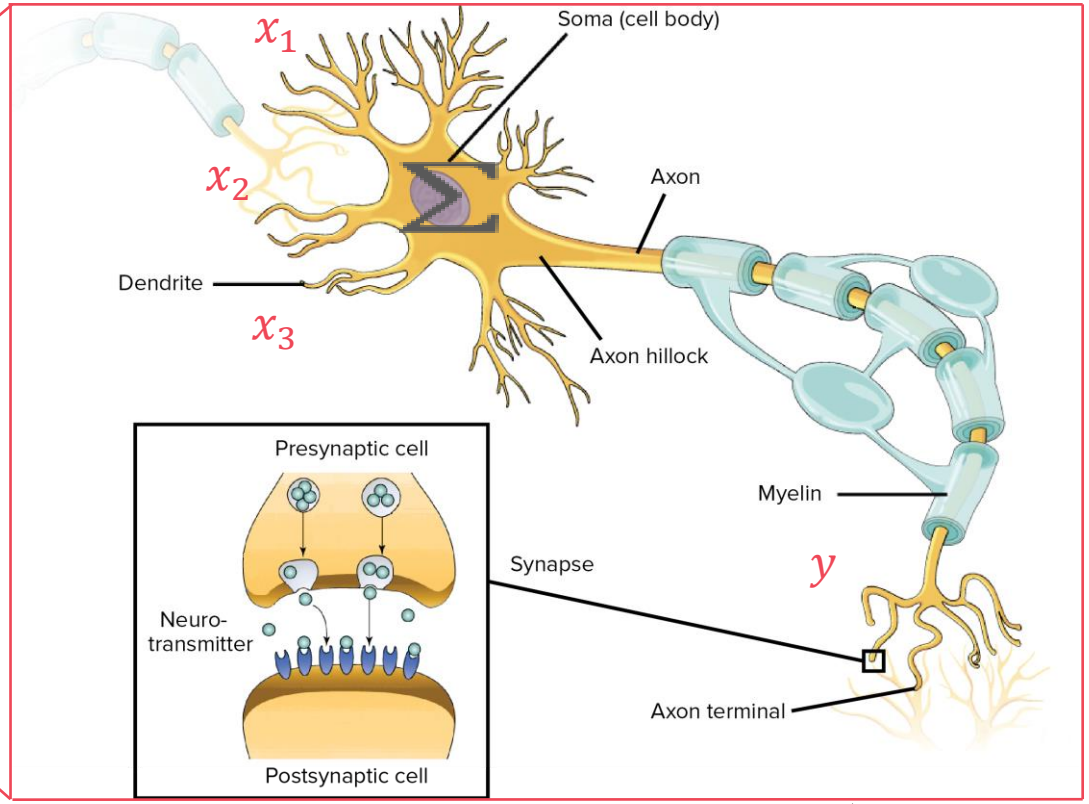


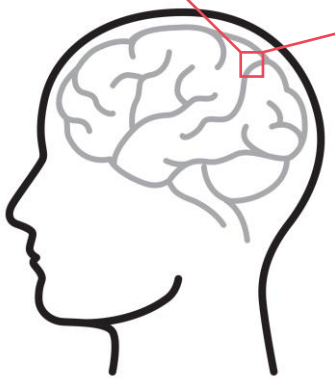
Features

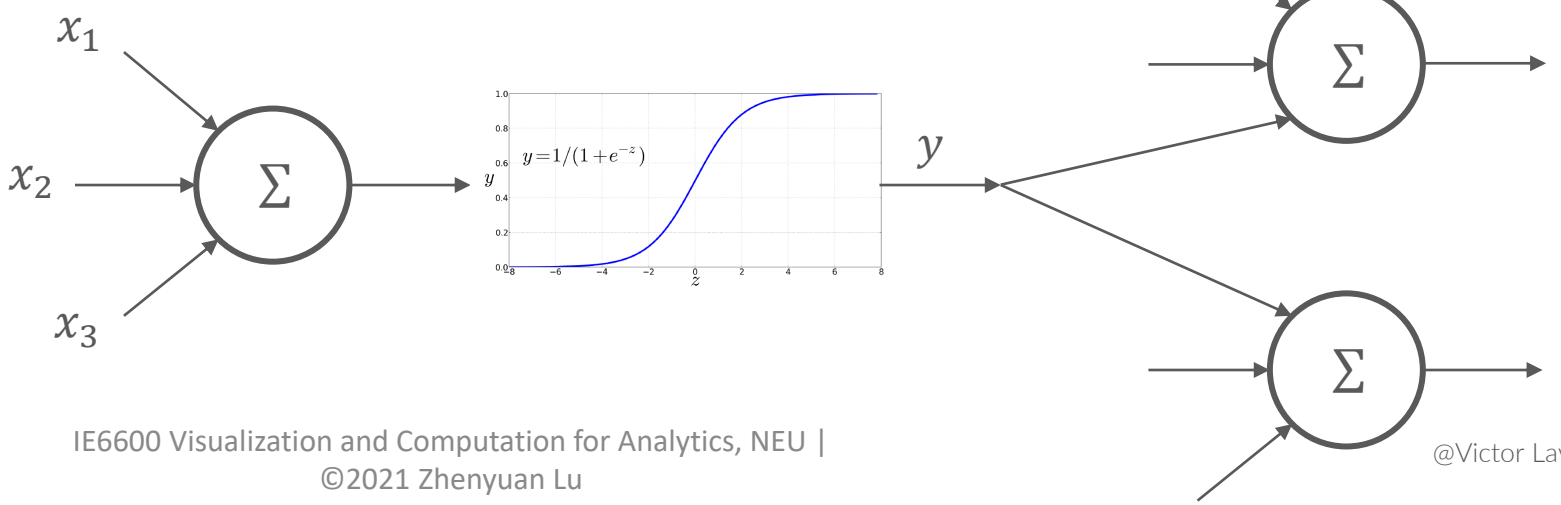
Human have the architecture of neural networks to deal with this!

Introduction *Neuron*









We don't need features

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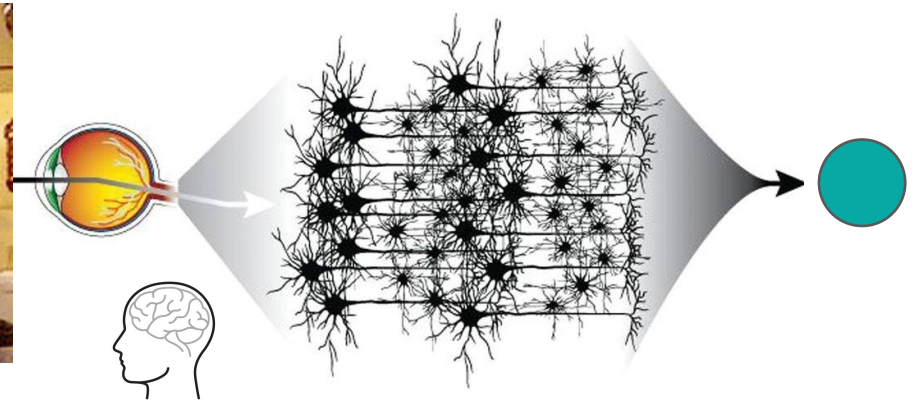
Introduction *Biological Neural Networks vs. Artificial Neural Networks*

Biological Neural Networks

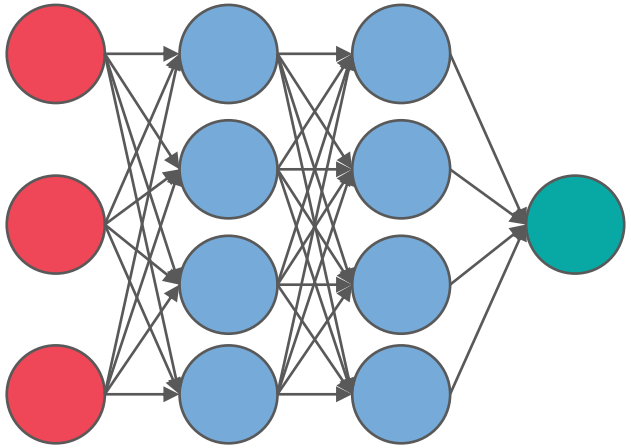
@Friends, Warner



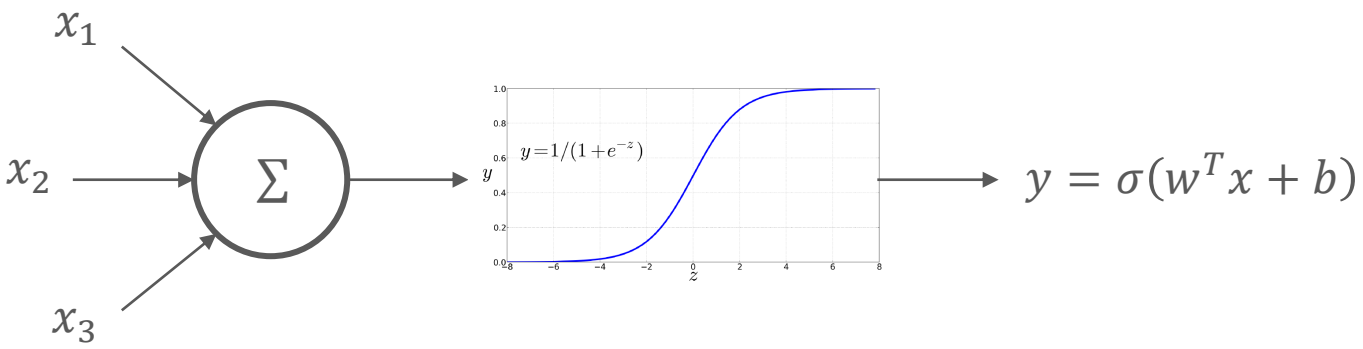
$$p(He's\ flirting) = 0.9$$

$$p(just\ saying\ Hi) = 0.1$$

Artificial Neural Networks



Introduction *Types of Neural Networks*



Single neuron: perceptron, linear/logistic regression

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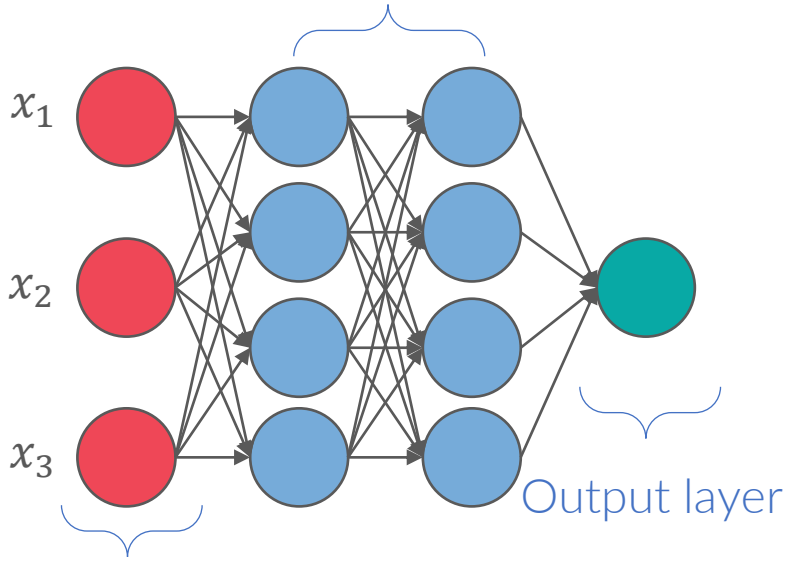
Introduction *Types of Neural Networks*

Hidden layers (Layer > 1, deep neural network)



Feed-forward network: no cycles,
Classification, and regression

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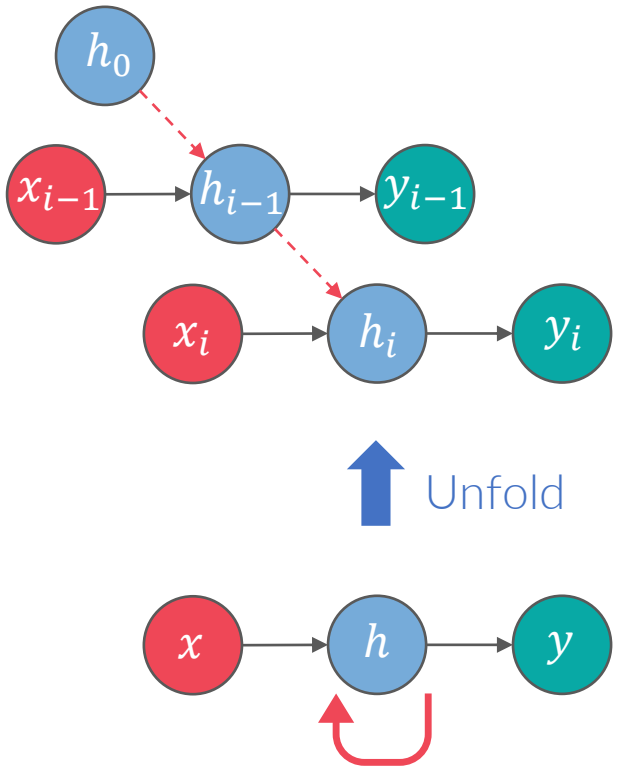
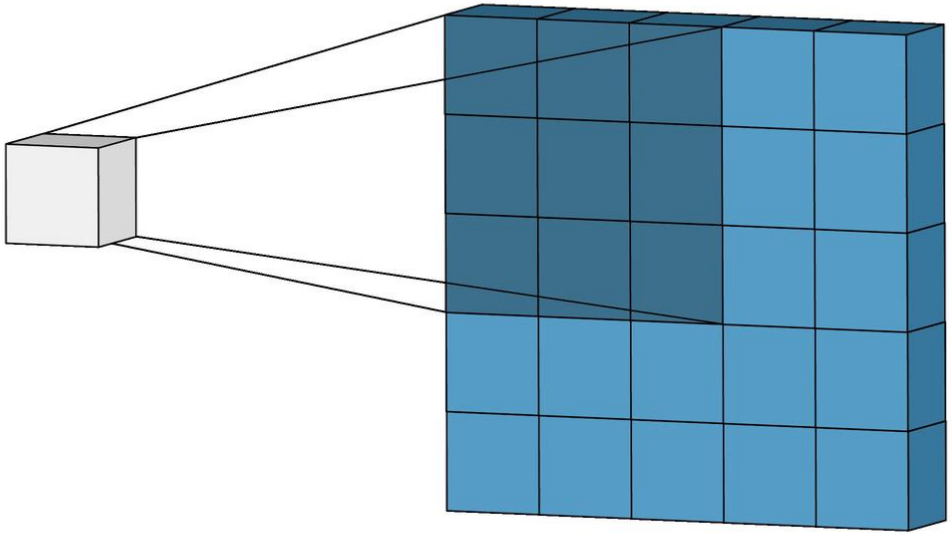
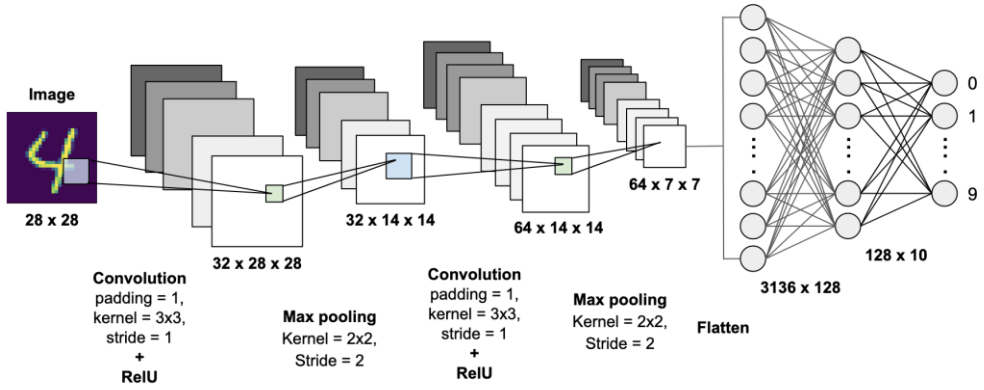
Introduction *Types of Neural Networks*



Recurrent Neural Network,
regression, and classification (NLP, etc.)

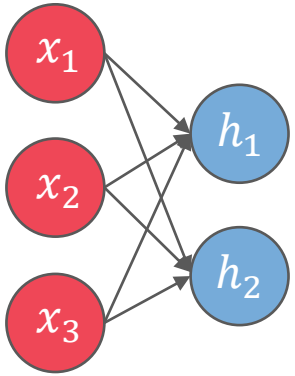
Introduction *Types of Neural Networks*





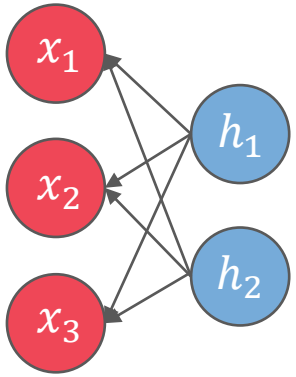
Convolutional Neural Network,
Classification (Computer vision, etc.)

Introduction *Types of Neural Networks*



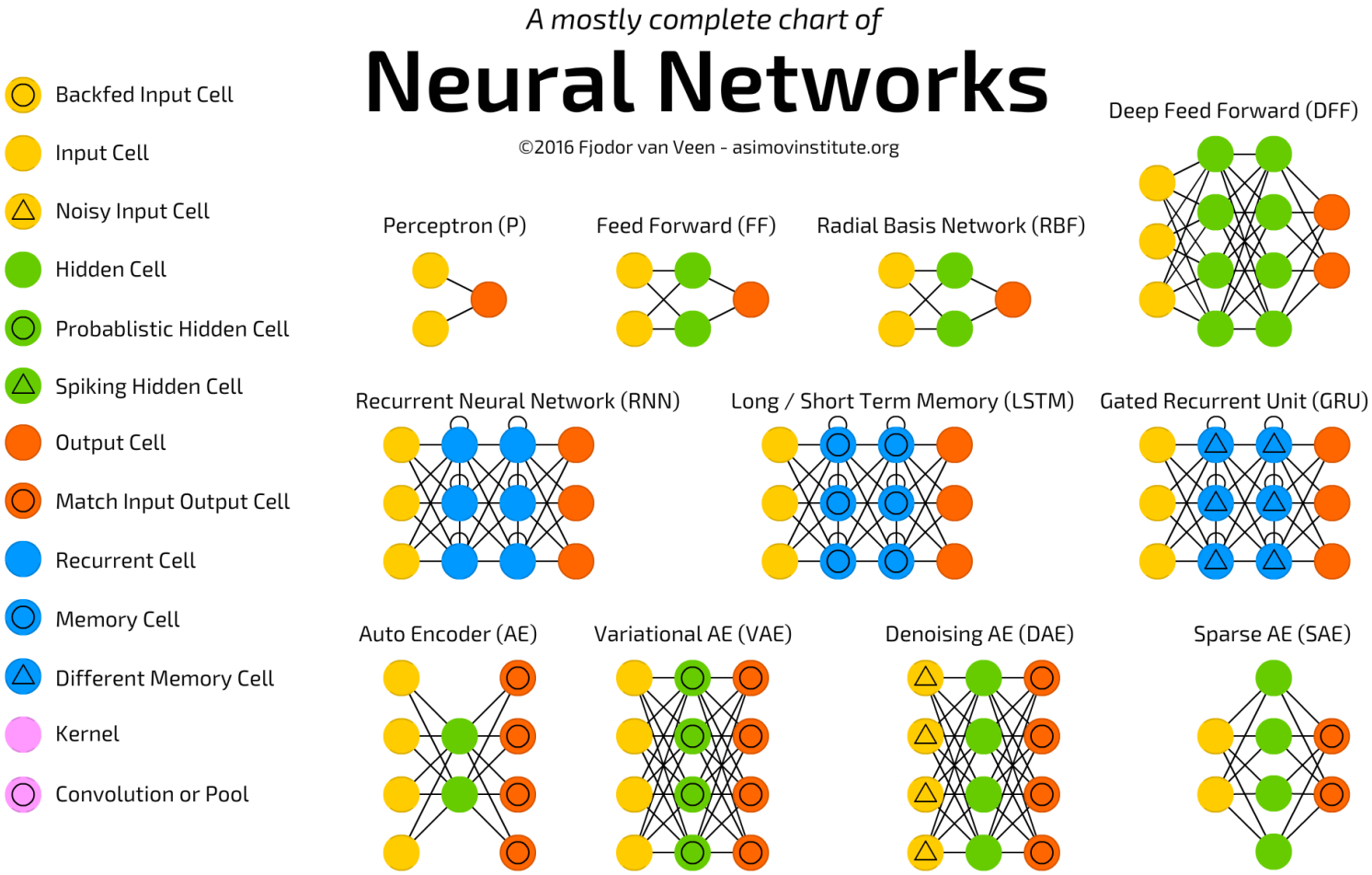
$$p(h_i|x_i) = \sigma(w^T x + b)$$

$$p(x_i|h_i) = \sigma(w^T h + B)$$

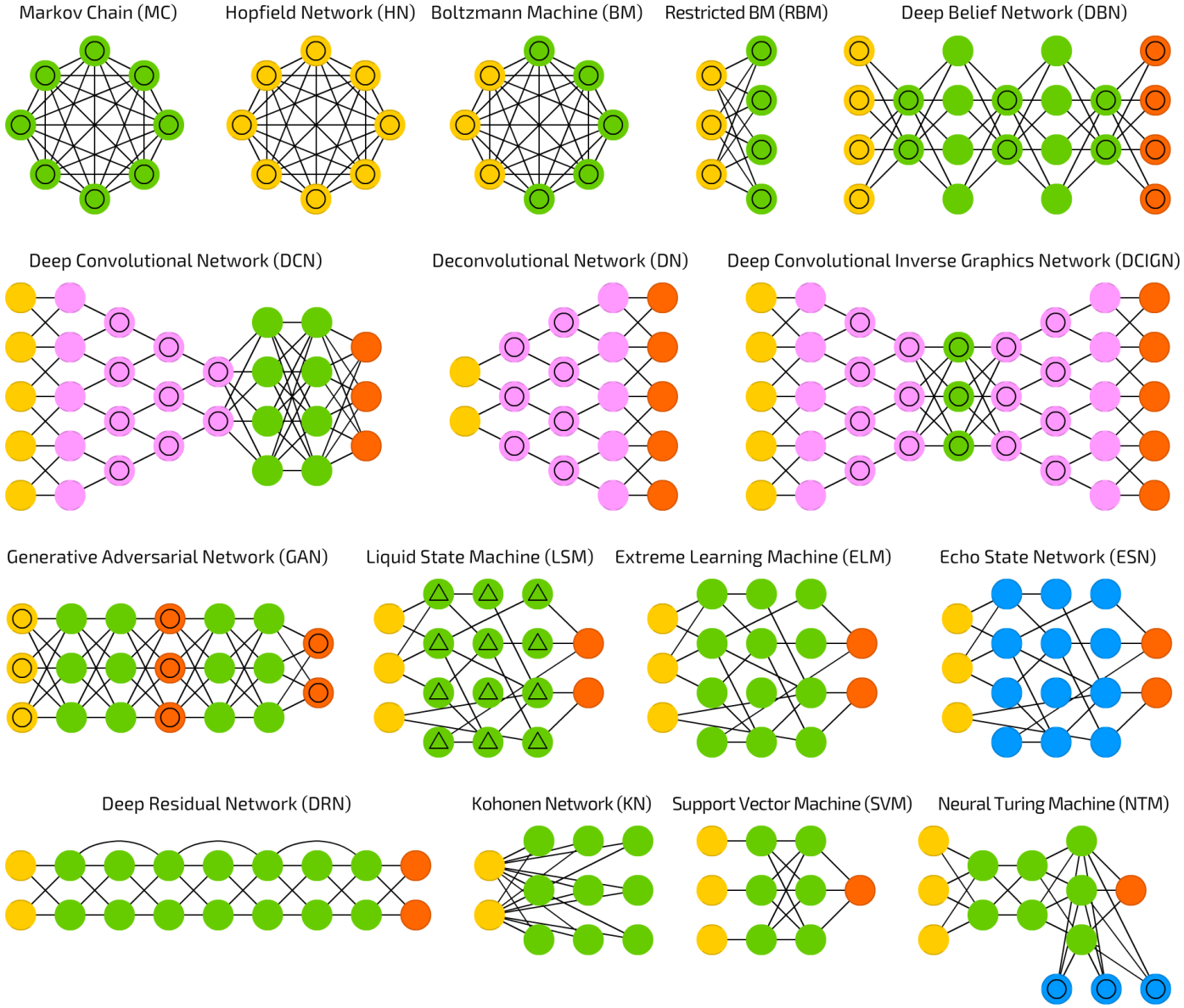


Symmetric (Restricted Boltzmann machine)
Unsupervised learning, trained to maximize the likelihood of input data

Introduction *Types of Neural Networks*



Introduction *Types of Neural Networks*



Introduction

The architecture will be introduced is called a feedforward network because the computation proceeds iteratively from one layer of units to the next. The use of modern neural nets is often called deep learning, because modern networks are often deep (have many layers).

1.Motivation of Modern Neural Network

Motivation

Neural Networks vs. Logistics Regression

Neural networks share much of the same mathematics as logistic regression. But neural networks are a more powerful classifier than logistic regression, and indeed a minimal neural network (technically one with a single 'hidden layer') can be shown to learn any function.

Units

Given a set of inputs $x_1, \ldots, x_n$, a unit has a set of corresponding weights $w_1, \ldots, w_n$ and a bias b, so the weighted sum z can be represented as:

$$z = b + \sum_i w_i x_i$$

$$z = b + w \cdot x$$

The output of this function as the activation value for the unit, α. Since we are just modeling a single unit, the activation for the node is in fact the final output of the network, which we'll generally call y.

$$y = \alpha = f(z)$$

Motivation

Activation function

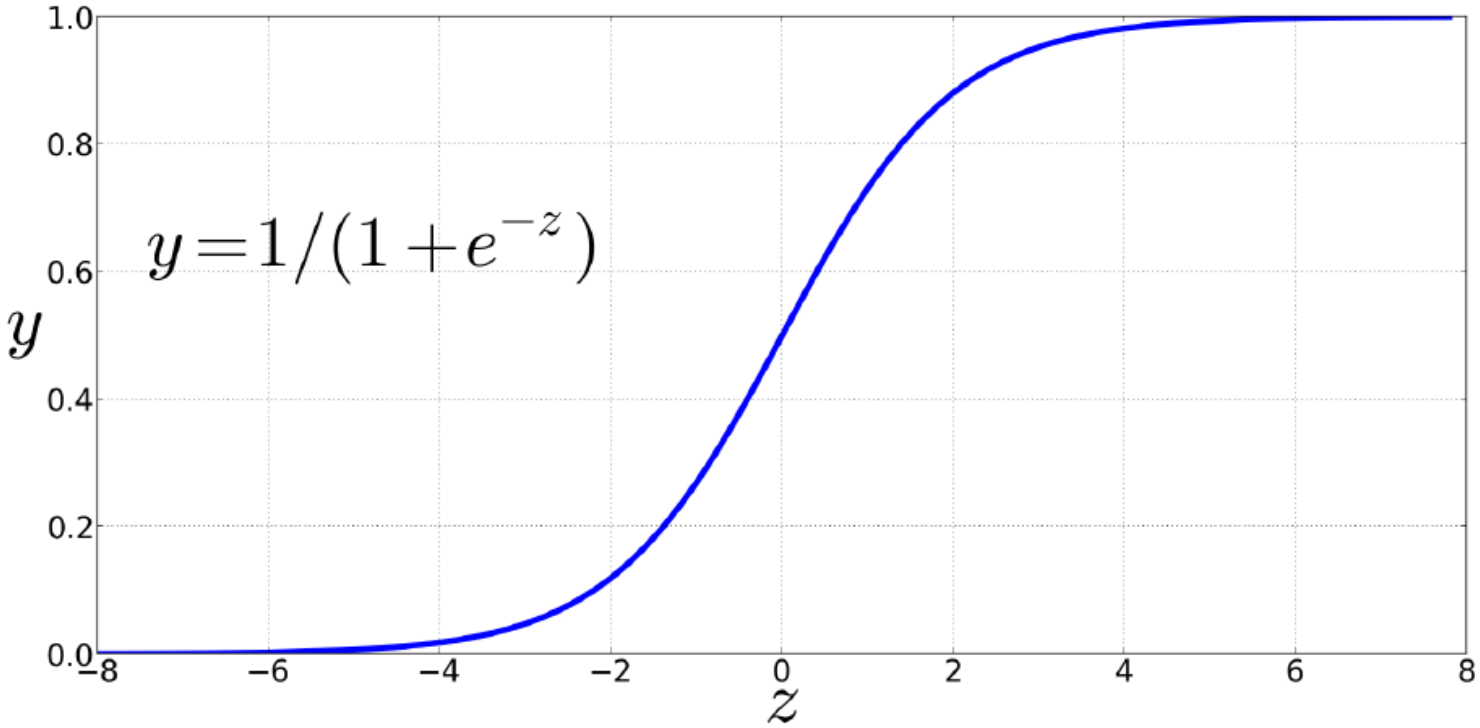
We'll discuss three popular non-linear functions $f()$,
the $sigmoid$, the $\tanh$, and the $rectified\ linear\ (ReLU)$. Here let's start with $sigmoid$

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

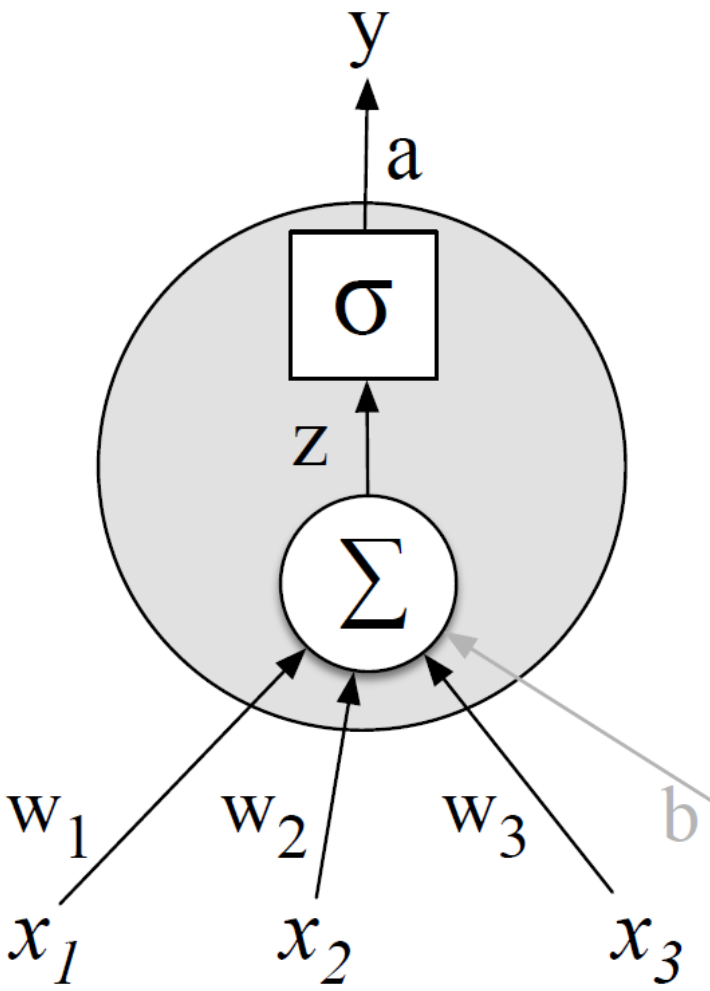
Activation Function *Sigmoid*

The range $[0,1]$, which is useful in squashing outliers toward 0 or 1.

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



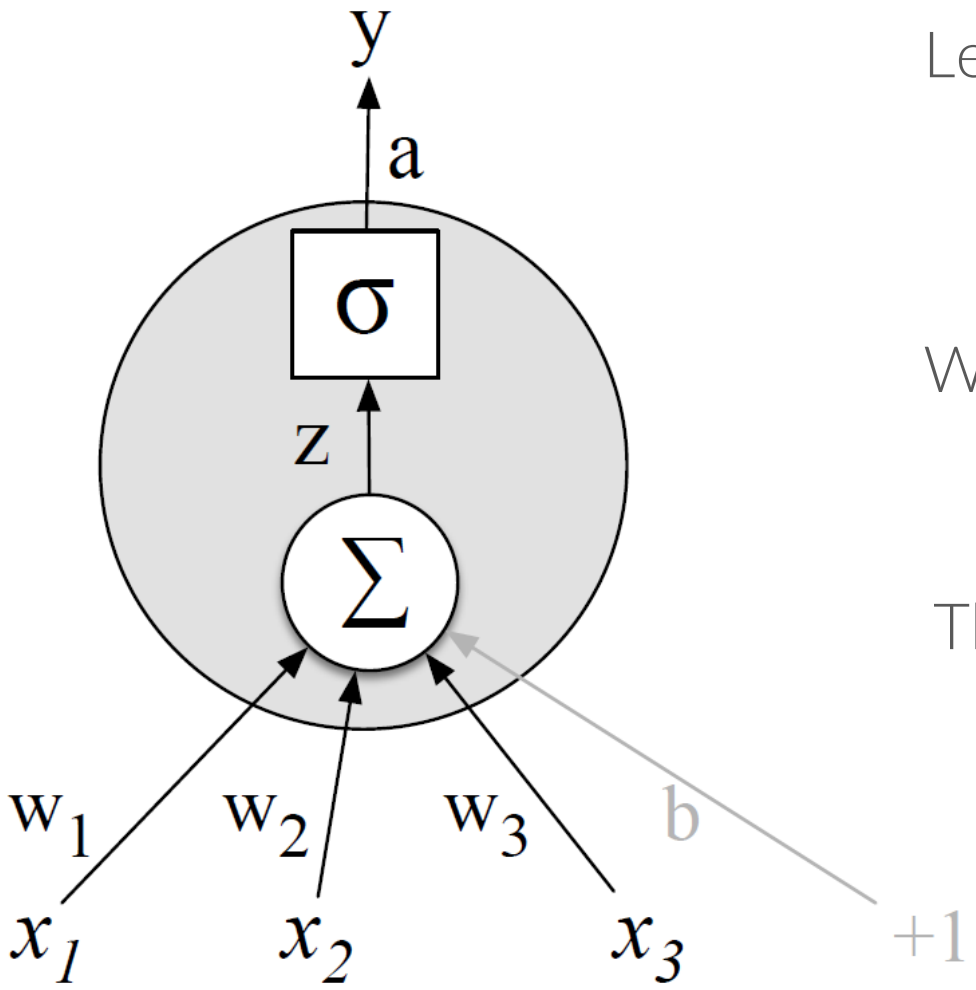
Neural Network *One single unit*



$$y = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-w \cdot x + b}}$$

$$z = w \cdot x + b$$
$$= w_1 x_1 + w_2 x_2 + w_3 x_3 + b$$

Neural Network *One single unit - Example*



Let's say

$$w = [0.2, 0.3, 0.9]$$
$$b = 0.5$$

We have input vector

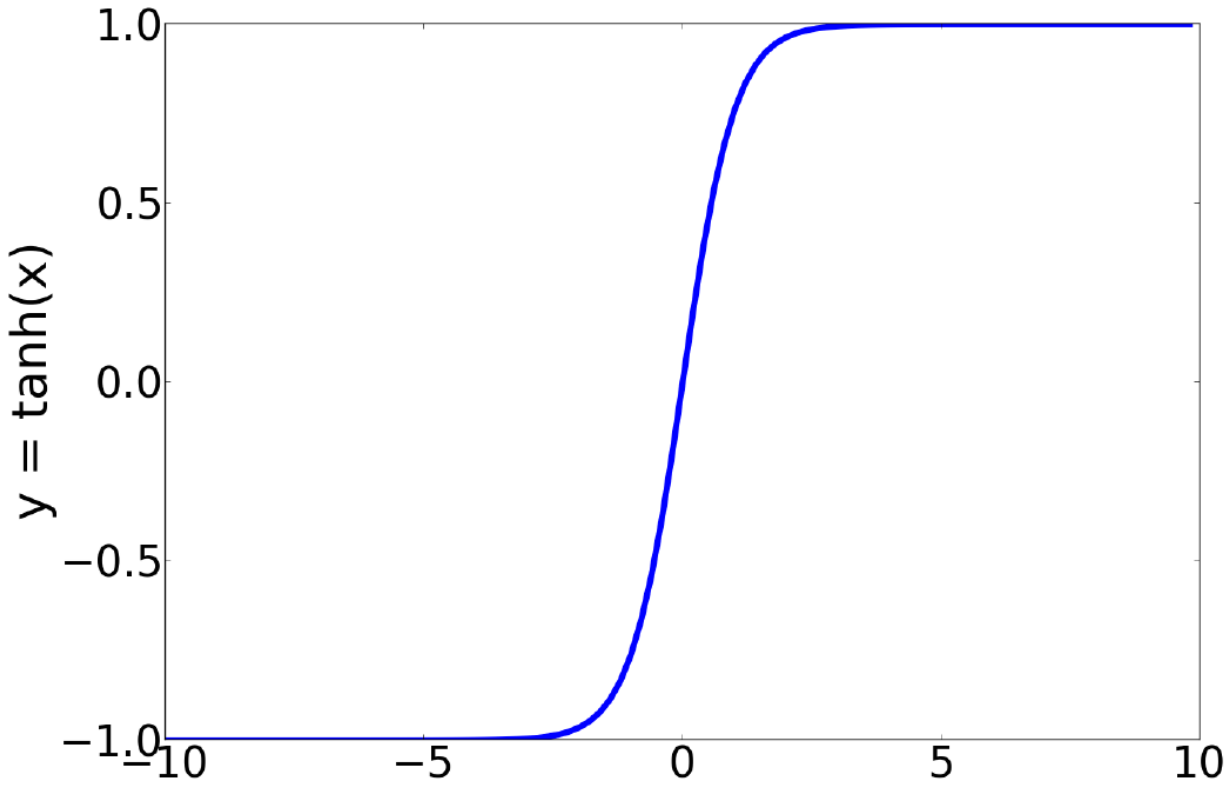
$$x = [0.5, 0.6, 0.1]$$

Then

$$y = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-w \cdot x + b}}$$
$$= \frac{1}{1 + e^{-.5*.2+.6*.3+.1*.9+.5}} = e^{-0.87} = .7$$

Other Functions *tanh*

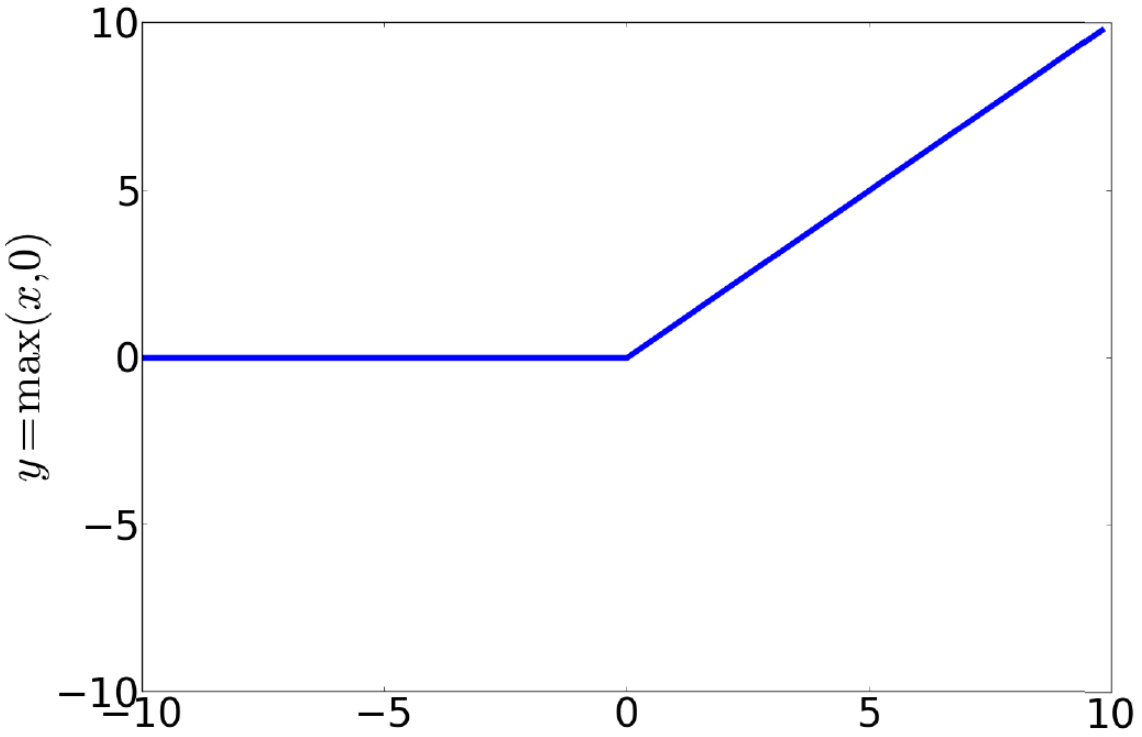
A function that is very similar but almost always better is the tanh function, tanh is a variant of the sigmoid that ranges from -1 to +1:



$$y = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$$

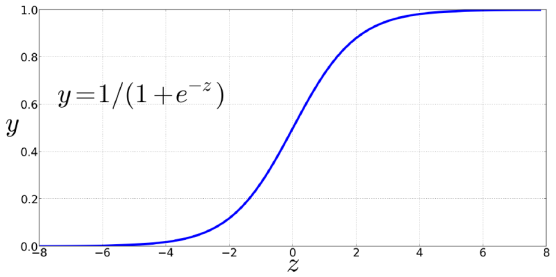
Other Functions *ReLu*

The simplest activation function, and perhaps the most commonly used, is the rectified linear unit, also called the ReLU. It's just the same as x when x is positive, and 0 otherwise:

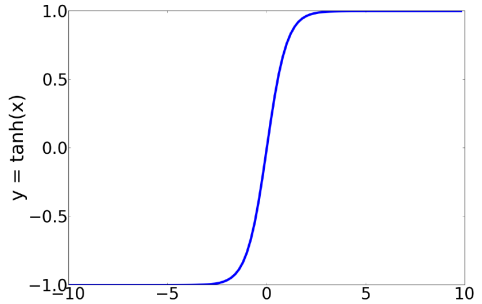


$$y = \max(x, 0)$$

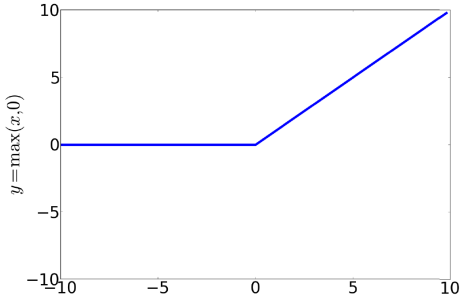
Activation Functions *Comparison*



sigmoid, very high values of z result in values of y that are saturated, extremely close to 1



tanh, being smoothly differentiable and mapping outlier values toward the mean

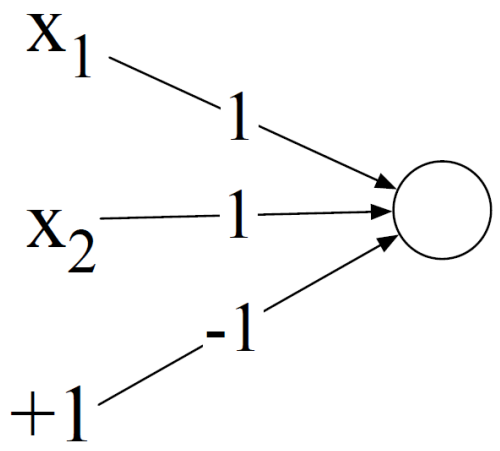


ReLu, close to linear, handy, won't be saturated

Motivation *The AND problem*

AND		
x1	x2	y
0	0	0
0	1	0
1	0	0
1	1	1

$$y = \begin{cases} 0, if\ w \cdot x + b \leq 0 \\ 1, if\ w \cdot x + b > 0 \end{cases}$$



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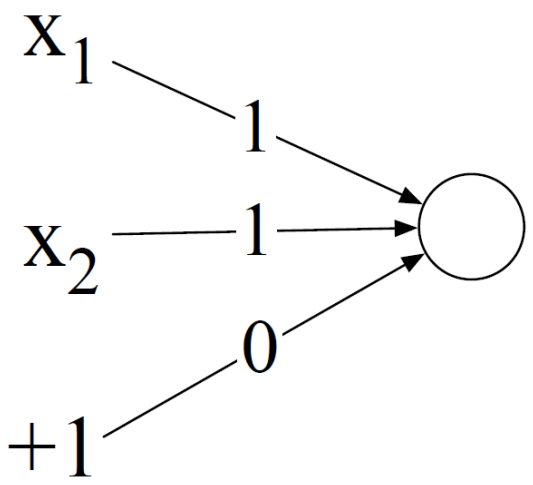
Motivation *The OR problem*

OR		
x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	1

$$y = \begin{cases} 0, if\ w \cdot x + b \leq 0 \\ 1, if\ w \cdot x + b > 0 \end{cases}$$



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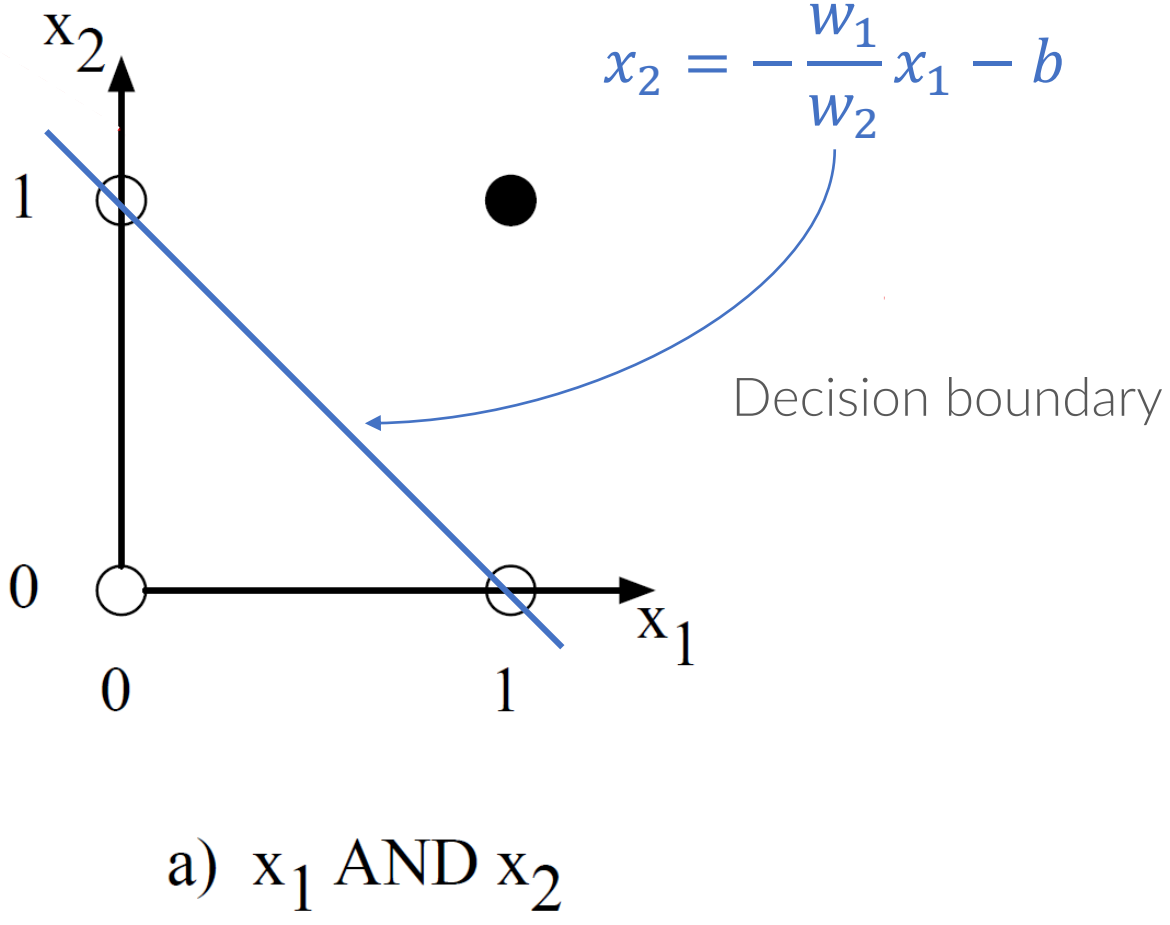
Motivation *The OR problem*

$$w_1 x_1 + w_2 x_2 + b = 0$$



a) x_1 AND x_2

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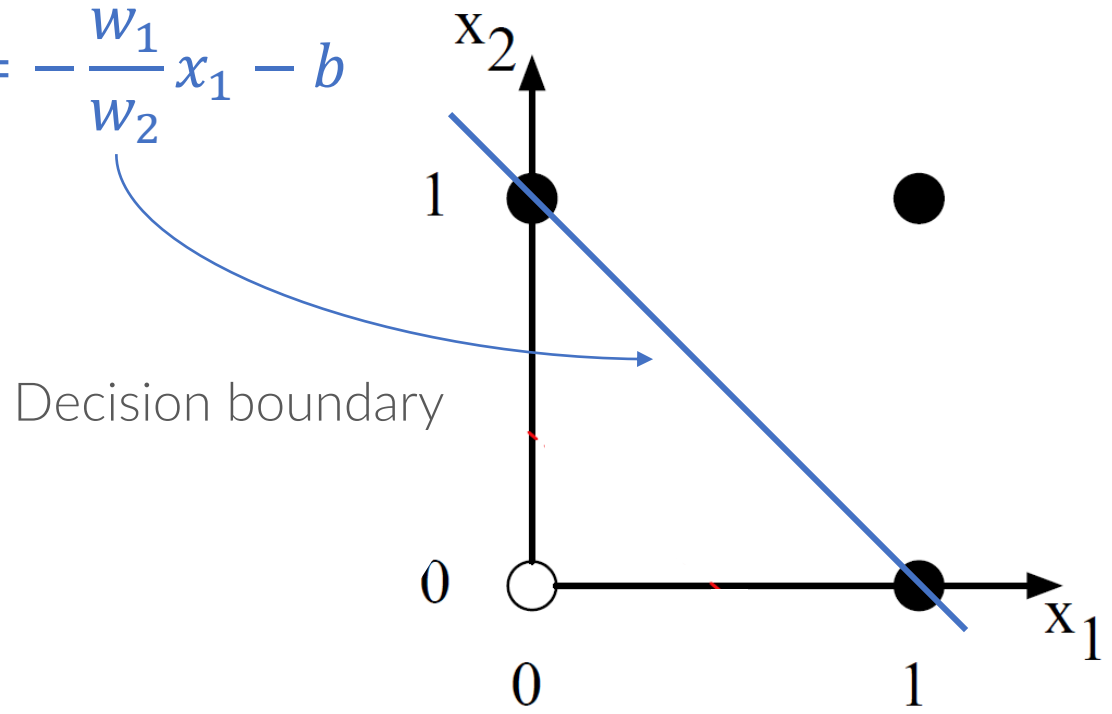
Motivation *The OR problem*

$$w_1 x_1 + w_2 x_2 + b = 0$$

$$x_2 = -\frac{w_1}{w_2} x_1 - b$$



b) x_1 OR x_2

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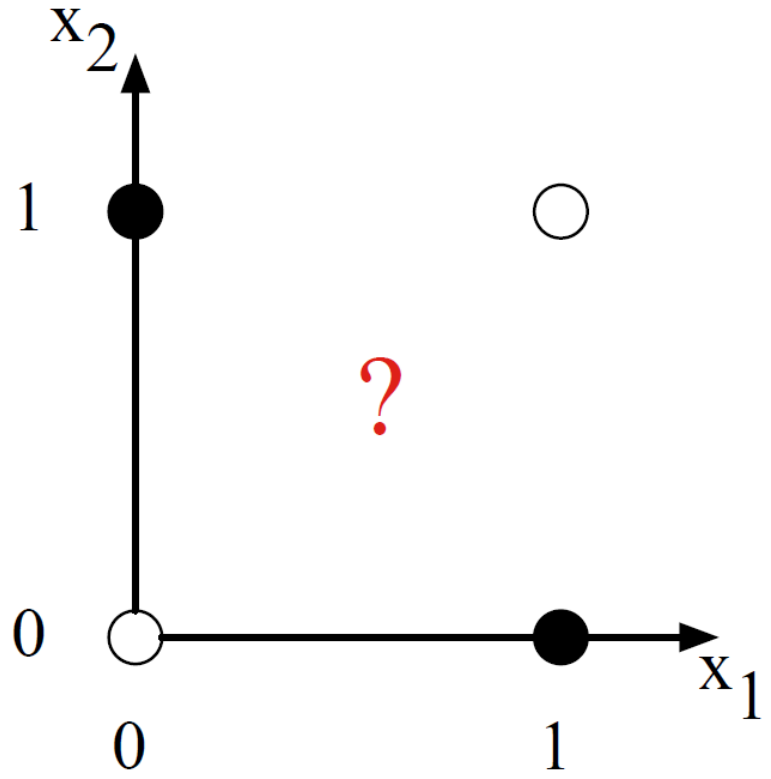
Motivation *The XOR problem*

XOR is not a linearly separable function

XOR		
x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0



c) x_1 XOR x_2

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Motivation *The XOR problem*

XOR is not a linearly separable function

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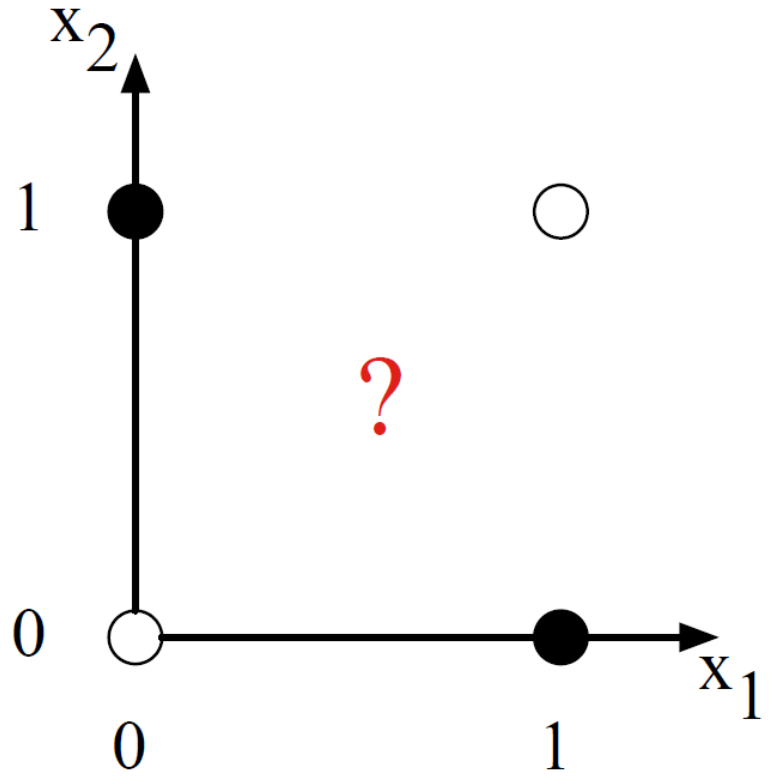

c) x_1 XOR x_2

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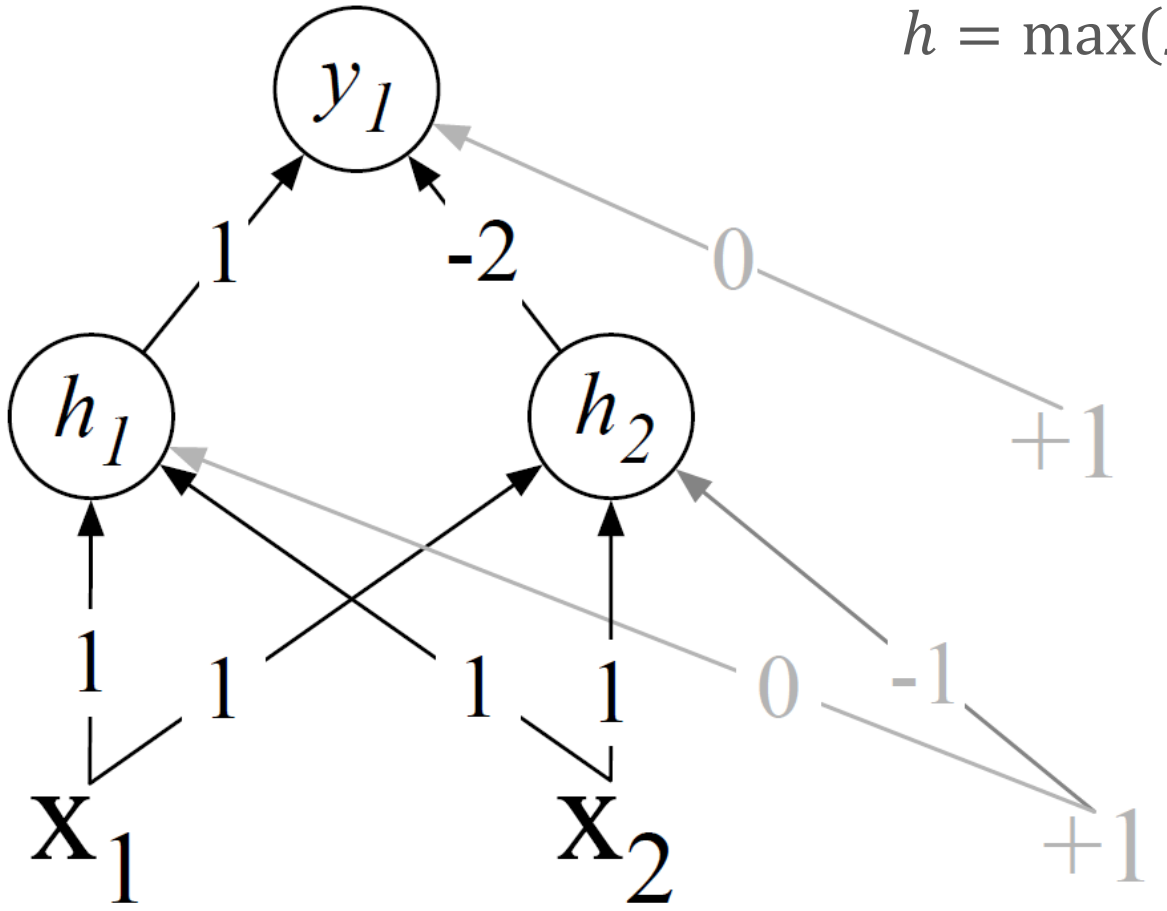
Motivation *The XOR problem*

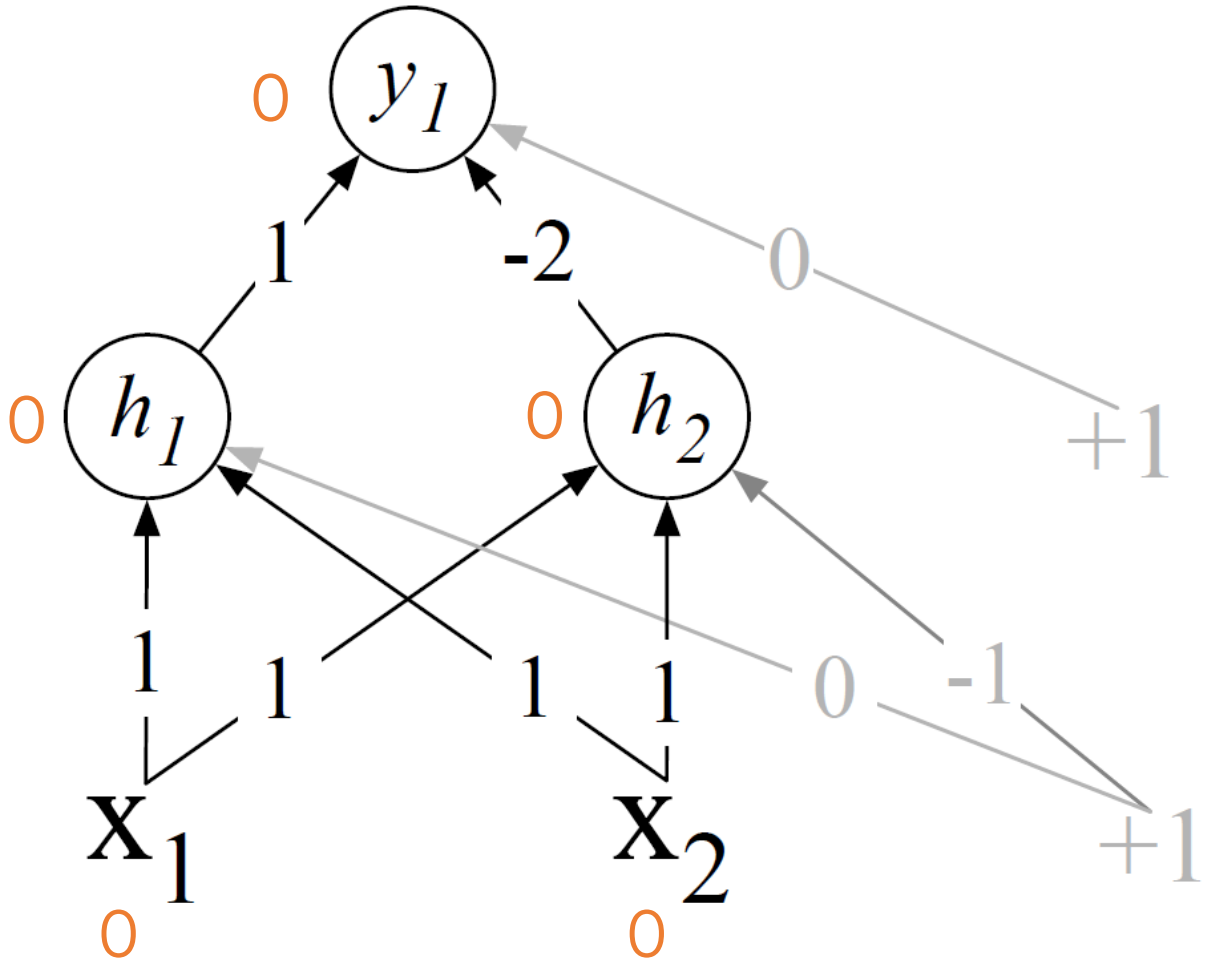


$$h = \max(x, 0)$$

XOR		
x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

Goodfellow et al. 2016

Motivation *The XOR problem*



XOR		
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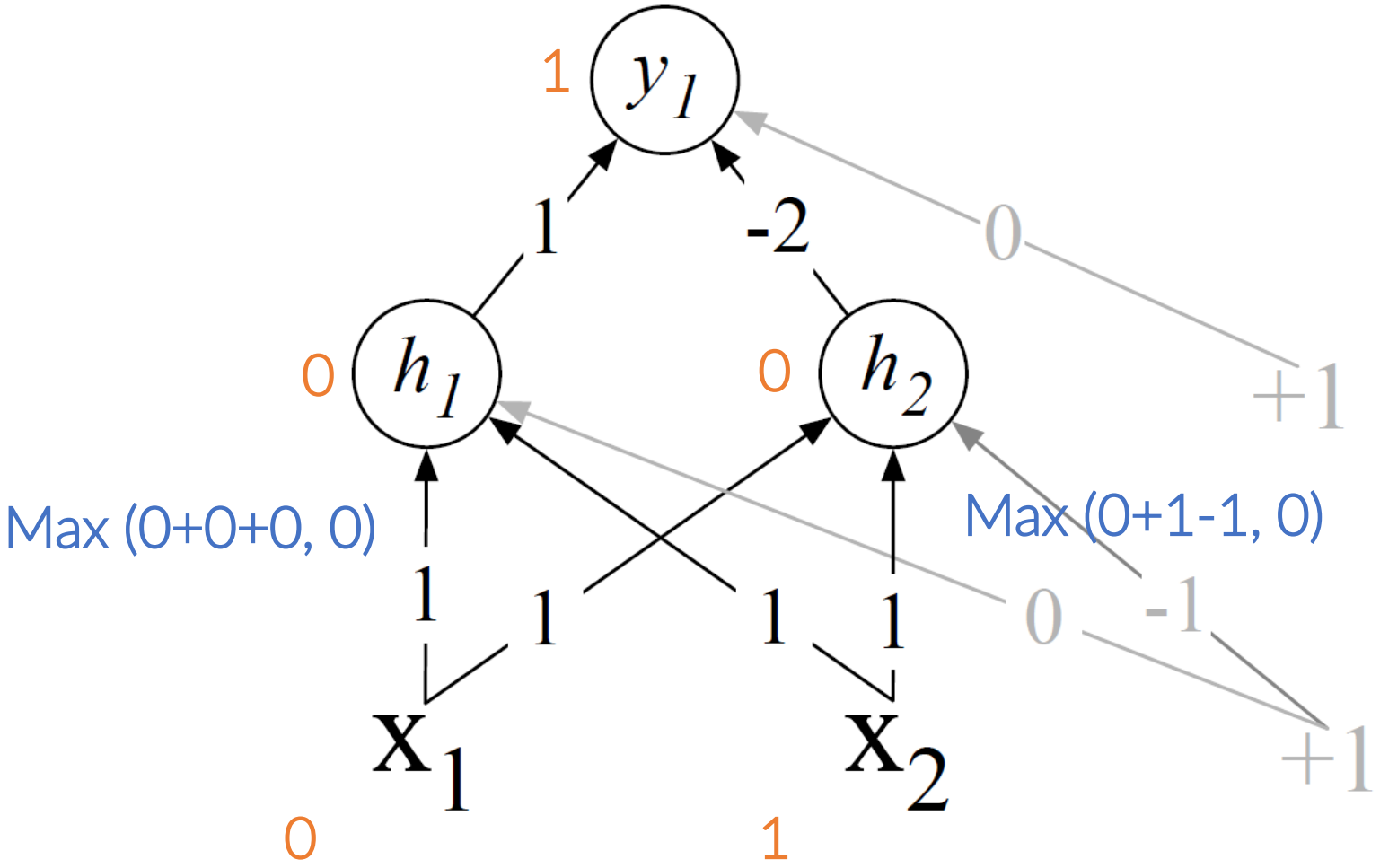
Goodfellow et al. 2016

Motivation *The XOR problem*



XOR		
x1	x2	y
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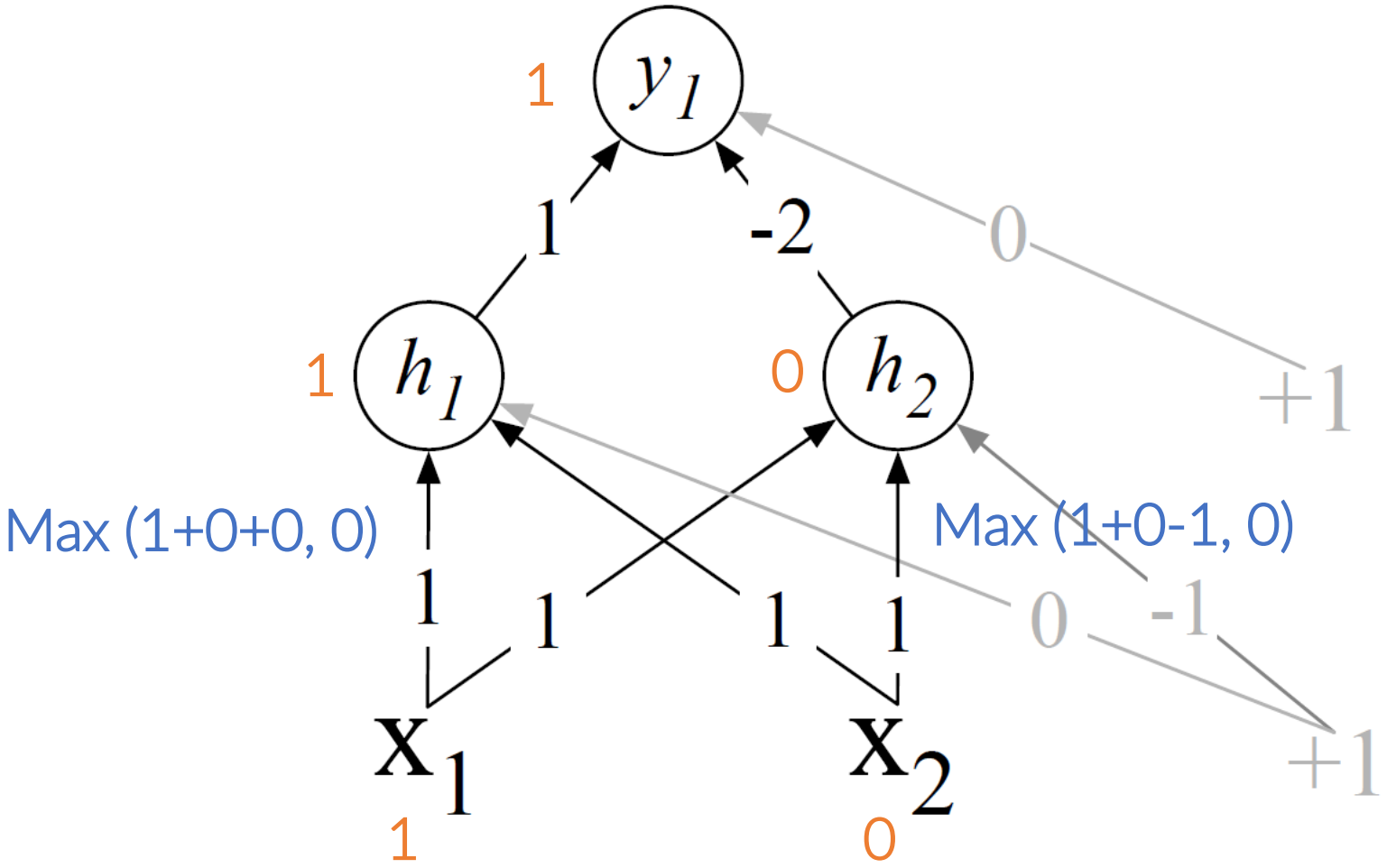
1	0	1
1	1	0

Goodfellow et al. 2016

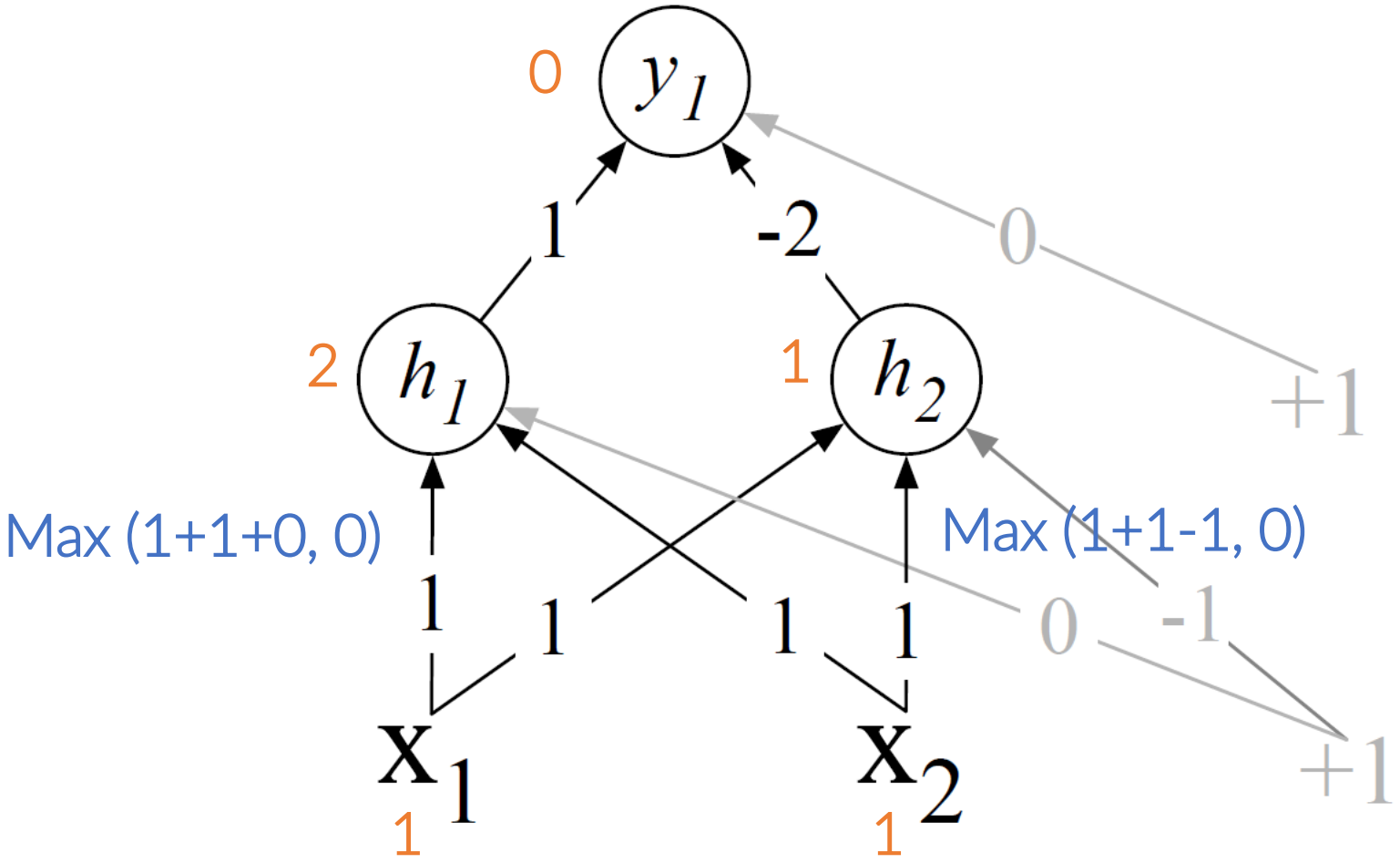
Motivation *The XOR problem*



XOR		
x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

Goodfellow et al. 2016

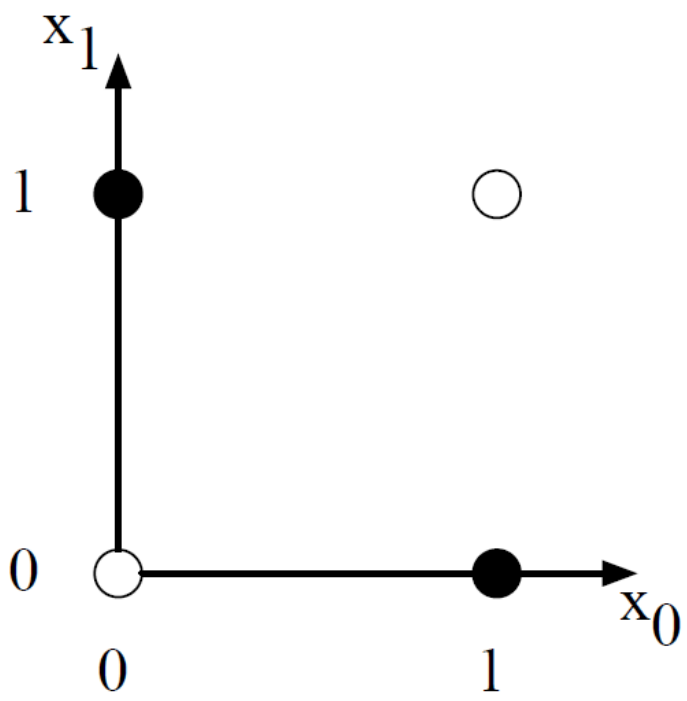
Motivation *The XOR problem*



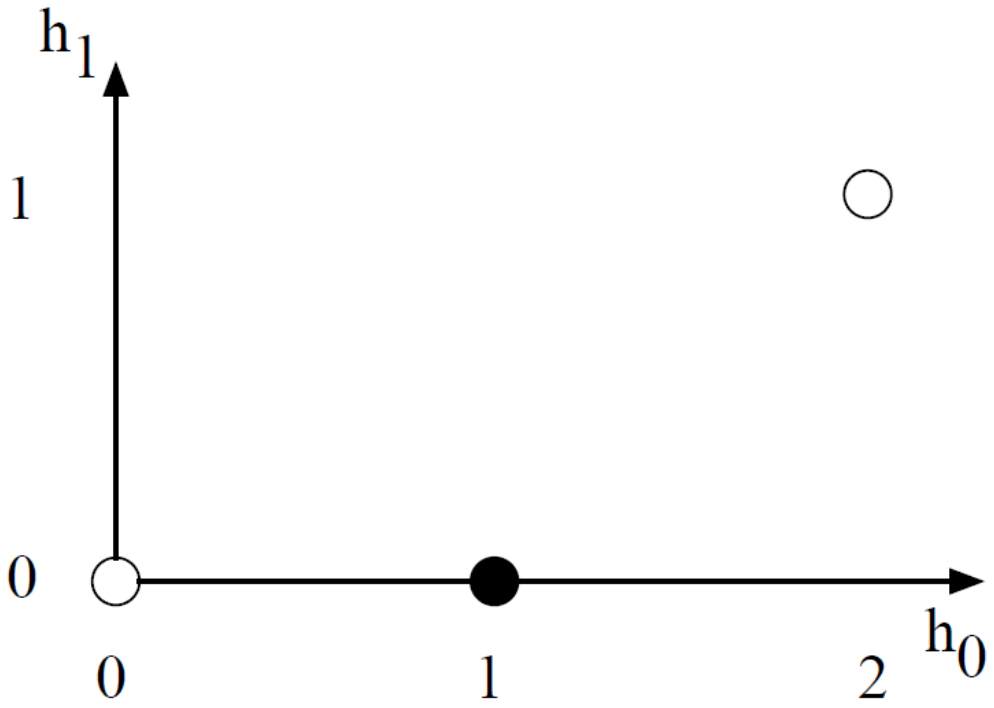
XOR		
x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

Goodfellow et al. 2016

Motivation *The solution*



a) The original x space



b) The new h space

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2. Feedforward Neural Networks

For historical reasons multilayer networks, especially feedforward networks, are sometimes called multi-layer perceptrons (or MLPs); this is a technical misnomer, since the units in modern multilayer networks aren't perceptrons (perceptrons are purely linear, but modern networks are made up of units with non-linearities like sigmoids), but at some point the name stuck.

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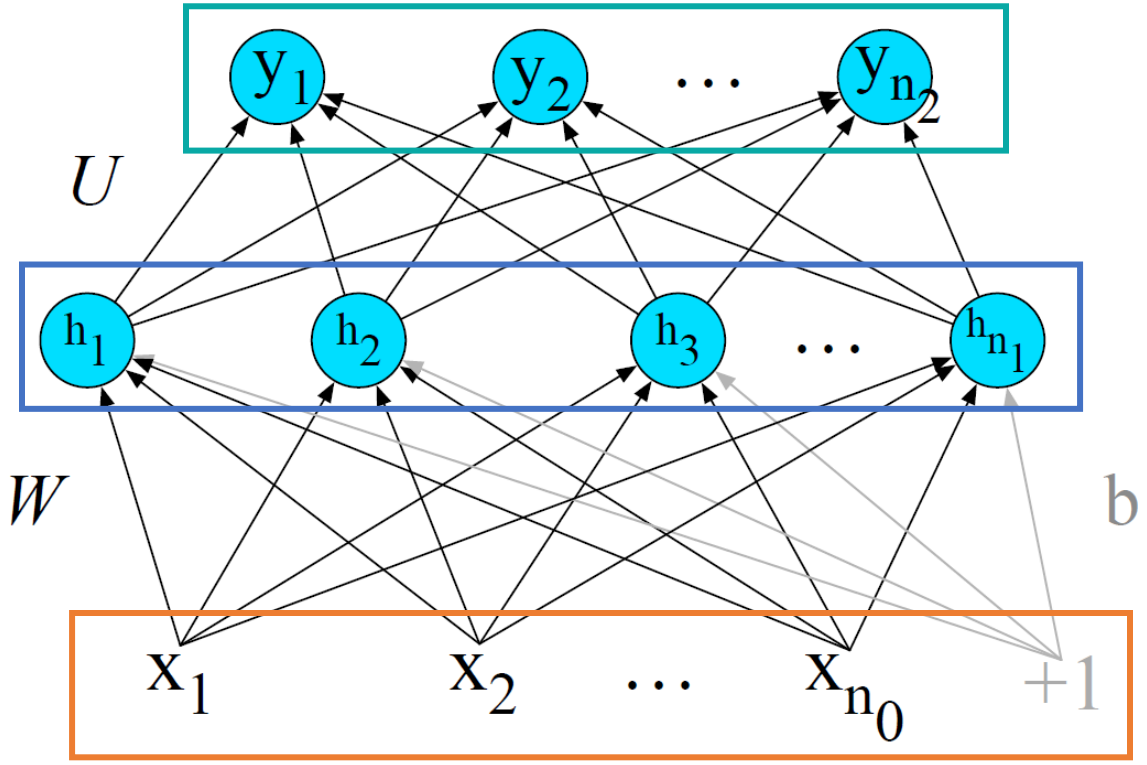
Neural Networks *Feed-Forward Neural Networks*

Simple feedforward networks have three kinds of nodes: input units, hidden units, and output units



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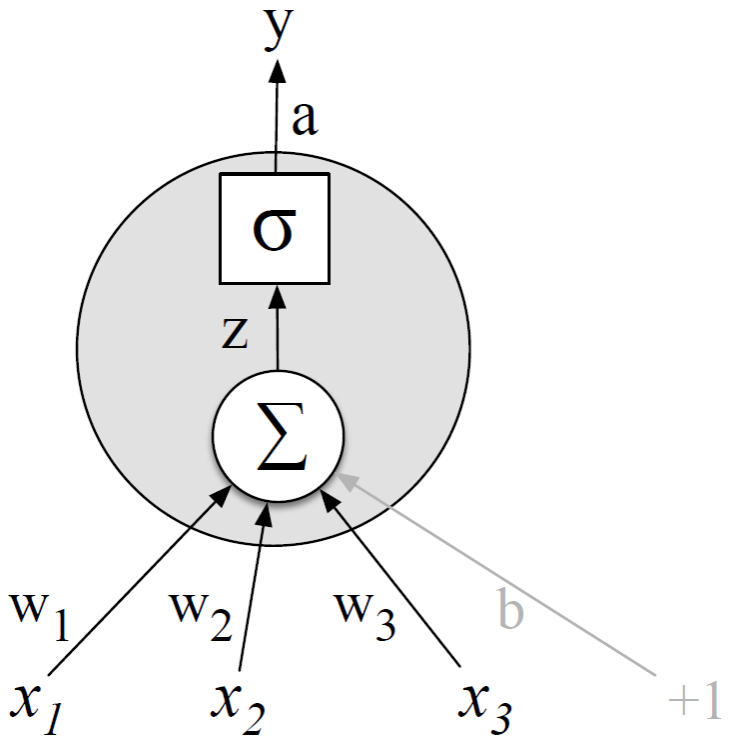
Neural Networks *1-layer network*

$$y = sigmoid(z)$$

$$z = Wx + b$$

Logistic regression is a 1-layer network



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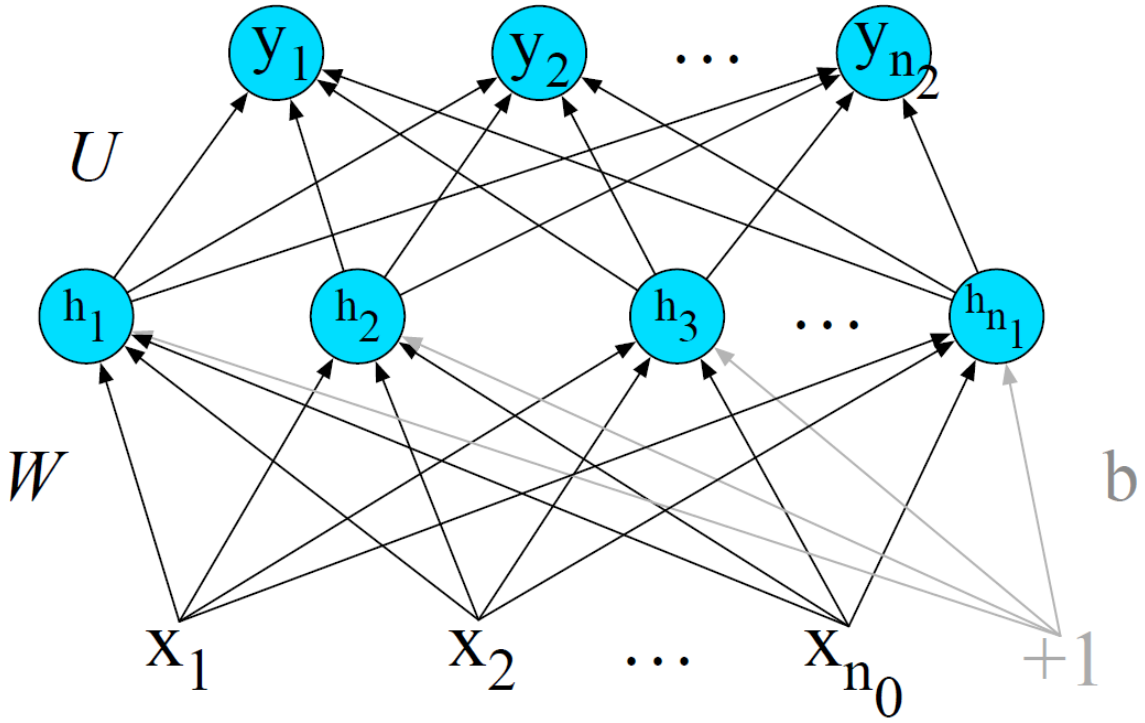
Neural Networks *Feed-Forward Neural Networks*

$$y = softmax(z)$$

$$z = Uh$$

$$h = \sigma(Wx + b)$$

We call this a 2-layer network



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Re-represent with some notations

$$y = softmax(z)$$

$$z = Uh$$

$$h = \sigma(Wx + b)$$

$$\hat{y} = a^{[2]}$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$

$$a^{[1]} = g^{[1]}(z^{[1]})$$

$$z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$$

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Neural Networks *Feed-Forward Neural Networks*

Superscripts in square brackets to mean layer numbers, starting at 0 for the input layer.

So $W^{[1]}$ will mean the weight matrix for the (first) hidden layer, and $b^{[1]}$ will mean the bias vector for the (first) hidden layer.

$g()$ to stand for the activation function, which will tend to be $ReLU$ or $tanh$ for intermediate layers and $softmax$ for output layers.

$$\hat{y} = a^{[2]}$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$

$$a^{[1]} = g^{[1]}(z^{[1]})$$

$$z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$$

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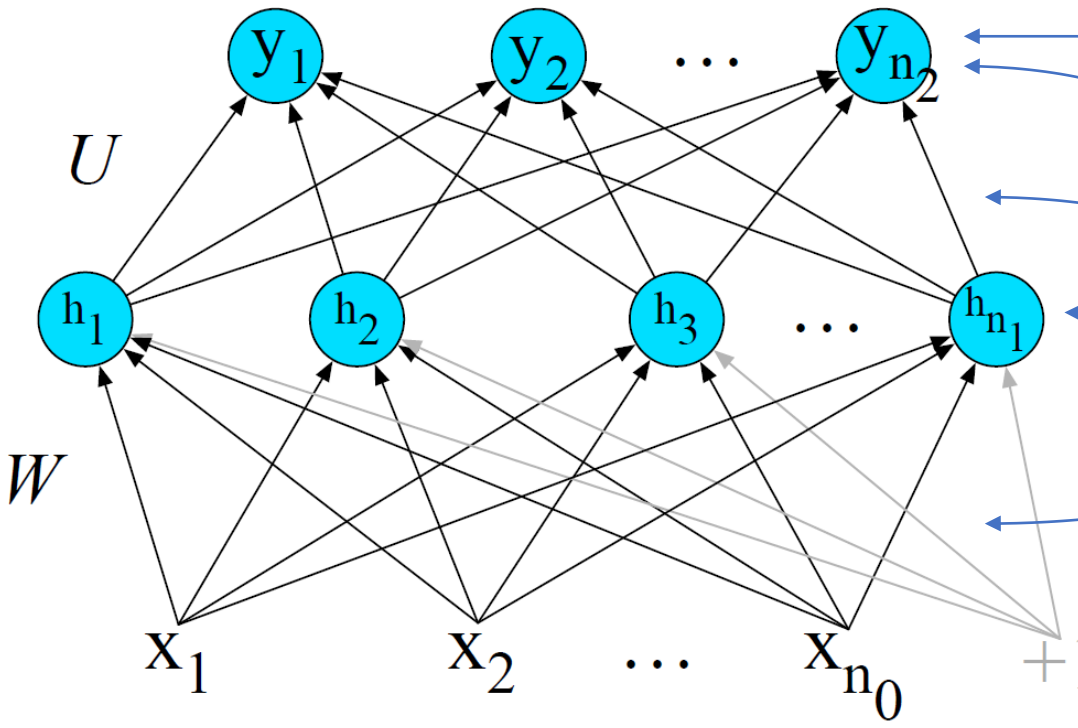
Neural Networks *Feed-Forward Neural Networks*



$$\hat{y} = a^{[2]}$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$

$$a^{[1]} = g^{[1]}(z^{[1]})$$

$$z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$$

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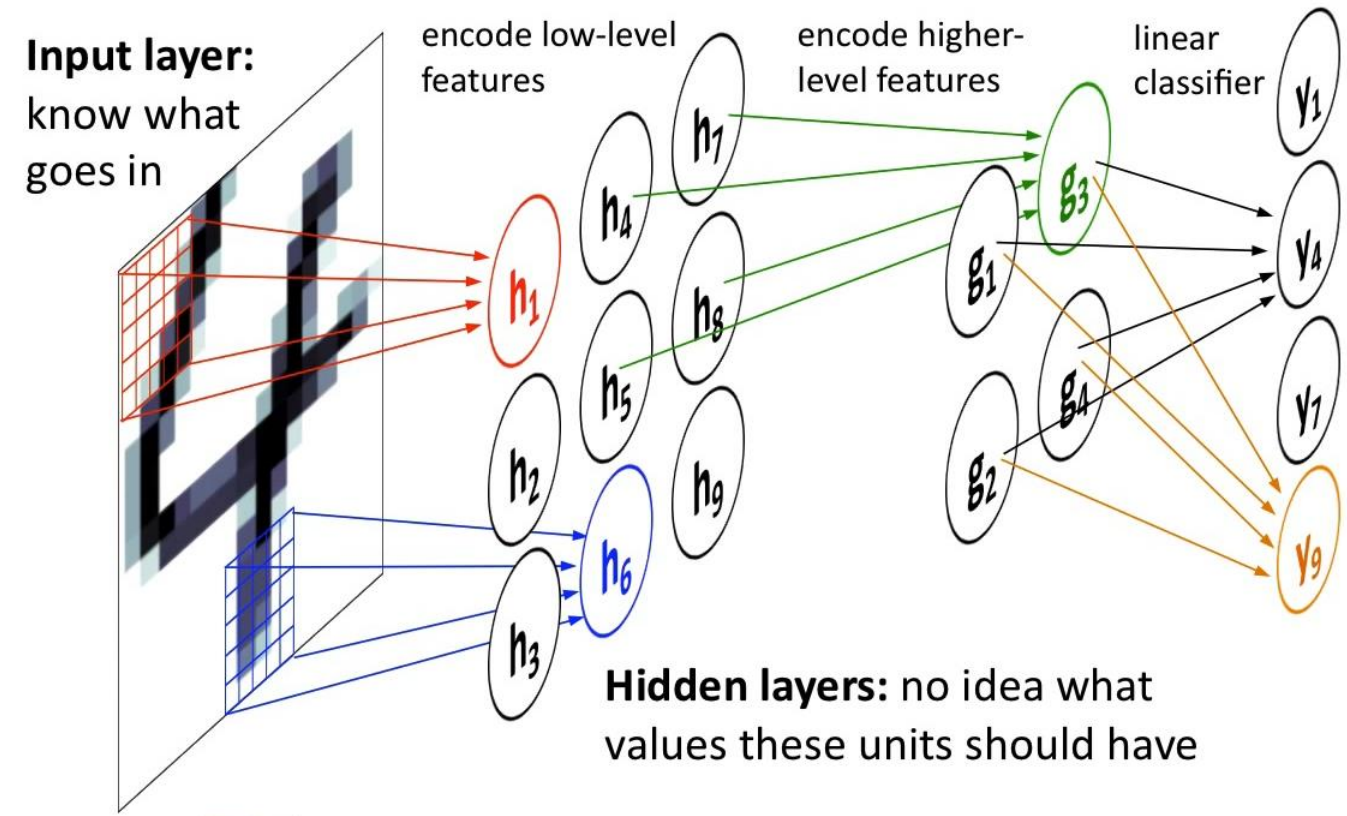
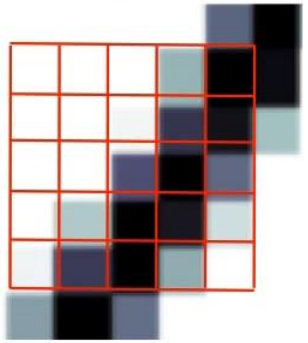
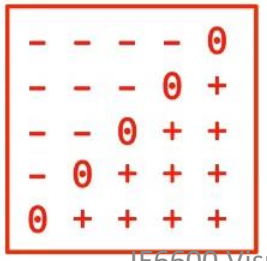
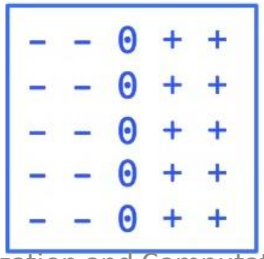
Neural Networks *Hidden layers*









Can encode just about any feature this way

Victor Lavrenko 2014

The algorithm for computing the forward step in an n-layer feedforward network, given the input vector $a^{[0]}$:

for i **in** 1..n

$$z^{[i]} = W^{[i]} a^{[i-1]} + b^{[i]}$$

$$a^{[i]} = g^{[i]}(z^{[i]})$$

$$\hat{y} = a^{[n]}$$

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3. Training Neural Nets

Logistic Regression *Derivation*

Given:

1. Y is Boolean, governed by a Bernoulli distribution, with parameter $\pi = P(Y = 1)$
2. $X = \{X_1, \dots, X_n\}$, each X_i is a continuous random variable
3. For X_i, $P(X_i|Y = y_k)$ is a Gaussian distribution of the form $N(\mu_{ik}, \sigma_i)$, assume $\sigma_{ik} = \sigma_i$
4. $\forall i \; and \; j \neq i$, X_i and X_j are conditionally independent given Y

Goal: Derive $P(Y = y_k|X)$

$$P(Y = 1|X) = \frac{P(Y = 1)P(X|Y = 1)}{P(Y = 1)P(X|Y = 1) + P(Y = 0)P(X|Y = 0)}$$

$$= \frac{1}{1 + \frac{P(Y = 0)P(X|Y = 0)}{P(Y = 1)P(X|Y = 1)}}$$

$$= \frac{1}{1 + \exp\left(\ln \frac{P(Y = 0)P(X|Y = 0)}{P(Y = 1)P(X|Y = 1)}\right)}$$

$$= \frac{1}{1 + \exp\left(\left(ln \frac{1 - \pi}{\pi}\right) + \sum_i \ln \frac{P(X_i|Y = 0)}{P(X_i|Y = 1)}\right)}$$

Logistic Regression *Derivation*

$$P(Y=1|X)=\frac{1}{1+\exp\left(\left(ln\frac{1-\pi}{\pi}\right)+\sum_i \ln\frac{P(X_i|Y=0)}{P(X_i|Y=1)}\right)}$$

$$P(X_i|Y=y_k)=\frac{1}{\sqrt{2\pi}\sigma_{ik}}\exp\{-\frac{\left(x_j-\mu_{ik}\right)^2}{2\sigma_{ik}^2}\}$$

$$lnP(X_i|Y=y_k)=\frac{1}{\sqrt{2\pi}\sigma_{ik}}+\left(-\frac{\left(x_j-\mu_{ik}\right)^2}{2\sigma_{ik}^2}\right)$$

$$\ln\frac{P(X_i|Y=0)}{P(X_i|Y=1)}=\frac{1}{\sqrt{2\pi}\sigma_{i0}}+\left(-\frac{\left(x_j-\mu_{i0}\right)^2}{2\sigma_{i0}^2}\right)-\frac{1}{\sqrt{2\pi}\sigma_{i1}}+\left(-\frac{\left(x_j-\mu_{i1}\right)^2}{2\sigma_{i1}^2}\right)$$

$$=\frac{1}{\sqrt{2\pi}\sigma_{i0}}-\frac{1}{\sqrt{2\pi}\sigma_{i1}}-\frac{x_i^2-2x_i\mu_{i0}+\mu_{i0}^2}{2\sigma_{i0}^2}+\frac{x_i^2-2x_i\mu_{i1}+\mu_{i1}^2}{2\sigma_{i1}^2}$$

Assume $\sigma_{ik}=\sigma_i$

$$=\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}X_i+\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}$$

Logistic Regression *Derivation*

$$P(Y=1|X)=\frac{1}{1+\exp\left(\left(ln\frac{1-\pi}{\pi}\right)+\sum_i \ln\frac{P(X_i|Y=0)}{P(X_i|Y=1)}\right)}$$

$$\ln\frac{P(X_i|Y=0)}{P(X_i|Y=1)}=\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}X_i+\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}$$

$$P(Y=1|X)=\frac{1}{1+\exp\left(\left(ln\frac{1-\pi}{\pi}\right)+\sum_i\left(\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}X_i+\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right)\right)}$$

Where weights are given by: $w_0=ln\frac{1-\pi}{\pi}+\sum_i\left(\frac{\mu_{i1}^2-\mu_{i0}^2}{2\sigma_i^2}\right), w_1=\frac{\mu_{i0}-\mu_{i1}}{\sigma_i^2}$

$$P(Y=1|X)=\frac{1}{1+\exp(w_0+\sum_{i=1}^n w_iX_i)}, P(Y=0|X)=\frac{\exp(w_0+\sum_{i=1}^n w_iX_i)}{1+\exp(w_0+\sum_{i=1}^n w_iX_i)}$$

Logistic Regression *Derivation*

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

$$P(Y=0|X) = \frac{\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

Then we get

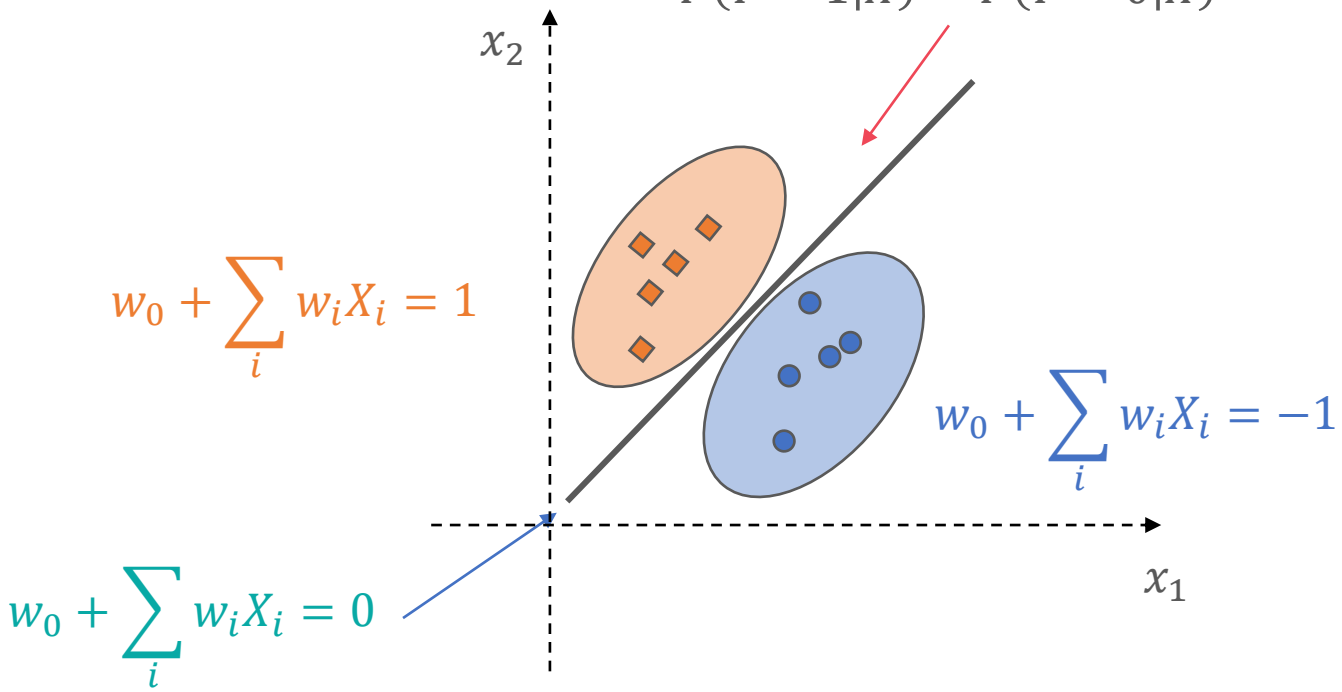
$$\frac{P(Y=0|X)}{P(Y=1|X)} = \exp\left(w_0 + \sum_i w_i X_i\right)$$

$$ln\frac{P(Y=0|X)}{P(Y=1|X)} = w_0 + \sum_i w_i X_i$$

Linear classification rule

$$z = ln\frac{P(Y=0|X)}{P(Y=1|X)} = 0$$

$$P(Y=1|X) = P(Y=0|X)$$



Logistic Regression *Derivation*

$$P(Y=1|X) = \frac{1}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

$$P(Y=0|X) = \frac{\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

Then we get

$$\frac{P(Y=0|X)}{P(Y=1|X)} = \exp\left(w_0 + \sum_i w_i X_i\right)$$

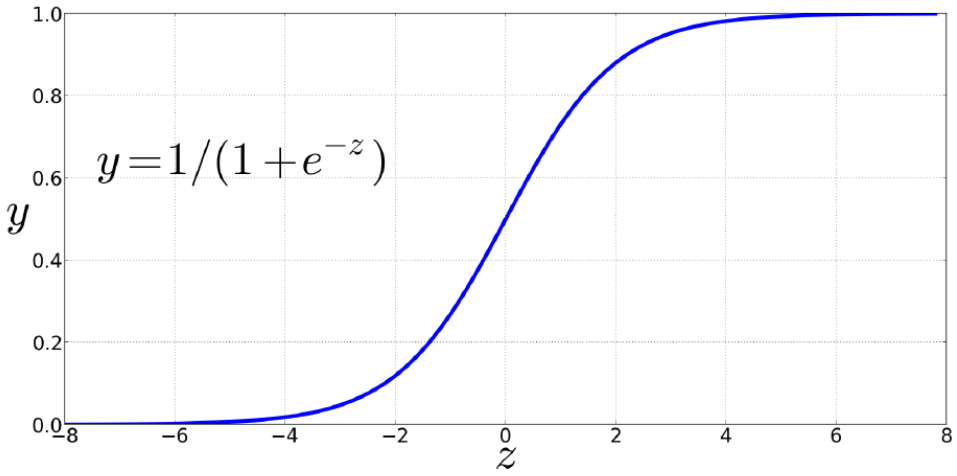
$$ln\frac{P(Y=0|X)}{P(Y=1|X)} = w_0 + \sum_i w_i X_i$$

This reflects the constraint that the probabilities sum to one

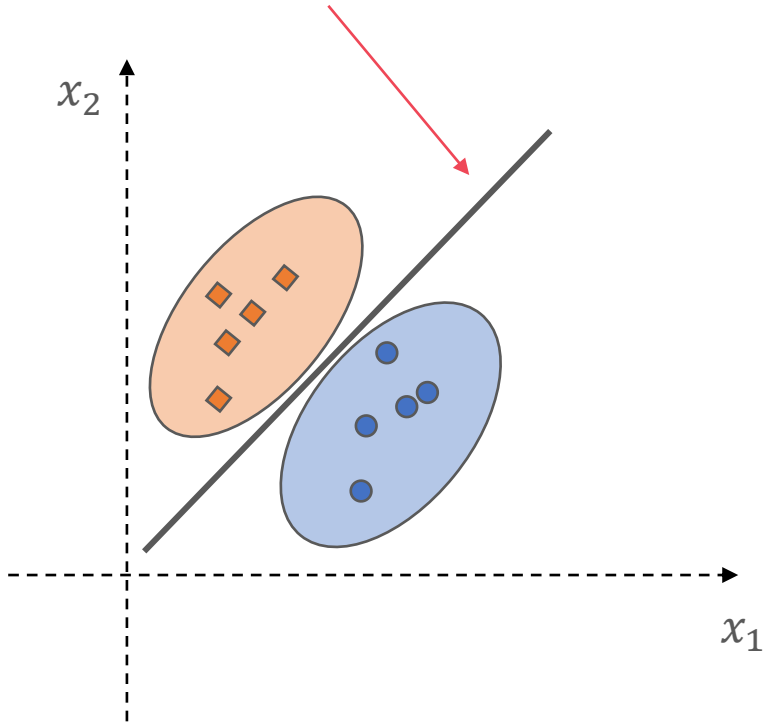
Log-odds or logit transformations

Logistic Regression *Derivation*

$$P(Y=0|X)=\frac{1}{1+\exp-(w_0+\sum_{i=1}^{n}w_iX_i)}$$



$$z=ln\frac{P(Y=0|X)}{P(Y=1|X)}=w_0+\sum_i w_iX_i=0$$



Logistic Regression *More general*

Given: Logistic regression when $Y = \{y_1, \dots y_K\}$

$$P(Y = y_K|X) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji} X_i)}$$

$$P(Y = y_k|X) = \frac{\exp(w_{k0} + \sum_{i=1}^{n} w_{ki} X_i)}{1 + \sum_{j=1}^{K-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji} X_i)}, k = 1, \dots, K-1$$

Training *The sigmoid function*

$$z = w_0 + \sum_i w_i X_i = w \cdot x + b \ (equivalent\ to\ w^T x + b)$$

The sigmoid function $\hat{y} = \sigma(w \cdot x + b) = \frac{1}{1+e^{-z}}$

Training *The cross-entropy loss function*

We need a loss function that expresses, for an observation x, how close the classifier output $\hat{y} = \sigma(w \cdot x + b)$ is to the correct output (y, which is 0 or 1). We'll call this:

$L(\hat{y}, y)$ =How much $\hat{y}$ differs from the true y

We do this via a loss function that prefers the correct class labels of the training examples to be *more likely*. This is called conditional maximum likelihood estimation: we choose the parameters w, b that maximize the log probability of the true y labels in the training data given the observations x. The resulting loss function is the negative log likelihood loss, generally called the cross-entropy loss.

Training *The cross-entropy loss function*

Given: $y = \{0, 1\}$, **Bernoulli distribution**, which can be expressed as probability $p(y|x)$. If $y = 1$, simplifies to $\hat{y}$; if $y = 0$, simplifies to $1 - \hat{y}$
Goal: Maximize the probability of $\hat{y}$

$$p(y|x) = \hat{y}^y(1 - \hat{y})^{1-y}$$

Now we take the log of both sides. This will turn out to be handy mathematically, and doesn't hurt us.

$$\log p(y|x) = \log[\hat{y}^y(1 - \hat{y})^{1-y}]$$
$$= y\log \hat{y} + (1 - y)\log(1 - \hat{y})$$

Training *The cross-entropy loss function*

$$\log p(y|x) = y\log\hat{y} + (1-y)\log(1-\hat{y})$$

This shows a log likelihood that should be maximized. In order to turn this into loss function (something that we need to minimize), we'll just flip the sign. The result is the cross-entropy loss L_{CE}

$$L_{CE}(\hat{y}, y) = -\log p(y|x) = -[y\log\hat{y} + (1-y)\log(1-\hat{y})]$$

Finally, we can plug in the definition of $\hat{y} = \sigma(w \cdot x + b)$:

$$L_{CE}(w, b) = -[y\log\sigma(w \cdot x + b) + (1-y)\log(1-\sigma(w \cdot x + b))]$$

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Logistic Regression *The cross-entropy loss function*

Why does minimizing this negative log probability do what we want?

A perfect classifier would assign probability 1 to the correct outcome (y=1 or y=0) and probability 0 to the incorrect outcome. That means the higher $\hat{y}$ (the closer it is to 1), the better the classifier; the lower $\hat{y}$ is (the closer it is to 0), the worse the classifier. The negative log of this probability is a convenient loss metric since it goes from 0 (negative log of 1, no loss) to infinity (negative log of 0, infinite loss). This loss function also ensures that as the probability of the correct answer is maximized, the probability of the incorrect answer is minimized; since the two sum to one, any increase in the probability of the correct answer is coming at the expense of the incorrect answer. It's called the cross-entropy loss,

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Training *Loss function*

The cross-entropy loss that is used in neural networks is the same one we saw for logistic regression. If the neural network is being used as a binary classifier, the loss function is exactly the same as the logistic regression

$$L_{CE}(\hat{y}, y) = -\log p(y|x) = -[y \log \hat{y} + (1-y)\log(1-\hat{y})]$$

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Training *Loss function*

If the neural network is being used as a multinomial classifier.

$$L_{CE}(\hat{y}, y) = -\sum_{i=1}^{c} y_i \log \hat{y}_i$$

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Training *Loss function*

$$L_{CE}(\hat{y}, y) = -\sum_{i=1}^{c} y_i \log \hat{y}_i$$

Assume this is a hard classification task, meaning that only one class is the correct one, and that there is one output unit in y for each class. If the true class is i, then y is a vector where $y_i = 1$ and $y_j = 0, \forall j \neq i$. A vector like this, with one value equals to 1 and the rest 0 is called a one-hot vector.

The sum will be 0 except for the true class. Hence the cross-entropy loss is simply the log probability of the correct class, and we therefore also call this the negative log likelihood loss:

$$L_{CE}(\hat{y}, y) = -\log \hat{y}_i$$

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Training *Loss function*

$$L_{CE}(\hat{y}, y) = -\log \hat{y}_i$$

$$softmax(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}}, 1 \leq i \leq k$$

Plugging in the SoftMax formula and with classes K

$$L_{CE}(\hat{y}, y) = -\log \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

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Training *Computing the Gradient*

For a network with one weight layer and sigmoid output (which is what logistic regression is), we could simply use the derivative of the loss that we used for logistic regression

$$\frac{\partial L_{CE}(w,b)}{\partial w_j} = [\sigma(w \cdot x + b) - y]x_j$$

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Training *Deriving the gradient equation*

Some basic calculus:

$$\frac{d}{dx}\ln(x) = \frac{1}{x}$$

The derivative of the sigmoid:

$$\frac{d\sigma(z)}{dz} = \sigma(z)\big(1 - \sigma(z)\big)$$

Chain rule of derivatives, suppose we are computing the derivative of a composite function $f\ (x)\ =\ u(v(x))$. The derivative of $f\ (x)$ is the derivative of $u(x)$ with respect to $v(x)$ times the derivative of $v(x)$ with respect to x:

$$\frac{df}{dx} = \frac{du}{dv} \cdot \frac{dv}{dx}$$

First, we want to know the derivative of the loss function with respect to a single weight w_j (we'll need to compute it for each weight, and for the bias):

$$\frac{\partial LL(w,b)}{\partial w_j} = \frac{\partial}{\partial w_j} - \left[ylog\sigma(w \cdot x + b) + (1-y)\log\big(1-\sigma(w \cdot x + b)\big)\right]$$

$$= -\left[\frac{\partial}{\partial w_j} ylog\sigma(w \cdot x + b) + \frac{\partial}{\partial w_j}(1-y)\log\big(1-\sigma(w \cdot x + b)\big)\right]$$

Next, using the chain rule, and relying on the derivative of log:

$$\frac{\partial LL(w,b)}{\partial w_j} = -\frac{y}{\sigma(w \cdot x + b)}\frac{\partial}{\partial w_j}\sigma(w \cdot x + b) - \frac{(1-y)}{\big(1-\sigma(w \cdot x + b)\big)}\frac{\partial}{\partial w_j}\big(1-\sigma(w \cdot x + b)\big)$$

Rearranging terms:

$$\frac{\partial LL(w,b)}{\partial w_j} = -\left[\frac{y}{\sigma(w \cdot x + b)} - \frac{(1-y)}{\big(1-\sigma(w \cdot x + b)\big)}\right]\frac{\partial}{\partial w_j}\sigma(w \cdot x + b)$$

And now plugging in the derivative of the sigmoid, and using the chain rule one more time

$$\frac{\partial LL(w,b)}{\partial w_j} = -\left[\frac{y-\sigma(w \cdot x + b)}{\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)}\right]\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)\frac{\partial(w \cdot x + b)}{\partial w_j}$$

$$= -\left[\frac{y-\sigma(w \cdot x + b)}{\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)}\right]\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)x_j$$

$$= -[y-\sigma(w \cdot x + b)]x_j$$

$$= [\sigma(w \cdot x + b) - y]x_j$$

Training *Computing the Gradient*

Or for a network with one hidden layer and SoftMax output, we could use the derivative of the SoftMax loss

$$\frac{\partial L_{CE}}{\partial w_j} = -\big(1\{y = k\} - p(y = k|x)\big)x_k$$

$$= -\left(1\{y = k\} - \frac{e^{w_c \cdot x + b_c}}{\sum_{j=1}^{k} e^{w_j \cdot x + b_j}}\right)x_k$$

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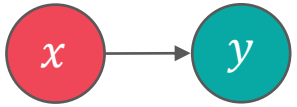
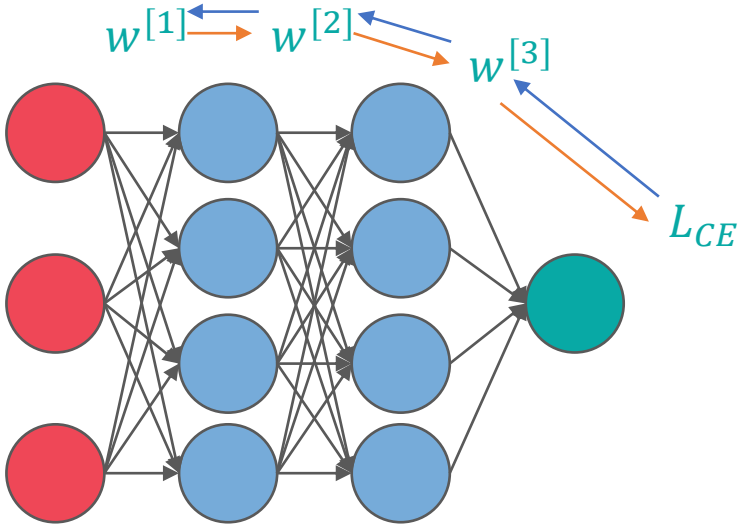
Training *Computing the Gradient*

But these derivatives only give correct updates for one weight layer: the last one!



For deep networks, computing the gradients for each weight is much more complex, since we are computing the derivative with respect to weight parameters that appear all the way back in the very early layers of the network, even though the loss is computed only at the very end of the network.



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Training *Gradient descent*

The intuition is that if you are hiking in a canyon and trying to descend most quickly down to the river at the bottom, you might look around yourself 360 degrees, find the direction where the ground is sloping the steepest, and walk downhill in that direction.

Training *Gradient descent – single scalar w*

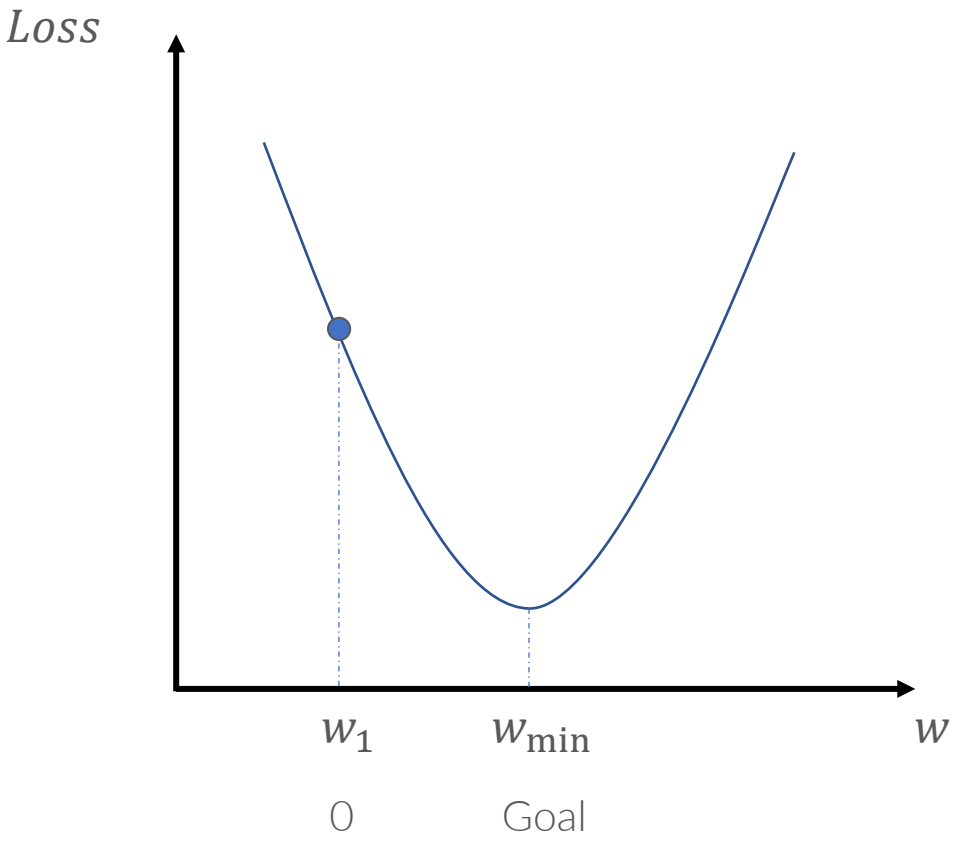
The algorithm (and the concept of gradient) are designed for *direction vectors*, let's first consider a visualization of the case where the parameter of our system is just a single scalar w

Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$

Training *Gradient descent – single scalar w*

Start at a random point

Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$

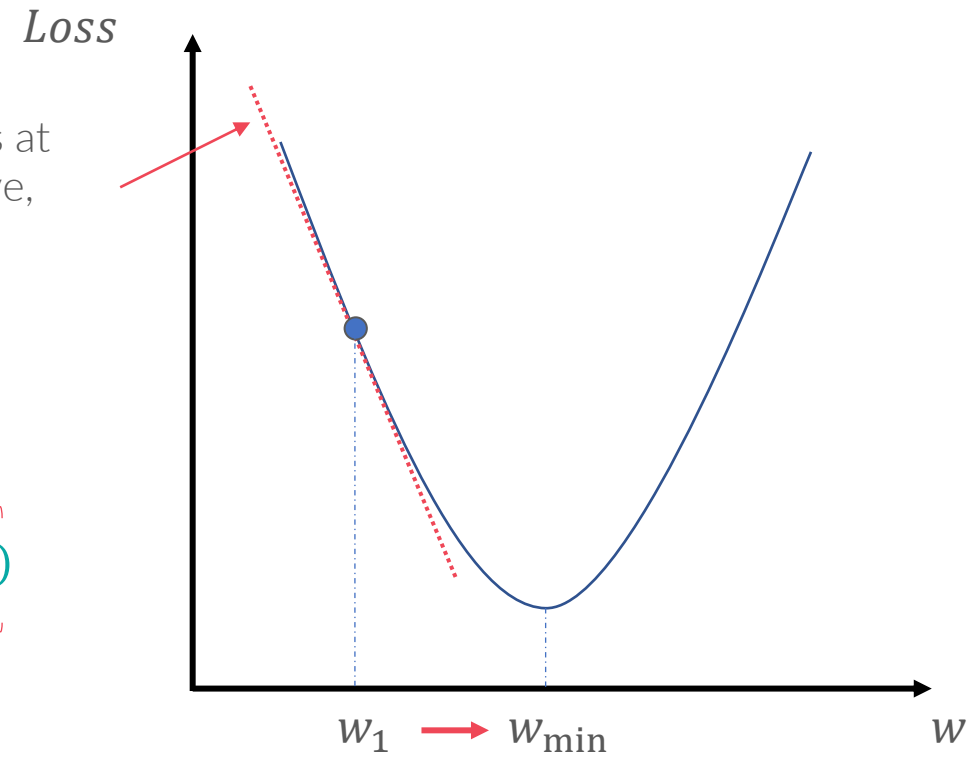


Training *Gradient descent – single scalar w*

Start at a random point

Determine a descent direction

Slope of loss at w_1 is negative, go right



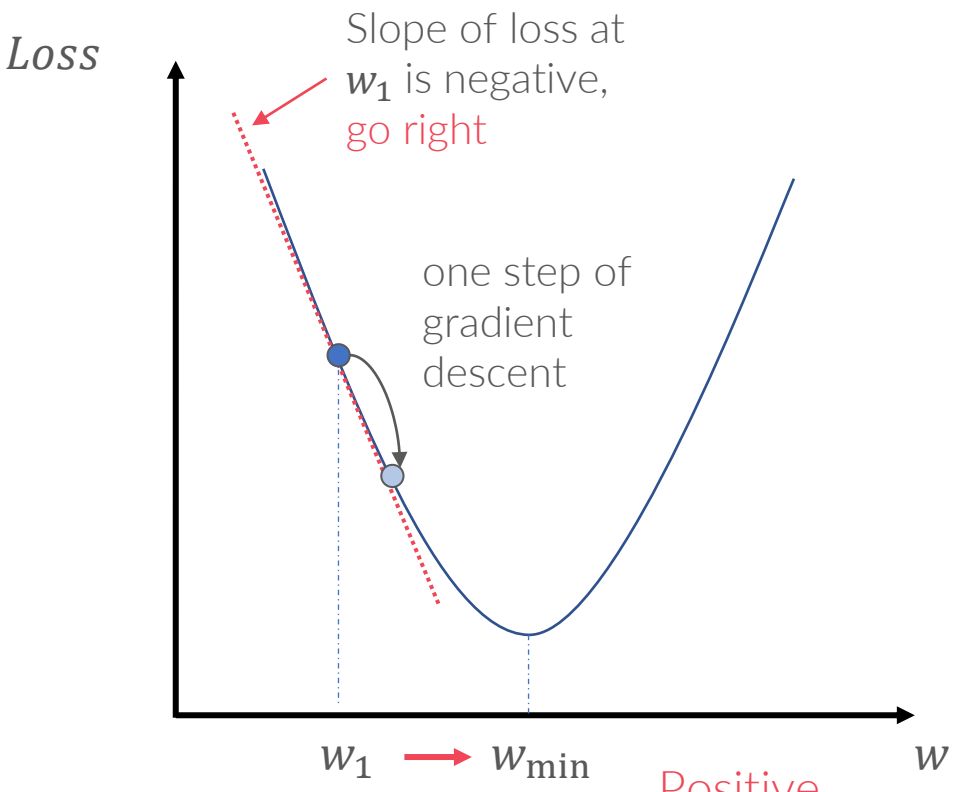
Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$

Positive

Negative

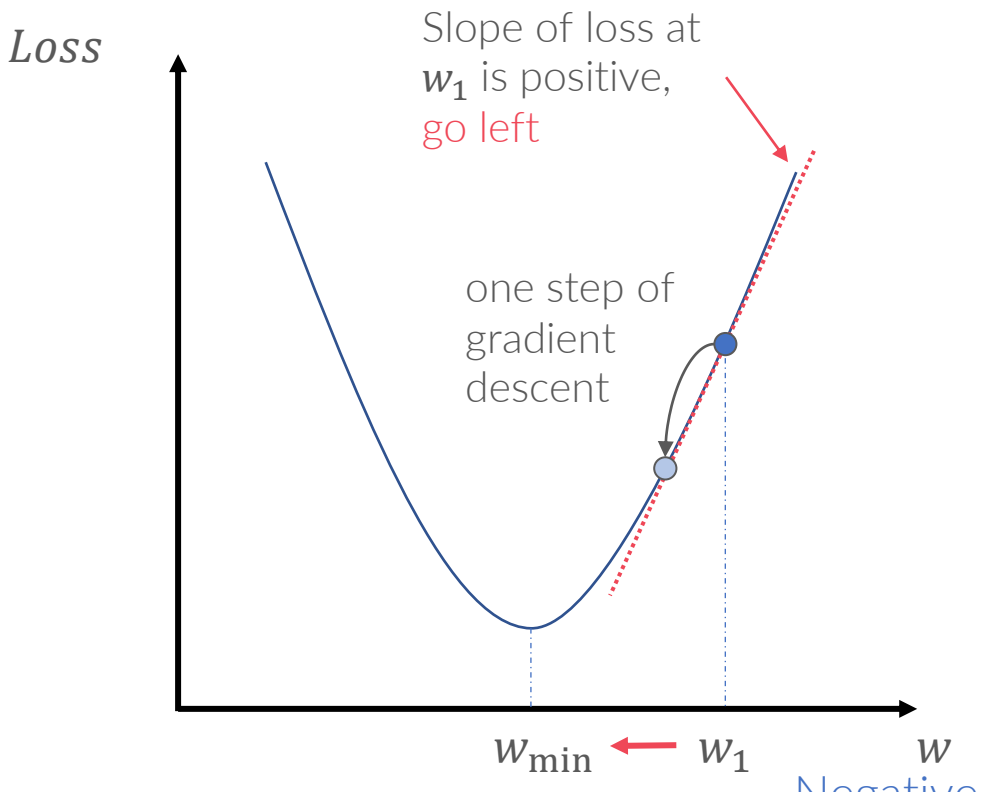
Training *Gradient descent – single scalar w*

Determine a descent direction



Update rule: $w_{t+1} = w_t - \eta \underbrace{\frac{\partial}{\partial w} f(x; w)}_{\text{Negative}}$

Positive



Update rule: $w_{t+1} = w_t - \eta \underbrace{\frac{\partial}{\partial w} f(x; w)}_{\text{Positive}}$

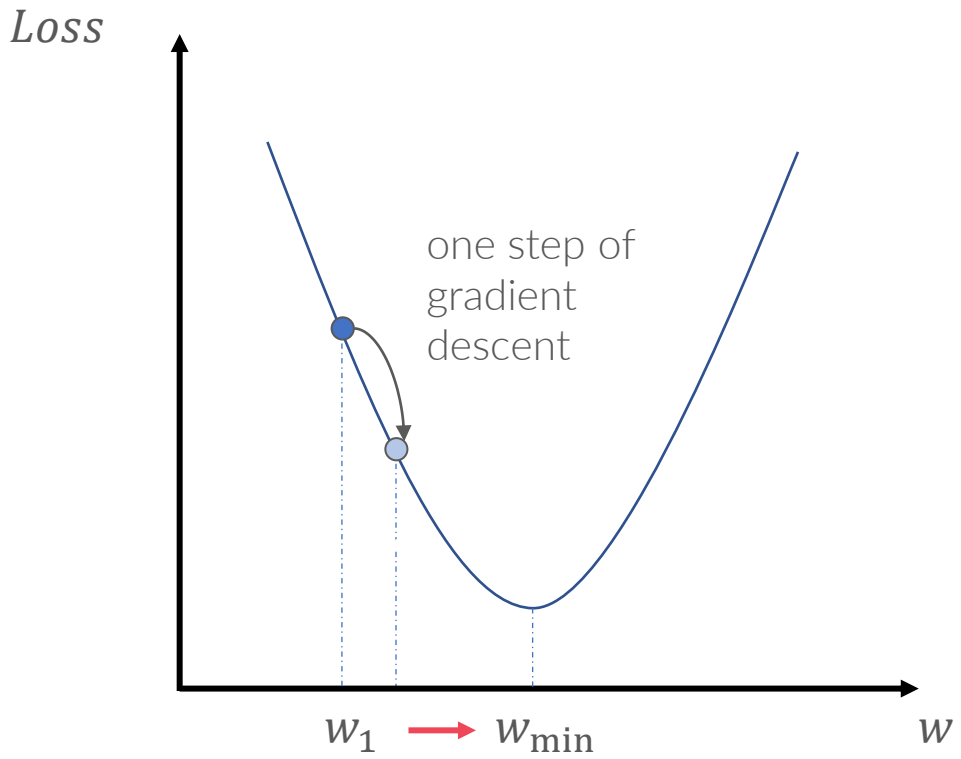
Negative

Training *Gradient descent – single scalar w*

Start at a random point

Determine a descent direction
Choose a step size

Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$

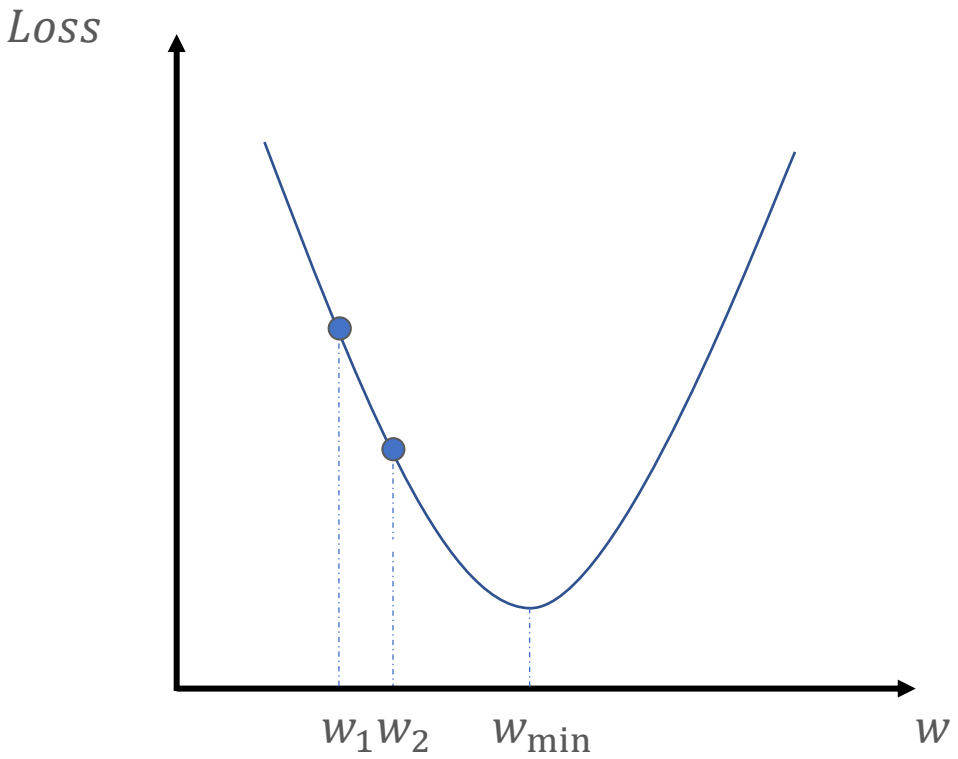


Training *Gradient descent – single scalar w*

Start at a random point

Determine a descent direction
Choose a step size
Update

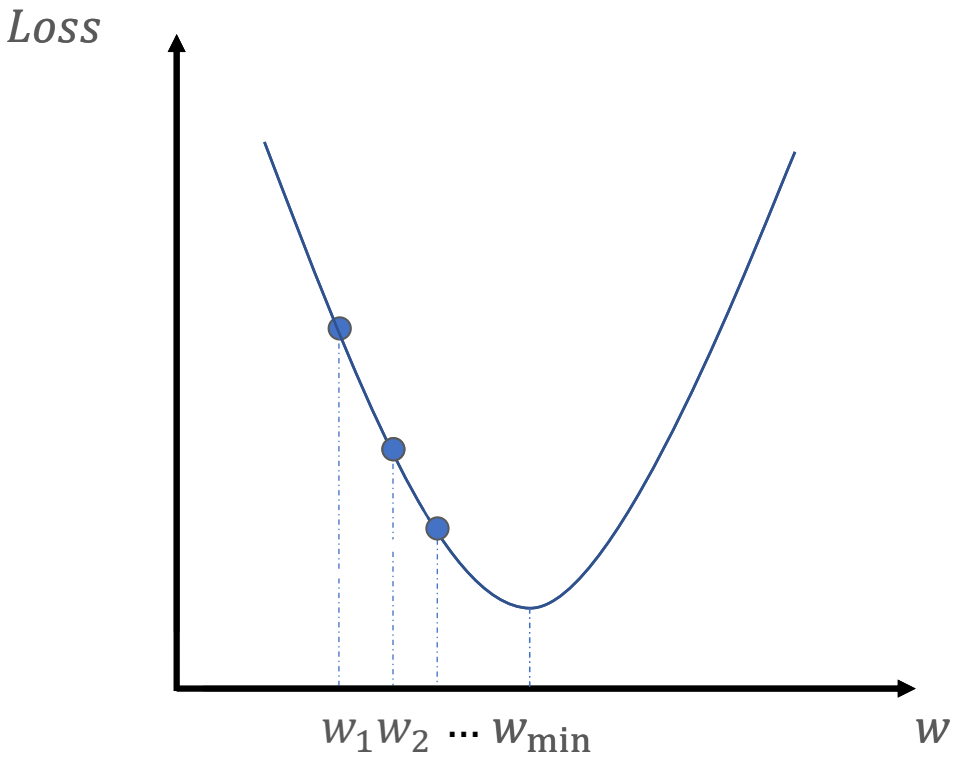
Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$



Training *Gradient descent – single scalar w*

Start at a random point
Repeat
    Determine a descent direction
    Choose a step size
    Update
Until
    Stopping criterion is satisfied

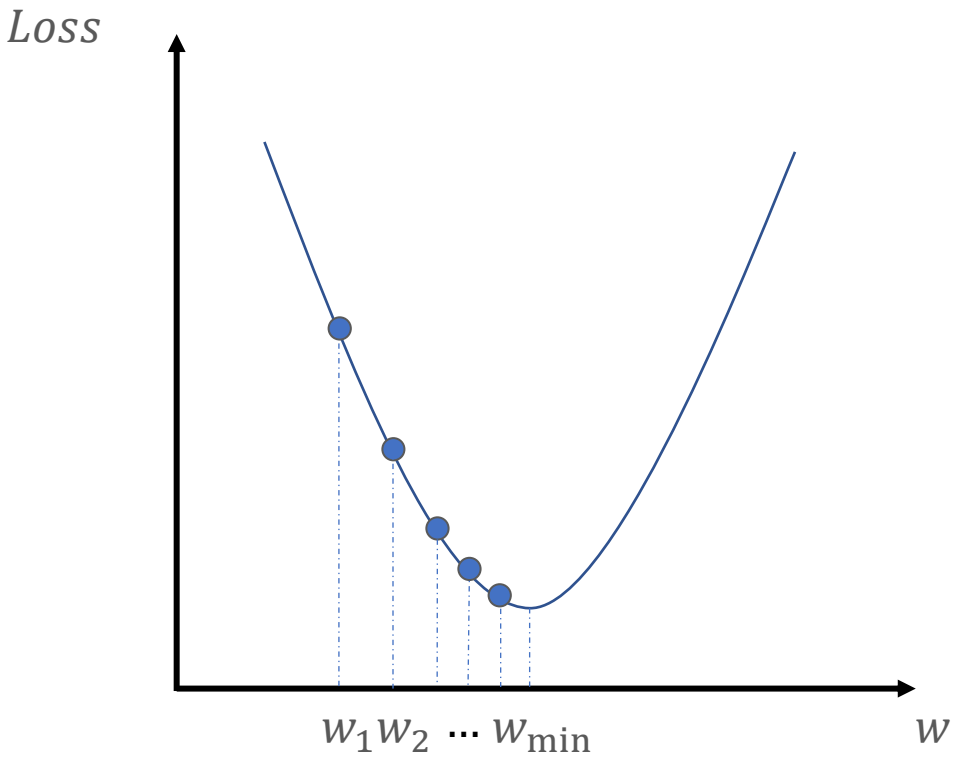
Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$



Training *Gradient descent – single scalar w*

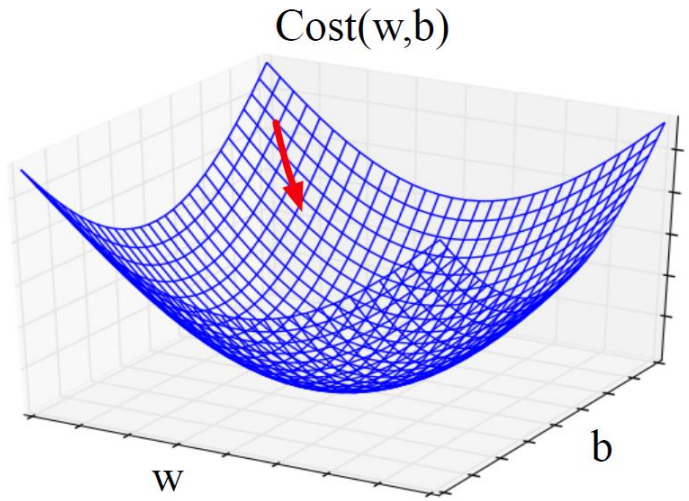
Start at a random point
Repeat
    Determine a descent direction
    Choose a step size
    Update
Until
    Stopping criterion is satisfied

Update rule: $w_{t+1} = w_t - \eta \frac{\partial}{\partial w} f(x; w)$



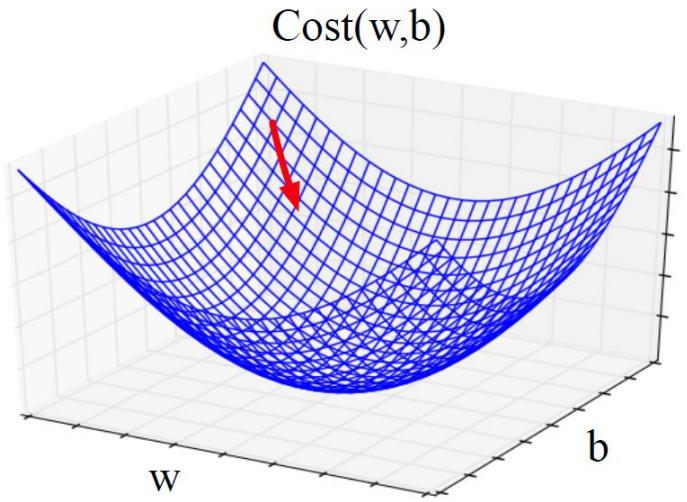
Training *Gradient descent – single scalar w*

Now let's extend the intuition from a function of one scalar variable w to many variables, because we don't just want to move left or right, we want to know where in the N-dimensional space (of the N parameters that make up θ) we should move. The gradient is just such a *vector*; it expresses the directional components of the sharpest slope along each of those N dimensions



Training *Gradient descent – single scalar w*

For each dimension/variable w_i in w (plus the bias b), the gradient will have a component that tells us the slope with respect to that variable.



In each dimension w_i , we express the slope as a partial derivative $\frac{\partial}{\partial w_i}$ of the loss function. The gradient is then defined as a vector of these partials. We'll represent w_i as $f(x;\theta)$ to make the dependence on θ more obvious:

$$\nabla_\theta L(f(x;\theta),y)) = \begin{bmatrix} \frac{\partial}{\partial w_1} L(f(x;\theta),y) \\ \frac{\partial}{\partial w_2} L(f(x;\theta),y) \\ \vdots \\ \frac{\partial}{\partial w_n} L(f(x;\theta),y) \end{bmatrix}$$

The final equation for updating q based on the gradient is thus

$$\theta_{t+1} = \theta_t - \eta \nabla L(f(x;\theta)y)$$

∇ denotes as standard derivative

Logistic Regression *Gradient descent for logistic regression*

Recall that the cross-entropy loss function for logistic regression is:

$$L_{CE}(w,b) = -[y\log\sigma(w\cdot x+b) + (1-y)\log(1-\sigma(w\cdot x+b))]$$

It turns out that the derivative of this function for one observation vector $\boldsymbol{x}$ is

$$\frac{\partial L_{CE}(w,b)}{\partial w_j} = [\sigma(w\cdot x+b) - y]x_j$$

Logistic Regression *Deriving the gradient equation*

Some basic calculus:

$$\frac{d}{dx}\ln(x) = \frac{1}{x}$$

The derivative of the sigmoid:

$$\frac{d\sigma(z)}{dz} = \sigma(z)\big(1 - \sigma(z)\big)$$

Chain rule of derivatives, suppose we are computing the derivative of a composite function $f(x) = u(v(x))$. The derivative of $f(x)$ is the derivative of $u(x)$ with respect to $v(x)$ times the derivative of $v(x)$ with respect to x:

$$\frac{df}{dx} = \frac{du}{dv} \cdot \frac{dv}{dx}$$

First, we want to know the derivative of the loss function with respect to a single weight w_j (we'll need to compute it for each weight, and for the bias):

$$\frac{\partial LL(w,b)}{\partial w_j} = \frac{\partial}{\partial w_j} - \left[ylog\sigma(w \cdot x + b) + (1-y)\log\big(1-\sigma(w \cdot x + b)\big)\right]$$

$$= -\left[\frac{\partial}{\partial w_j} ylog\sigma(w \cdot x + b) + \frac{\partial}{\partial w_j}(1-y)\log\big(1-\sigma(w \cdot x + b)\big)\right]$$

Next, using the chain rule, and relying on the derivative of log:

$$\frac{\partial LL(w,b)}{\partial w_j} = -\frac{y}{\sigma(w \cdot x + b)}\frac{\partial}{\partial w_j}\sigma(w \cdot x + b) - \frac{(1-y)}{\big(1-\sigma(w \cdot x + b)\big)}\frac{\partial}{\partial w_j}\big(1-\sigma(w \cdot x + b)\big)$$

Rearranging terms:

$$\frac{\partial LL(w,b)}{\partial w_j} = -\left[\frac{y}{\sigma(w \cdot x + b)} - \frac{(1-y)}{\big(1-\sigma(w \cdot x + b)\big)}\right]\frac{\partial}{\partial w_j}\sigma(w \cdot x + b)$$

And now plugging in the derivative of the sigmoid, and using the chain rule one more time

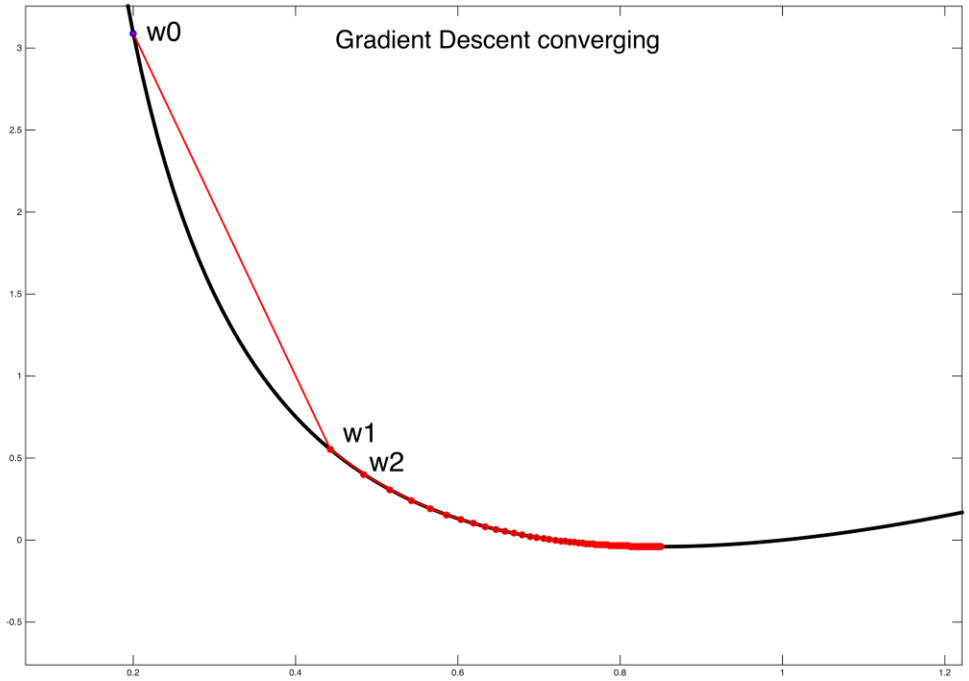
$$\frac{\partial LL(w,b)}{\partial w_j} = -\left[\frac{y-\sigma(w \cdot x + b)}{\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)}\right]\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)\frac{\partial(w \cdot x + b)}{\partial w_j}$$

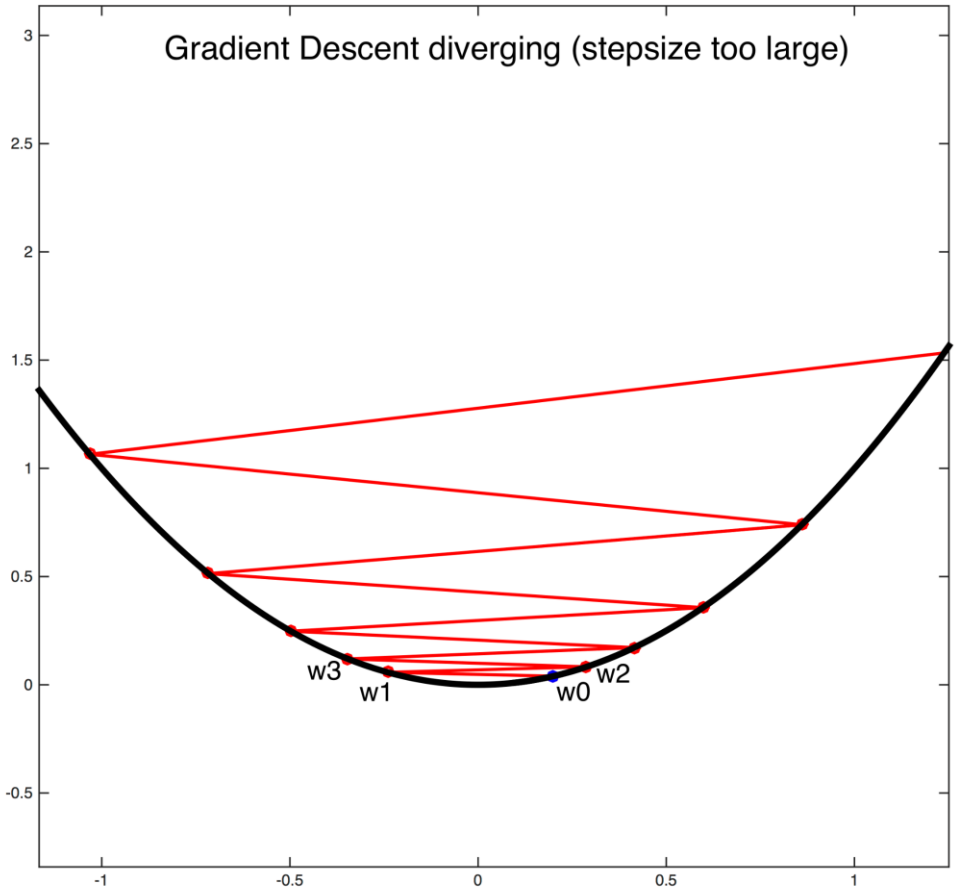
$$= -\left[\frac{y-\sigma(w \cdot x + b)}{\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)}\right]\sigma(w \cdot x + b)\big(1-\sigma(w \cdot x + b)\big)x_j$$

$$= -[y-\sigma(w \cdot x + b)]x_j$$

$$= [\sigma(w \cdot x + b) - y]x_j$$

Logistic Regression *Gradient descent diverging and converging*





Logistic Regression *Gradient descent for logistic regression*

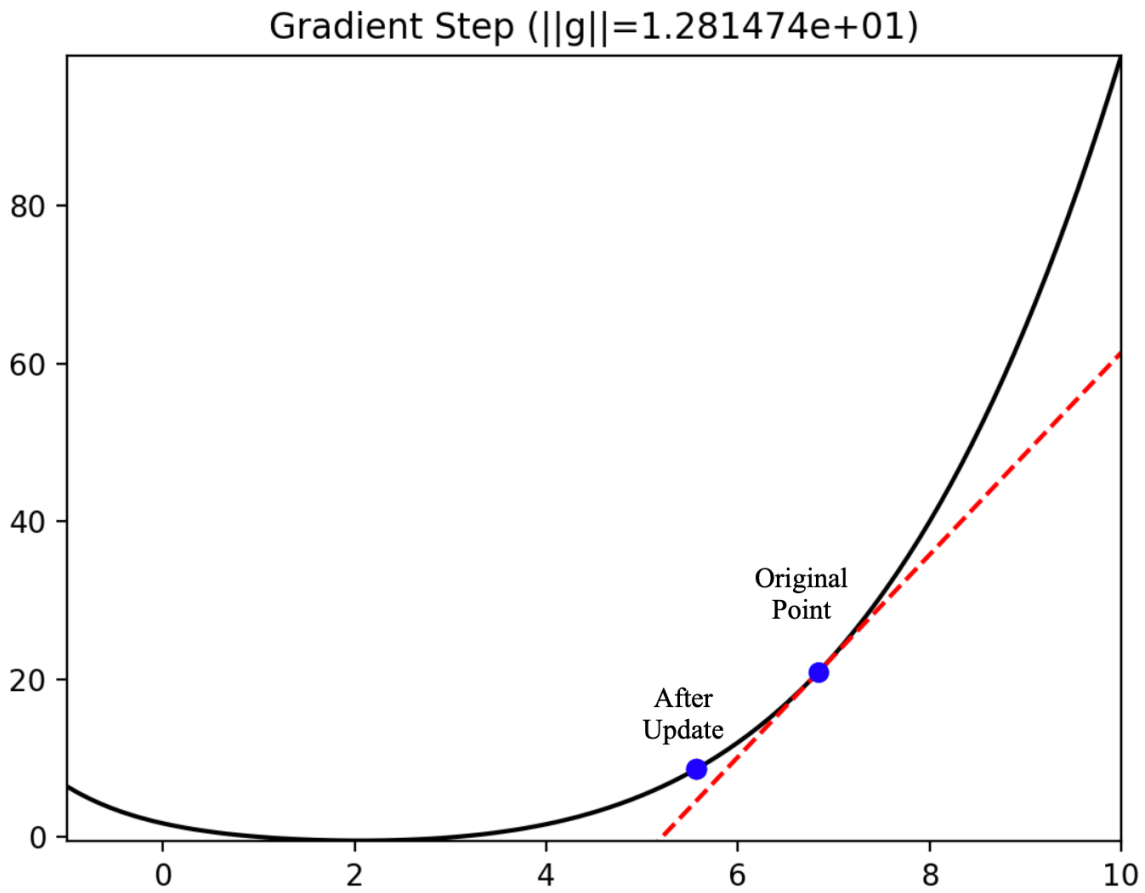
function STOCHASTIC GRADIENT DESCENT($L()$, $f()$, x, y) **returns** θ

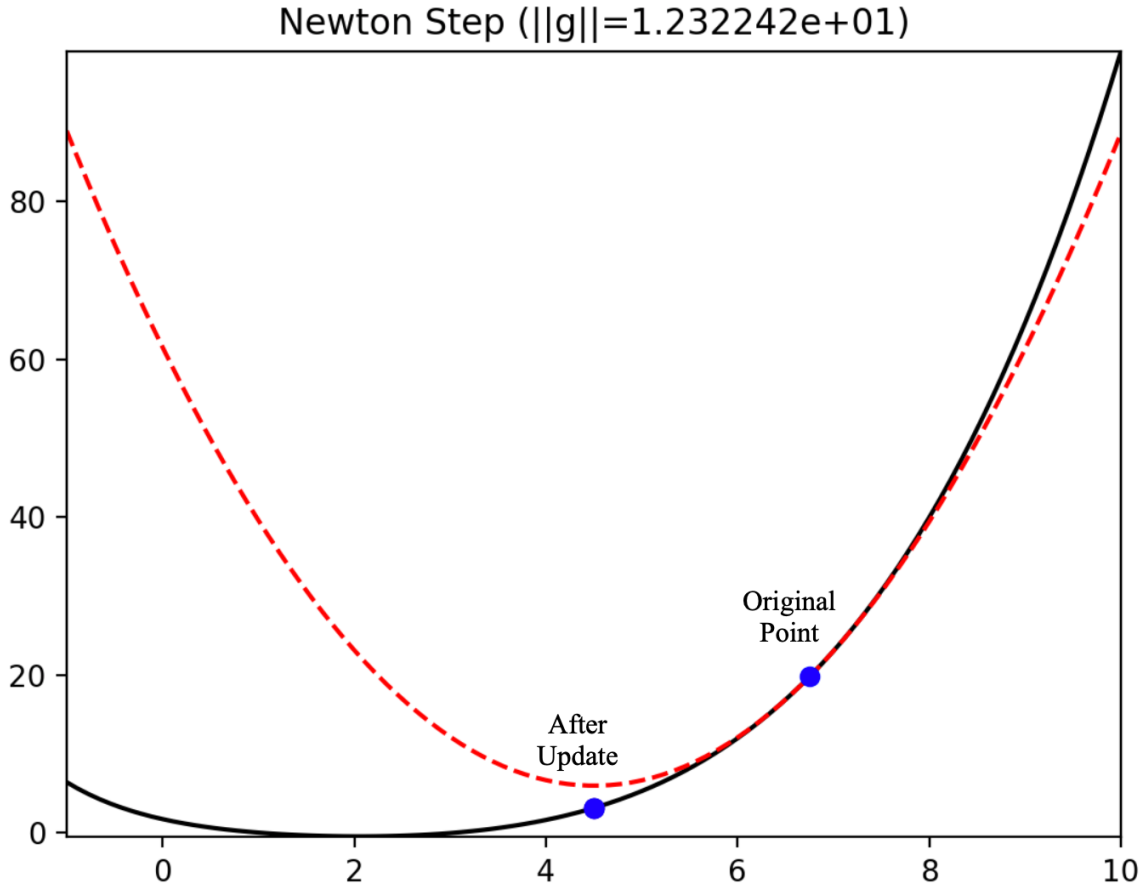
where: L is the loss function
f is a function parameterized by θ
x is the set of training inputs $x^{(1)}$, $x^{(2)}$,..., $x^{(n)}$
y is the set of training outputs (labels) $y^{(1)}$, $y^{(2)}$,..., $y^{(n)}$

$\theta \leftarrow 0$
repeat til done # see caption
For each training tuple $(x^{(i)}, y^{(i)})$ (in random order)
1. Optional (for reporting): # How are we doing on this tuple?
   Compute $\hat{y}^{(i)} = f(x^{(i)}; \theta)$ # What is our estimated output $\hat{y}$?
   Compute the loss $L(\hat{y}^{(i)}, y^{(i)})$ # How far off is $\hat{y}^{(i)}$) from the true output $y^{(i)}$?
2. $g \leftarrow \nabla_\theta L(f(x^{(i)}; \theta), y^{(i)})$ # How should we move θ to maximize loss?
3. $\theta \leftarrow \theta - \eta\, g$ # Go the other way instead
return θ

The stochastic gradient descent algorithm. Step 1 (computing the loss) is used to report how well we are doing on the current tuple. The algorithm can terminate when it converges, or when progress halts (for example when the loss starts going up on a held-out set).

Logistic Regression *Gradient descent vs. Newton Raphson*





$$l(\vec{w}+\vec{s}) = l(\vec{w}) + g(\vec{w})\vec{s} + \frac{1}{2}s^T H(\vec{w})\vec{s}$$

Training *Gradient descent - Example*

One single observation, whose correct class is $y = 1$, and with only two features:

$$x_1 = 3\ (Biomarker_1\ level)$$

$$x_2 = 2\ (Biomarker_2\ level)$$

Assume the initial weights and bias in θ^0 are all set to 0, and the initial learning rate η is 0.1:

$$w_1 = w_2 = b = 0$$

$$\eta = 0.1$$

Then compute

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta L(f(x_i; \theta) y_{\mathrm{i}})$$

Training *Gradient descent - Example*

In our mini example there are three parameters, so the gradient vector has 3 dimensions, for w_1, w_2, and b. We can compute the first gradient as follows:

$$\nabla_{w,b} = \begin{bmatrix} \frac{\partial L_{CE}(w,b)}{\partial w_1} \\ \frac{\partial L_{CE}(w,b)}{\partial w_2} \\ \frac{\partial L_{CE}(w,b)}{\partial b} \end{bmatrix} = \begin{bmatrix} (\sigma(w \cdot x + b) - y)x_1 \\ (\sigma(w \cdot x + b) - y)x_2 \\ \sigma(w \cdot x + b) - y \end{bmatrix} = \begin{bmatrix} (\sigma(0) - 1)x_1 \\ (\sigma(0) - 1)x_2 \\ \sigma(0) - 1 \end{bmatrix} = \begin{bmatrix} -0.5x_1 \\ -0.5x_2 \\ -0.5 \end{bmatrix} = \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix}$$

$$\theta^2 = \begin{bmatrix} w_1 \\ w_2 \\ b \end{bmatrix} - \eta \begin{bmatrix} -1.5 \\ -1.0 \\ -0.5 \end{bmatrix} = \begin{bmatrix} .15 \\ .1 \\ .05 \end{bmatrix}$$

Training *Backpropagation*

The solution to computing this gradient is an algorithm called error backpropagation or backprop (Rumelhart et al., 1986). While backprop was invented specially for neural networks, it turns out to be the same as a more general procedure called backward differentiation, which depends on the notion of computation graphs.

Jurafsky 2019

Training *Computation Graphs*

Consider computing the function $L(a, b, c) = c(a + 2b)$. If we make each of the component addition and multiplication operations explicit, and add names (d and e) for the intermediate outputs, the resulting series of computations is:

$$L(a, b, c) = c(a + \underbrace{2b}_{d})$$

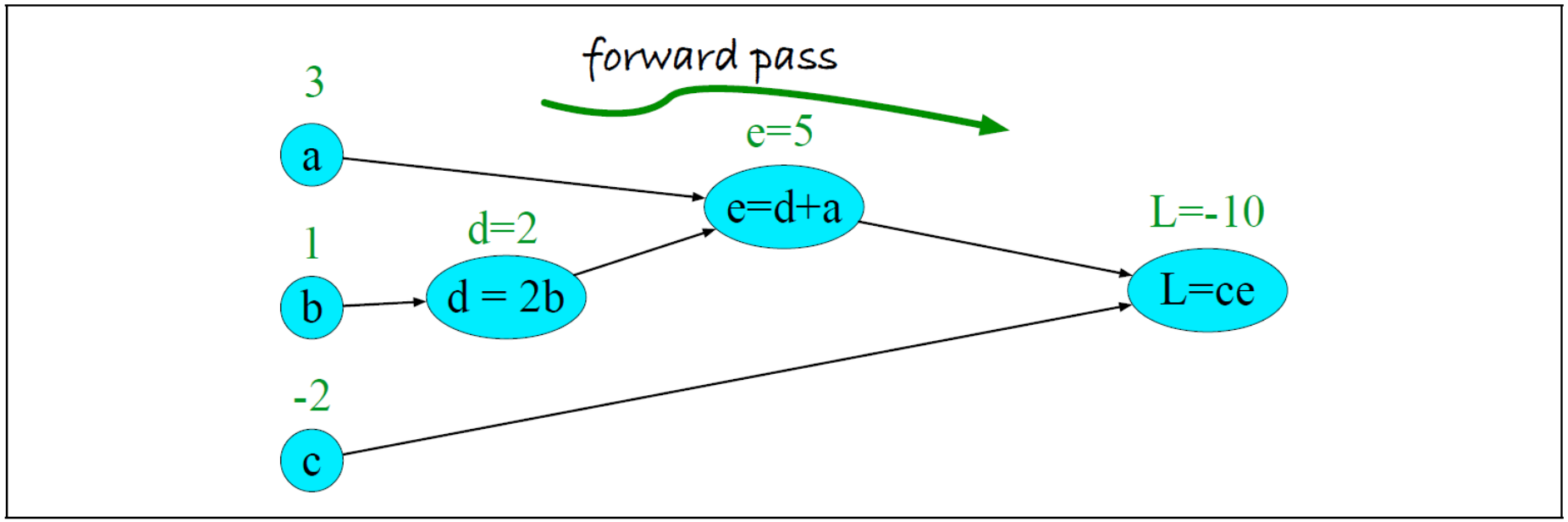
$$d = 2 * b$$
$$e = a + d$$
$$L = c * e$$

$$\underbrace{\underbrace{\underbrace{\quad}_{d}}_{e}}_{L}$$

Jurafsky 2019

Training *Computation Graphs*

$$b = 1 \qquad d = 2 * 1 = 2$$
$$a = 3 \qquad e = 3 + 2 = 5$$
$$c = -2 \qquad L = -2 * 5 = 10$$



Jurafsky 2019

Training *Computation Graphs*

$$L = ce \qquad \frac{\partial L}{\partial e} = c,\ \frac{\partial L}{\partial c} = e$$

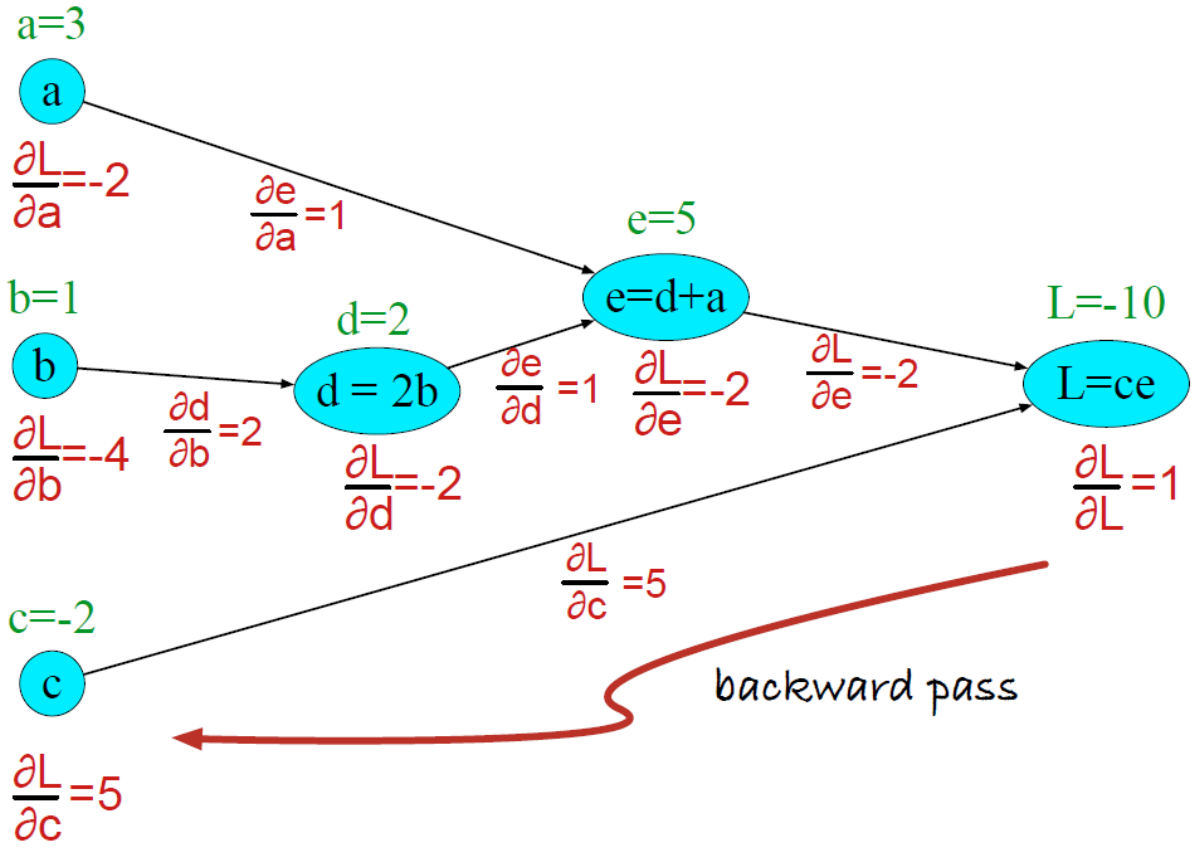
$$e = a + d \qquad \frac{\partial e}{\partial a} = 1,\ \frac{\partial e}{\partial d} = 1$$

$$d = 2b \qquad \frac{\partial L}{\partial c} = 2$$

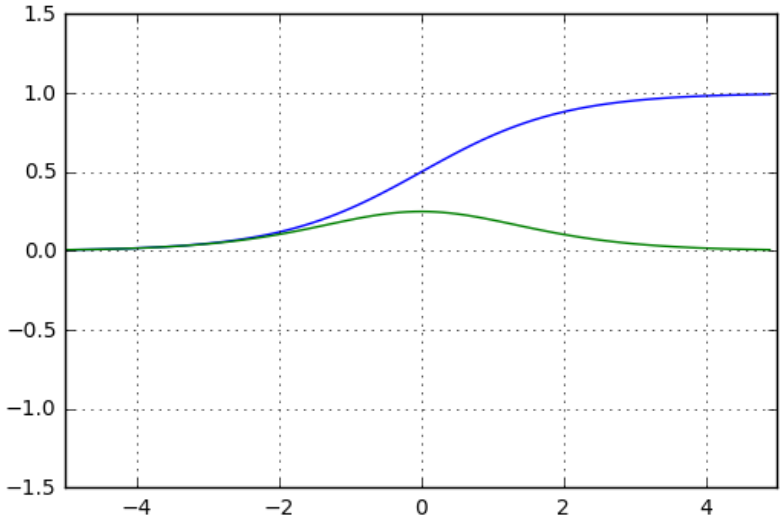
Chain Rule

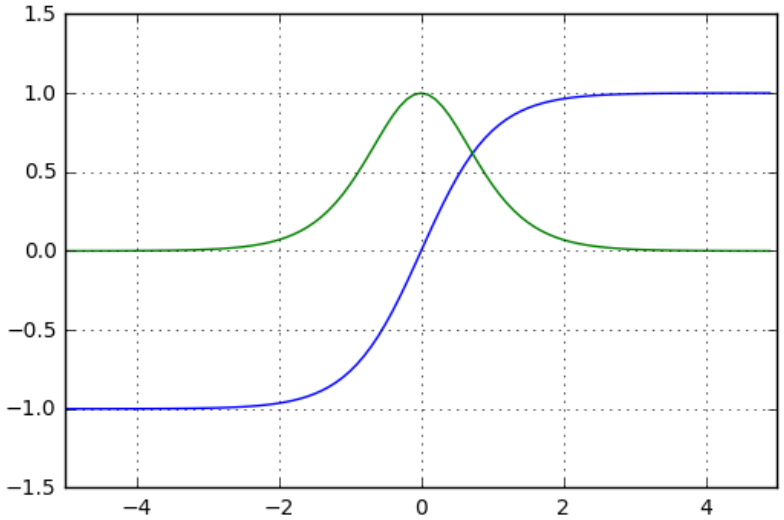
$$\frac{\partial L}{\partial a} = \frac{\partial L}{\partial e}\frac{\partial e}{\partial a}$$

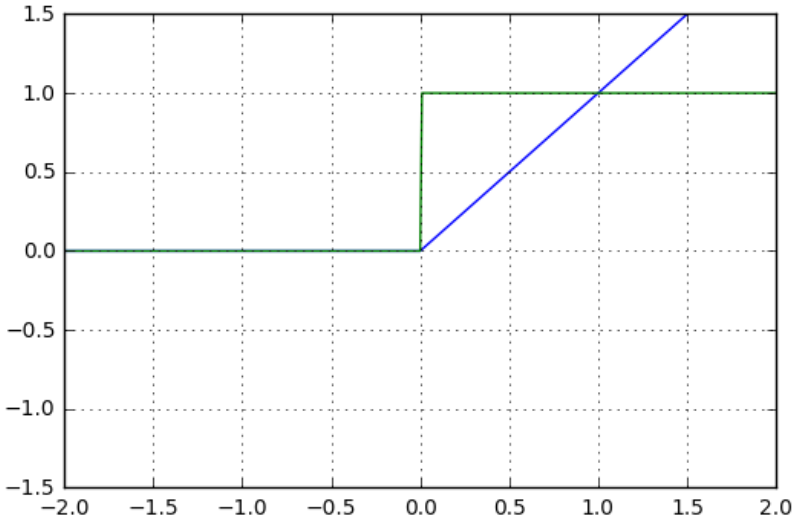
$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial e}\frac{\partial e}{\partial d}\frac{\partial d}{\partial b}$$



Training *Computation Graphs*







$$\text{sigm}(x) = \frac{1}{1+e^{-x}}$$

$$\text{sigm}'(x) = \text{sigm}(x)(1-\text{sigm}(x))$$

$$\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$$

$$\tanh'(x) = 1-\tanh(x)^2$$

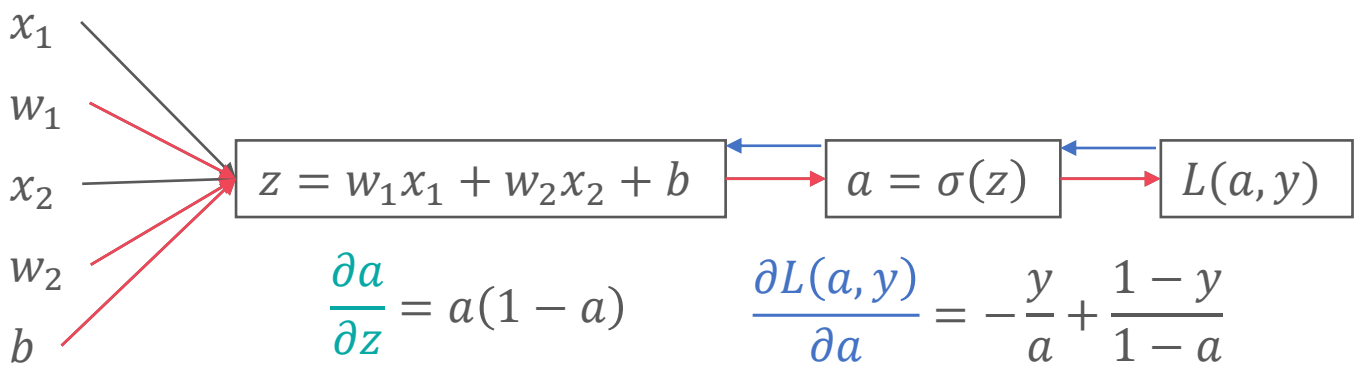
$$\text{relu}(x) = \max(0,x)$$

$$\text{relu}'(x) = 1_{x>0}$$

Green: derivative
Blue: activation function

Charles Ollion - Olivier Grisel

Training *Computation Graphs*



$$\frac{\partial a}{\partial z} = a(1-a) \qquad \frac{\partial L(a,y)}{\partial a} = -\frac{y}{a} + \frac{1-y}{1-a}$$

$$\frac{\partial L}{\partial z} = \frac{\partial L}{\partial a}\frac{\partial a}{\partial z}$$

$$= a - y$$

$$\frac{\partial L}{\partial w_1} = x_1 \frac{\partial L}{\partial z} \qquad w_1 := w_1 - \alpha \frac{\partial L}{\partial w_1}$$

$$\frac{\partial L}{\partial w_2} = x_2 \frac{\partial L}{\partial z} \qquad w_2 := w_2 - \alpha \frac{\partial L}{\partial w_2}$$

$$\partial b = \frac{\partial L}{\partial z} \qquad b := b - \alpha \frac{\partial L}{\partial z}$$

Andrew Ng 2017

Training *Batch training vs. Mini-batch training*

Batch gradient descent (batch training): compute $L_{CE}(w, b)$ over entire training set M to find the perfect direction

1. Compute the gradient: $\nabla L(f(x;\theta)y)$
2. Update the vector of parameters: $\theta_{t+1} = \theta_t - \eta \nabla L(f(x;\theta)y)$

Stochastic gradient descent (mini- batch): compute $L_{CE}(w, b)$ over single training example $m \in M$

1. Choose (with replacement) a random training example $\mathrm{d} \in D$
2. Compute the gradient: $\nabla L_d(f(x;\theta)y)$
3. Update the vector of parameters: $\theta_{t+1} = \theta_t - \eta \nabla L_d(f(x;\theta)y)$

When D is very large, Stochastic gradient is faster.
If m is the size of the dataset, then we are doing batch gradient descent; if m = 1, we are back to doing stochastic gradient descent.

Training *Mini-batch training of m examples*

We make the assumption that the training examples are independent

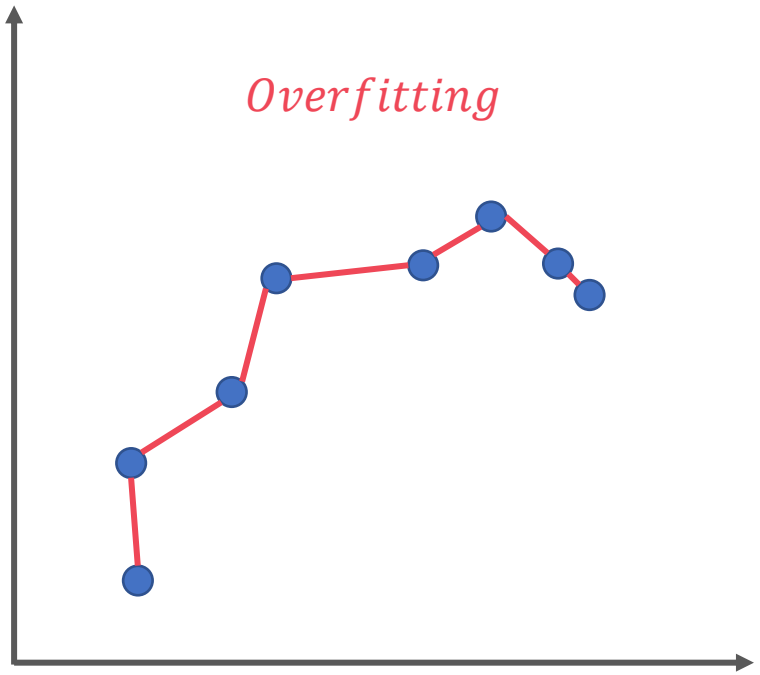
$$log\ p(training\ labels) = log \prod_{i=1}^{m} p(y_i|x_i) = \sum_{i=1}^{m} logp(y_i|x_i) = -\sum_{i=1}^{m} L_{CE}(\hat{y}, y)$$

Now the cost function for the mini-batch of m examples is the average loss for each example:

$$cost(w, b) = \frac{1}{m} \sum_{i=1}^{m} L_{CE}(\hat{y}, y)$$

$$= \frac{1}{m} \sum_{i=1}^{m} -[y_i \log \sigma(w \cdot x_i + b) + (1 - y_i) \log\big(1 - \sigma(w \cdot x_i + b)\big)]$$

Neural Networks *Regularization*



A good model should be able to generalize well from the training data to the unseen test set, but a model that overfits will have poor generalization.

To avoid overfitting, a new regularization term $R(\theta)$ is added to the objective function $\hat{\theta} = \arg\min_{\theta} \frac{1}{m} \sum_{i=1}^{m} L_{CE}(y_i, x_i; \theta)$

Slightly rewritten to be maximizing log probability rather than minimizing loss, and removing the $\frac{1}{m}$ term

$$\hat{\theta} = \arg\max_{\theta} \sum_{i=1}^{m} logP(y_i|x_i) - \alpha R(\theta)$$

The new regularization term R(q) is used to penalize large weights.

Mathematics *Distance*

From the general $L_p - norm$ we can define the corresponding $L_p - distance$ function, given as follows

$$\sigma_p(a,b) = \left|\left|a-b\right|\right|_{\mathrm{p}}$$

Mathematics *Distance*

1. Euclidean Distance*, L_2
2. Manhattan Distance, L_1
3. Hamming Distance, L_0
4. Minkowski Distance, L_p
5. Cosine Distance(similarity)

Euclidean Distance* is the most popular method

Mathematics *Euclidean distance*

Euclidean Distance

$$L_2 - norm: \left|\left|x_i - y_i\right|\right|_2 = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

Mathematics *Manhattan distance*

Manhattan Distance

$$L_1 - norm: \left|\left|x_i - y_i\right|\right|_1 = \sum_{i=1}^{n} |x_i - y_i|$$

Neural Networks *L2 Regularization*

$L2\ regularization$ is a quadratic function of Regularization the weight values, named because it uses the (square of the) L2 norm of the weight values. The L2 norm, $||\theta||_2$, is the same as the Euclidean distance of the vector θ from the origin. If θ consists of n weights, then:

$$R(\theta) = ||\theta||_2^2 = \sum_{j=1}^{n} \theta_j^2$$

Plug in

$$\hat{\theta} = \arg\max_{\theta} \sum_{i=1}^{m} logP(y_i|x_i) - \alpha \sum_{j=1}^{n} \theta_j^2$$

Neural Networks *L1 Regularization*

$L1\ regularization$ is a linear function of the weight values, named after the L1 norm Regularization $||\theta||_1$, the sum of the absolute values of the weights, or Manhattan distance (the Manhattan distance is the distance you'd have to walk between two points in a city with a street grid like New York):

$$R(\theta) = ||\theta||_1 = \sum_{i=1}^{n} |\theta_i|$$

Plug in

$$\hat{\theta} = \arg\max_{\theta} \sum_{i=1}^{m} logP(y_i|x_i) - \alpha \sum_{i=1}^{n} |\theta_i|$$

Neural Networks

Multinomial logistic regression

For classes more than two, we use multinomial logistic regression, also called SoftMax regression (or, historically, the maxent classifier) using a generalization of the sigmoid. We want to know the probability of y being in each potential class $c \in C, p(y = c|x)$. The SoftMax function takes a vector $z = [z_1, \dots, z_k]$ of k arbitrary values and maps them to a probability distribution, with each value in the range (0,1), and all the values summing to 1. Like the sigmoid, it is an exponential function.

$$softmax(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}}, 1 \leq i \leq k$$

Neural Networks

SoftMax is an extension of the sigmoid

Let's say, we have two classes:

$$Softmax(z_i) = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}} = \frac{e^{z_1}}{e^{z_1} + e^{z_2}} = \frac{e^{z_1 - z_2}}{e^{z_1 - z_2} + 1}$$

Sigmoid

Neural Networks *Multinomial logistic regression*

The SoftMax of an input vector $z = [z_1, \dots, z_k]$ is thus a vector itself:

$$softmax(z) = \left[\frac{e^{z_1}}{\sum_{i=1}^{k} e^{z_i}}, \dots, \frac{e^{z_k}}{\sum_{i=1}^{k} e^{z_i}}\right]$$

The denominator $\sum_{i=1}^{k} e^{z_i}$ is used to normalize all the values into probabilities.
Thus for example given a vector:

$$z = [0.6, 1.1, -1.5, 1.2, 3.2, -1.1]$$

The result $softmax(z)$ is

$$[0.055, 0.090, 0.0067, 0.10, 0.74, 0.010]$$

Neural Networks

Multinomial logistic regression

Like the sigmoid, the SoftMax has the property of squashing values toward 0 or 1. Thus if one of the inputs is larger than the others, it will tend to push its probability toward 1, and suppress the probabilities of the smaller inputs

$$p(y = c|x) = \frac{e^{w_c \cdot x + b_c}}{\sum_{j=1}^{k} e^{w_j \cdot x + b_j}}$$

Neural Networks *Learning in SoftMax*

Like the sigmoid, the SoftMax has the property of squashing values toward 0 or 1. Thus if one of the inputs is larger than the others, it will tend to push its probability toward 1, and suppress the probabilities of the smaller inputs

$$L_{CE}(\hat{y}, y) = -\sum_{k=1}^{K} 1\{y = k\} log p(y = k|x)$$

$$= -\sum_{k=1}^{K} 1\{y = k\} \log \frac{e^{w_c \cdot x + b_c}}{\sum_{j=1}^{k} e^{w_j \cdot x + b_j}}$$

This makes use of the function $1\{\}$ which evaluates to 1 if the condition in the brackets is true and to 0 otherwise.

Gradient

$$\frac{\partial L_{CE}}{\partial w_j} = -\big(1\{y = k\} - p(y = k|x)\big)x_k$$

$$= -\left(1\{y = k\} - \frac{e^{w_c \cdot x + b_c}}{\sum_{j=1}^{k} e^{w_j \cdot x + b_j}}\right)x_k$$

Encoding Methods

One-hot encoding

```
df <- tibble(
  ID = c(1:5),
  Employed = c("Yes", "Yes", "No", "Yes", "No"),
  Education = c(
    "Graduate",
    "High School",
    "Undergrad",
    "High School",
    "Undergrad"
  ),
  Marital = c("Single", "Single", "Married", "Married",
"Divorced"),
  Credit = c("Great", "Bad", "Bad", "Good", "Bad")
)
```

ID	Employed	Education	Marital Status	Credit
1	Yes	Graduate	Single	Great
2	Yes	High School	Single	Bad
3	No	Undergrad	Married	Bad
4	Yes	High School	Married	Good
5	No	Undergrad	Divorced	Bad

```
df %>% mutate(oneHot=1) %>%
spread(Education, oneHot, fill=0)
```

```
# A tibble: 5 x 7
     ID Employed Marital  Credit Graduate `High School` Undergrad
  <int> <chr>    <chr>    <chr>      <dbl>         <dbl>     <dbl>
1     1 Yes      Single   Great          1             0         0
2     2 Yes      Single   Bad            0             1         0
3     3 No       Married  Bad            0             0         1
4     4 Yes      Married  Good           0             1         0
5     5 No       Divorced Bad            0             0         1
```

Label encoding

ID	Employed	Education	Marital Status	Credit Worthy
1	Yes	Graduate	Single	Yes
2	Yes	High School	Single	No
3	No	Undergrad	Married	No
4	Yes	High School	Married	Yes
5	No	Undergrad	Divorced	No

```
df %>% mutate(Education =
                ifelse(Education == "Graduate", 1,
                       ifelse(Education =="Undergrad", 2, 3)))
```

```
# A tibble: 5 x 5
     ID Employed Education   Marital  Credit
  <int> <chr>    <chr>       <chr>    <chr>
1     1 Yes      Graduate    Single   Great
2     2 Yes      High School Single   Bad
3     3 No       Undergrad   Married  Bad
4     4 Yes      High School Married  Good
5     5 No       Undergrad   Divorced Bad
```

```
# A tibble: 5 x 5
     ID Employed Education Marital  Credit
  <int> <chr>        <dbl> <chr>    <chr>
1     1 Yes              1 Single   Great
2     2 Yes              3 Single   Bad
3     3 No               2 Married  Bad
4     4 Yes              3 Married  Good
5     5 No               2 Divorced Bad
```

Ordinal encoding

ID	Employed	Education	Marital Status	Credit Worthy
1	Yes	Graduate	Single	Yes
2	Yes	High School	Single	No
3	No	Undergrad	Married	No
4	Yes	High School	Married	Yes
5	No	Undergrad	Divorced	No

```
df %>% mutate(Education =
           ifelse(Education == "Graduate", 3,
                  ifelse(Education =="Undergrad", 2, 1)))
```

```
# A tibble: 5 x 5
     ID Employed Education   Marital  Credit
  <int> <chr>    <chr>       <chr>    <chr>
1     1 Yes      Graduate    Single   Great
2     2 Yes      High School Single   Bad
3     3 No       Undergrad   Married  Bad
4     4 Yes      High School Married  Good
5     5 No       Undergrad   Divorced Bad
```

```
# A tibble: 5 x 5
     ID Employed Education Marital  Credit
  <int> <chr>        <dbl> <chr>    <chr>
1     1 Yes              3 Single   Great
2     2 Yes              1 Single   Bad
3     3 No               2 Married  Bad
4     4 Yes              1 Married  Good
5     5 No               2 Divorced Bad
```

Frequency encoding

ID	Employed	Education	Marital Status	Credit Worthy
1	Yes	Graduate	Single	Yes
2	Yes	High School	Single	No
3	No	Undergrad	Married	No
4	Yes	High School	Married	Yes
5	No	Undergrad	Divorced	No

```
1    df %>% group_by(Education) %>%
     mutate(EdFreq=n()/nrow(.))
```

```
1    # A tibble: 5 x 5
2         ID Employed Education   Marital  Credit
3      <int> <chr>    <chr>       <chr>    <chr>
4    1     1 Yes      Graduate    Single   Great
5    2     2 Yes      High School Single   Bad
6    3     3 No       Undergrad   Married  Bad
7    4     4 Yes      High School Married  Good
8    5     5 No       Undergrad   Divorced Bad
```

```
# A tibble: 5 x 6
# Groups:   Education [3]
     ID Employed Education   Marital  Credit EdFreq
  <int> <chr>    <chr>       <chr>    <chr>   <dbl>
1     1 Yes      Graduate    Single   Great     0.2
2     2 Yes      High School Single   Bad       0.4
3     3 No       Undergrad   Married  Bad       0.4
4     4 Yes      High School Married  Good      0.4
5     5 No       Undergrad   Divorced Bad       0.4
```

1. one-hot encoding
2. label encoding
3. ordinal encoding
4. frequency encoding
5. mean encoding
6. weight of evidence encoding
7. probability ratio encoding

Acknowledgements and Resources

Acknowledgements and Resources

All the lectures materials borrowed from the following resources with/without modifications:

Textbook:

Galit Shmueli, Peter C. Bruce, Inbal Yahav, Nitin R. Patel, Kenneth C. Lichtendahl Jr., Data Mining for Business Analytics: Concepts, Techniques, and Applications in R (DMBA), Wiley, 1st Edition, ISBN-10: 1118879368, ISBN-13: 978-1118879368.

Additional Textbooks:

R For Data Science (open license, R4DS), Wickham, Hadley, and Garrett Grolemund

R Markdown (open license, RMD), Xie, Yihui, et al.

James, Gareth, et al. An Introduction to Statistical Learning: with Applications in R. Springer, 2017. (open license, ISL)

Mohammed J. Zaki, Wagner Meira, Jr., Data Mining and Analysis: Fundamental Concepts and Algorithms (DMA), Cambridge University Press, May 2014 (NEU library link)

David Hand, Heikki Mannila, Padhraic Smyth. Principles of Data Mining (PDM), The MIT Press, 2001, ISBN-10: 026208290X, ISBN-13: 978-0262082907. (NEU library link)

Tan, Pang-Ning, et al. Introduction to Data Mining (DM). Pearson Education, 2006. (official link)

Hastie, T., Friedman, J., & Tisbshirani, R. (2017). The Elements of statistical learning: data mining, inference, and prediction (ESL). New York: Springer. (open license)