MAE 688: Machine Learning for Mechanical Engineers

Lecture 2- Introduction to Deep Learning

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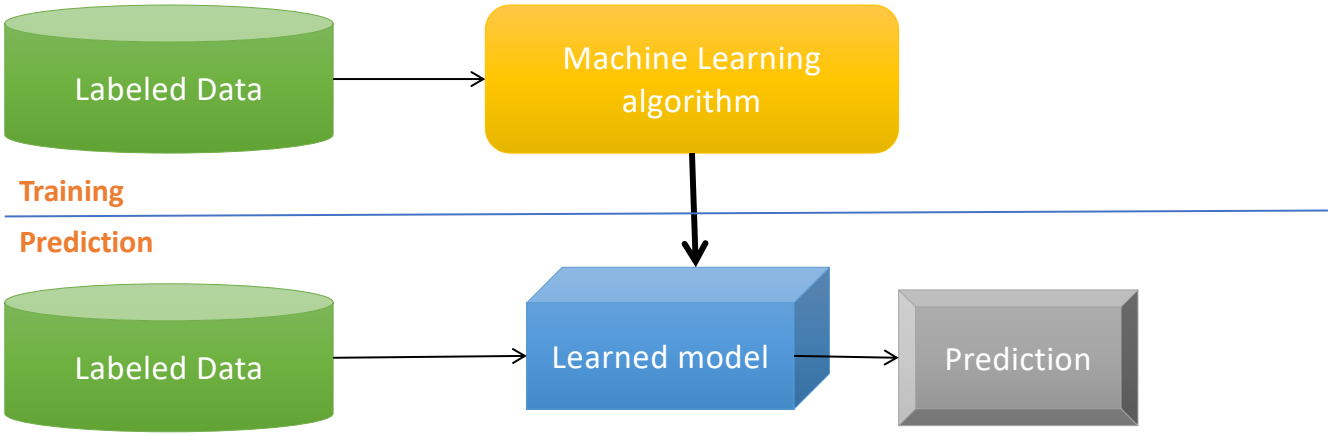
What is Machine Learning?

Machine learning is a field of computer science that gives computers the ability to **learn without being explicitly programmed**



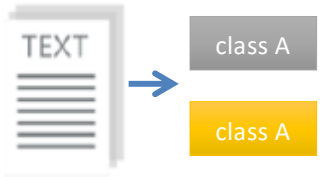
Methods that can learn from and make predictions on data

Types of Machine Learning

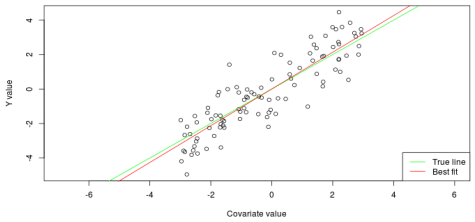
Supervised: Learning with a **labeled training** set
Example: email *classification* with already labeled emails

Unsupervised: Discover **patterns** in **unlabeled** data
Example: *cluster* similar documents based on text

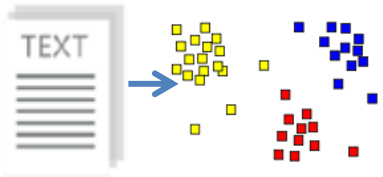
Reinforcement learning: learn to **act** based on **feedback/reward**
Example: learn to play Go, reward: *win or lose*



Classification



Regression



Clustering

Anomaly Detection
Sequence labeling
…

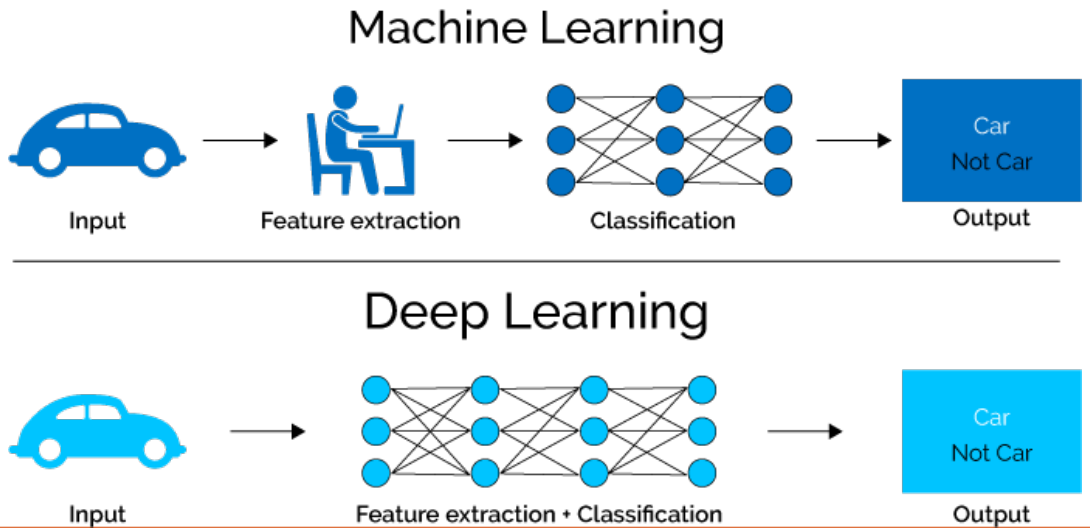
http://mbjoseph.github.io/2013/11/27/measure.html

What is Deep Learning?

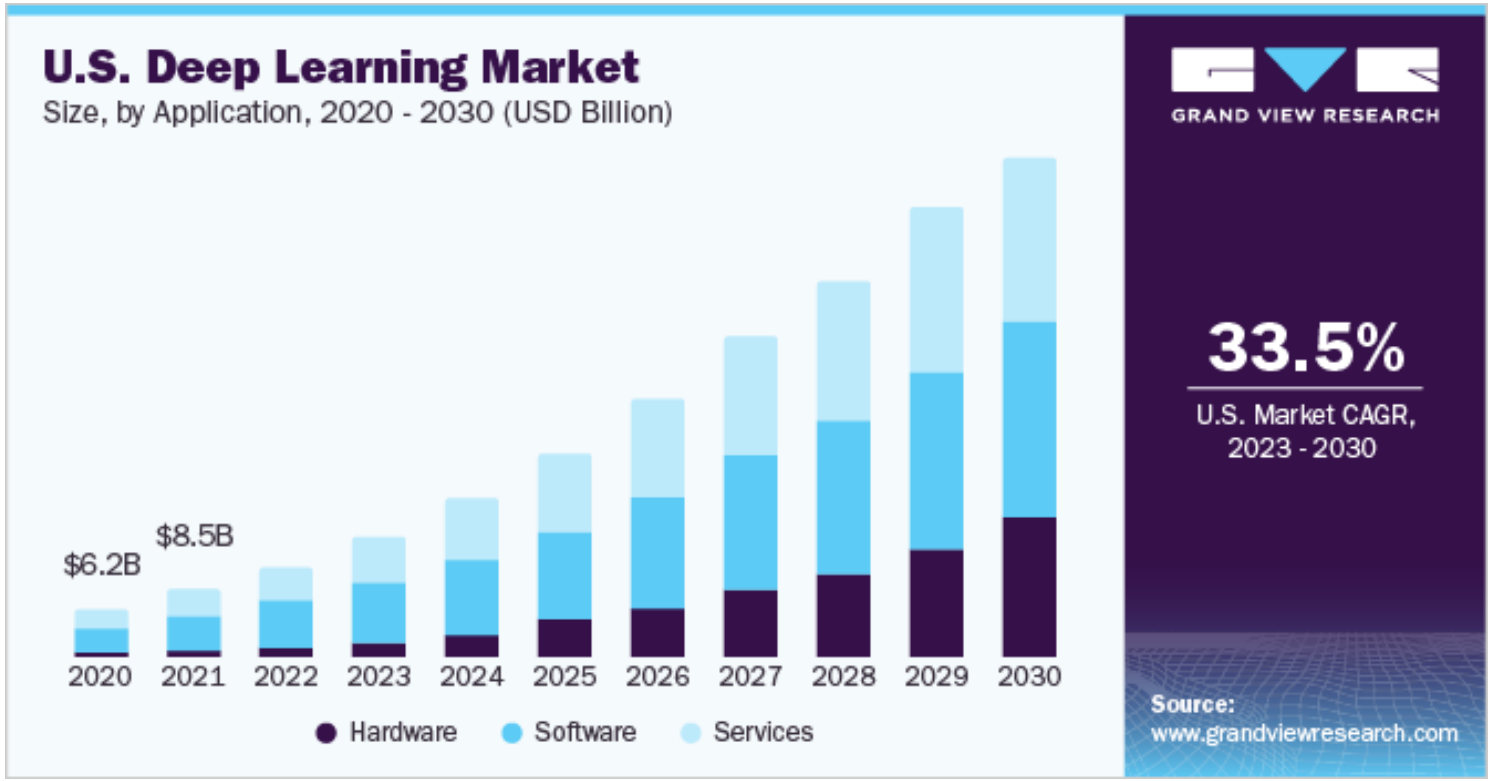
A machine learning subfield of learning **representations** of data. Exceptional effective at **learning patterns**.

Deep learning algorithms attempt to learn (multiple levels of) representation by using a **hierarchy of multiple layers**

If you provide the system **tons of information**, it begins to understand it and respond in useful ways.



Deep learning attracts lots of attention



The History of Deep Learning

1958: Perceptron (linear model)

1969: Perceptron has limitation

1980s: Multi-layer perceptron

Do not have significant difference from DNN today

1986: Backpropagation

Usually more than 3 hidden layers is not helpful

1989: 1 hidden layer is "good enough", why deep?

2006: RBM initialization

2009: GPU

2011: Start to be popular in speech recognition

2012: win ILSVRC image competition

2015.2: Image recognition surpassing human-level performance

2016.3: Alpha GO beats Lee Sedol

2016.10: Speech recognition system as good as humans

Hinton, G.E., 1986, August. Learning distributed representations of concepts. In *Proceedings of the eighth annual conference of the cognitive science society* (Vol. 1, p. 12).

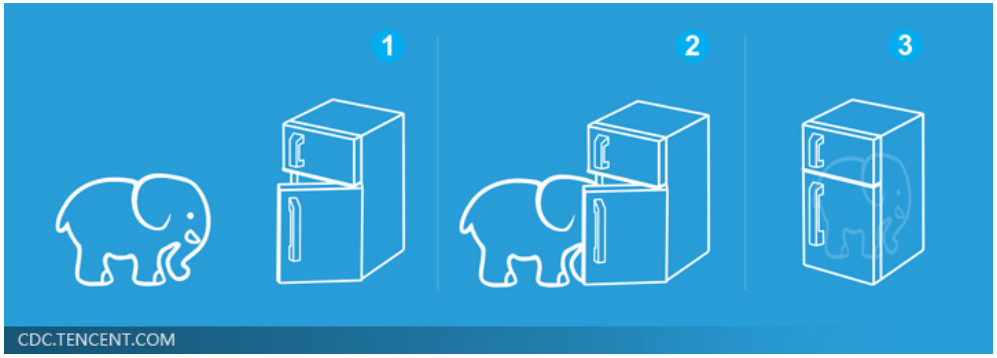
Hinton, G.E. and Salakhutdinov, R.R., 2006. Reducing the dimensionality of data with neural networks. *science*, *313*(5786), pp.504-507.

Restricted boltzmann machines

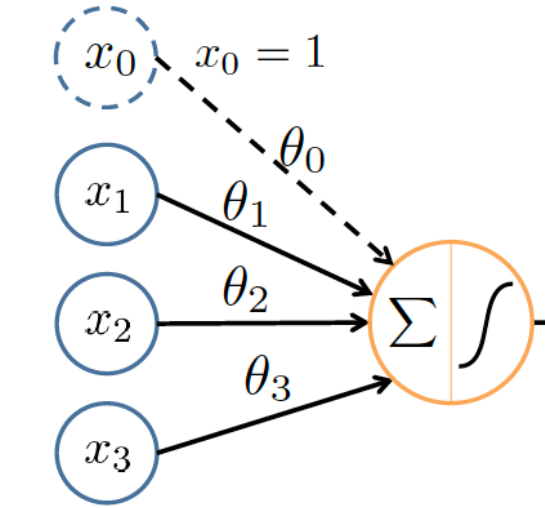
Three ”SIMPLE” steps for deep learning

Three ”SIMPLE” steps for deep learning

Deep Learning is so simple ……



Single Node



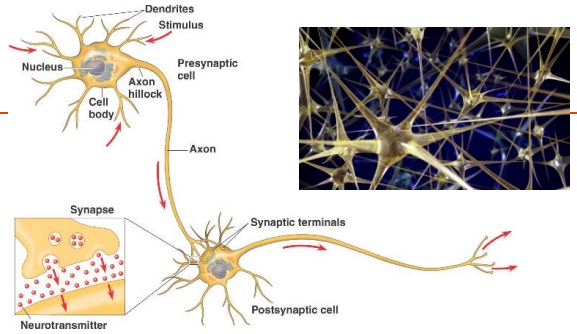
$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

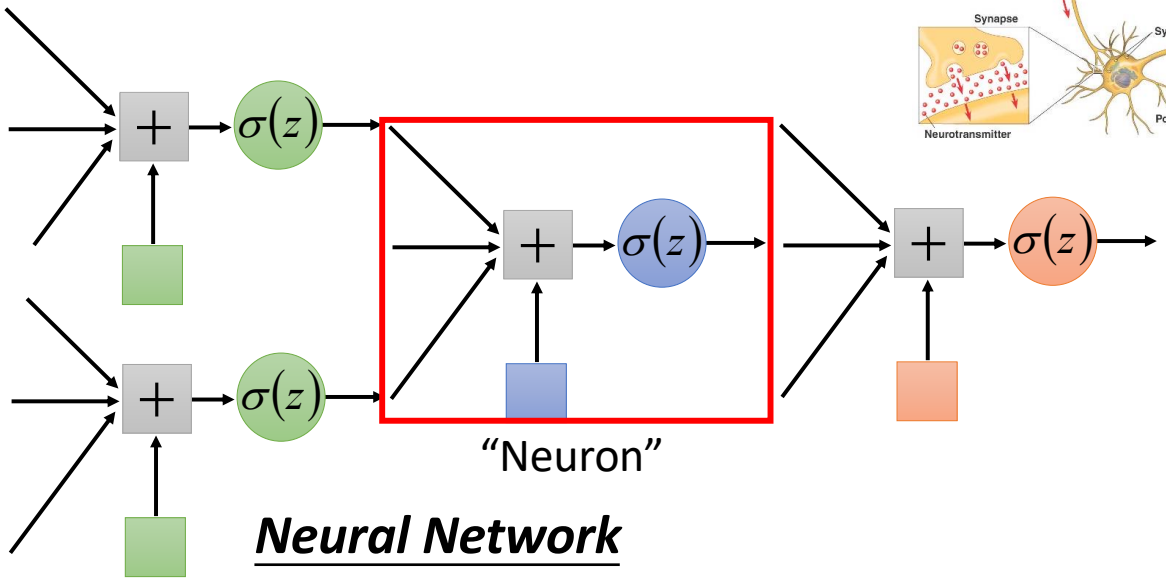
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}\right) = \frac{1}{1 + e^{-\boldsymbol{\theta}^{\mathsf{T}}\mathbf{x}}}$$

Binary Logistic Regression

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

Neural Network





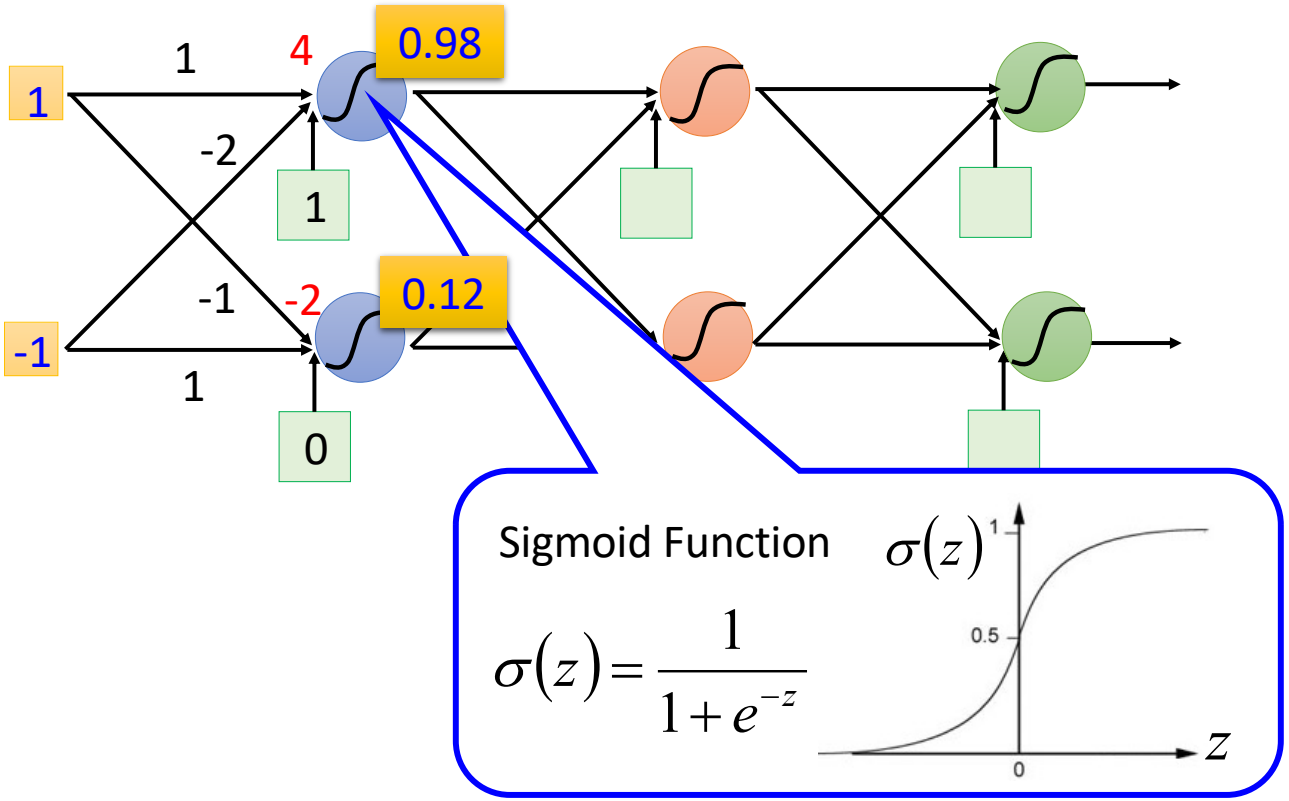
"Neuron"

Neural Network

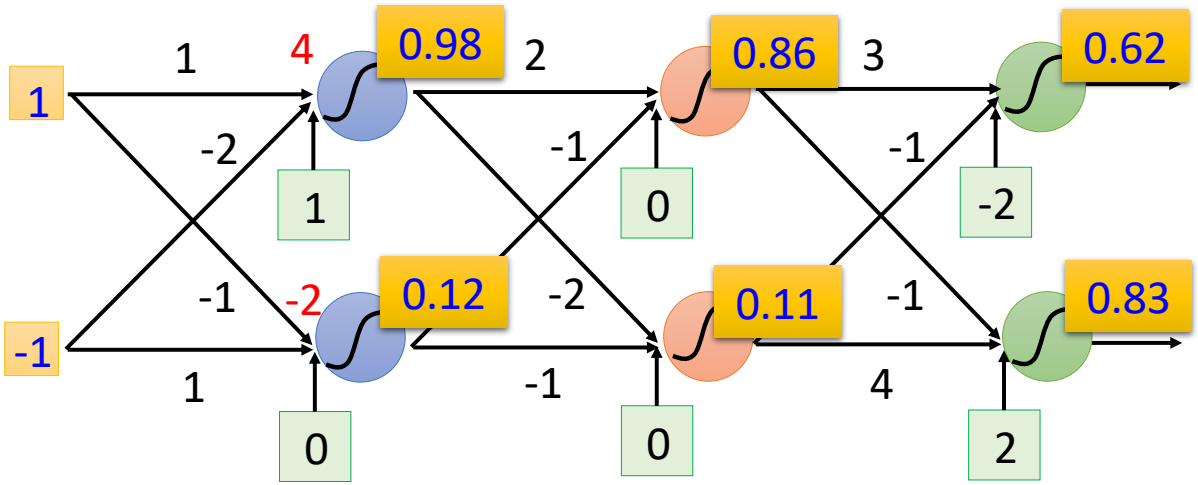
Different connection leads to different network structures

Network parameter θ: all the weights and biases in the "neurons"

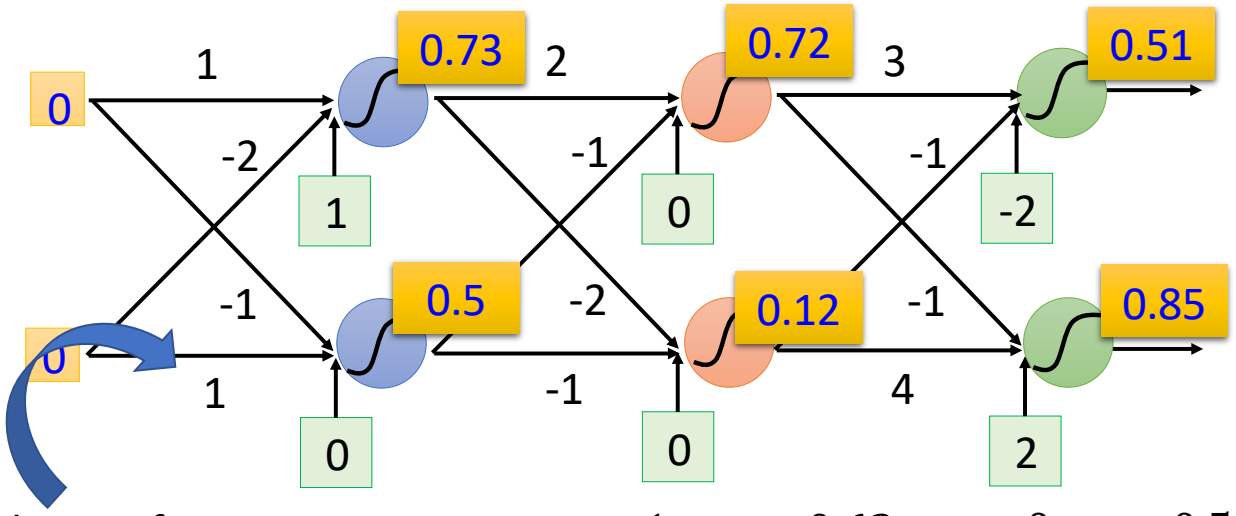
Fully Connect Feedforward Network



Fully Connect Feedforward Network



Fully Connect Feedforward Network



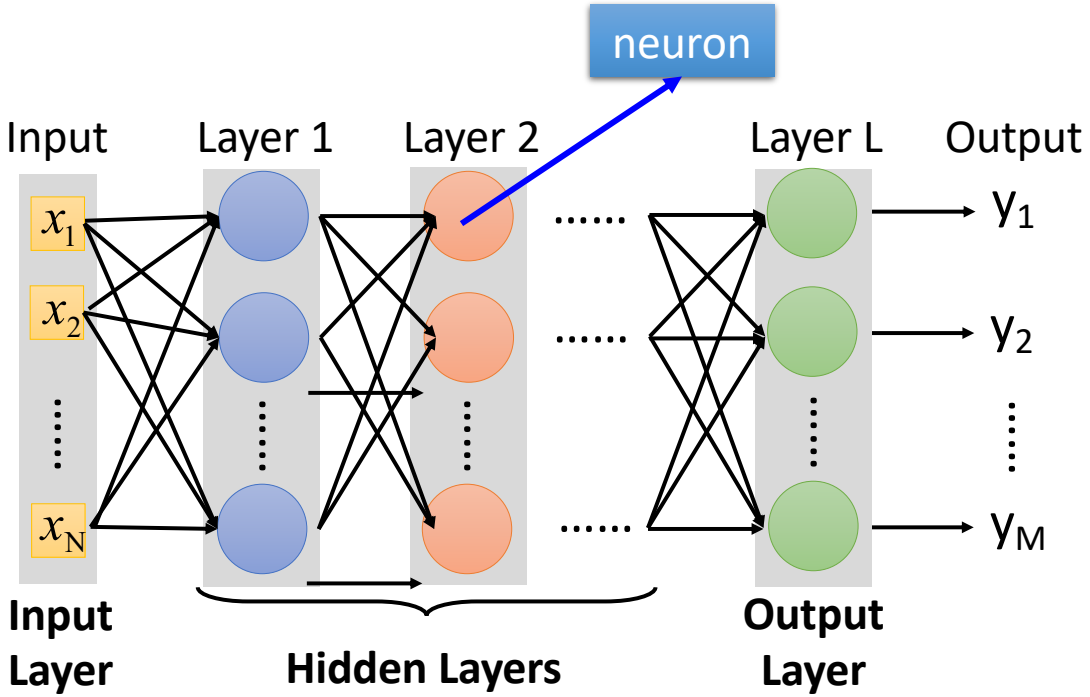
This is a function.

Input vector, output vector

$$f\left(\begin{bmatrix}1\\-1\end{bmatrix}\right)=\begin{bmatrix}0.62\\0.83\end{bmatrix} \quad f\left(\begin{bmatrix}0\\0\end{bmatrix}\right)=\begin{bmatrix}0.51\\0.85\end{bmatrix}$$

Given network structure, define ***a function set***

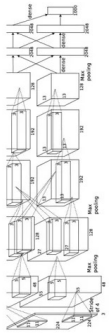
Fully Connect Feedforward Network



Deep = Many Many hidden la

Large Scale Visual Recognition Challenge (ILSVRC)

8 layers



16.4%

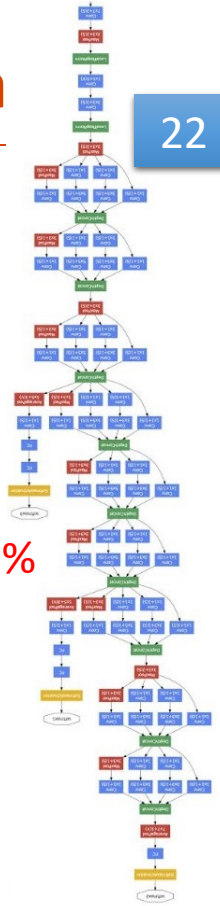
AlexNet (2012)

19 layers

7.3%

VGG (2014)

22 layers

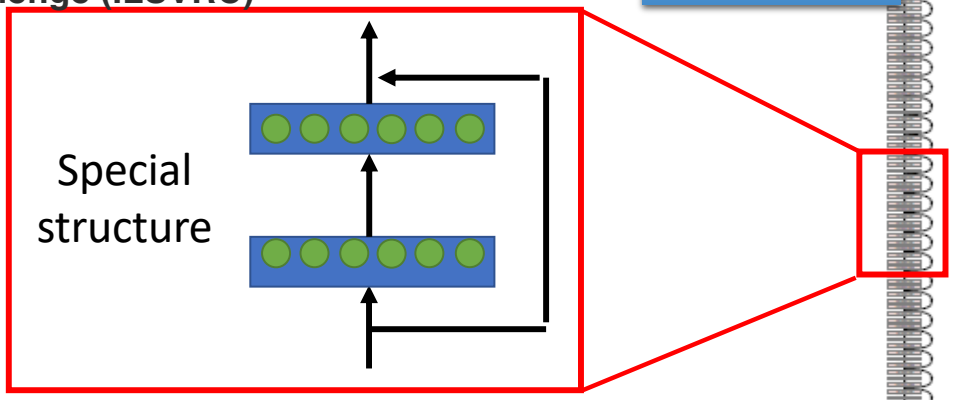


6.7%

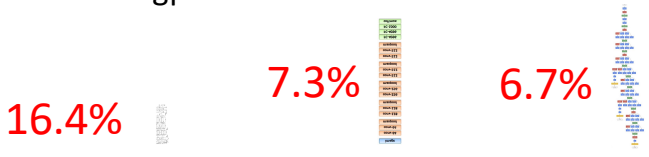
GoogleNet (2014)

Deep = Many Many hidden layers

Large Scale Visual Recognition Challenge (ILSVRC)



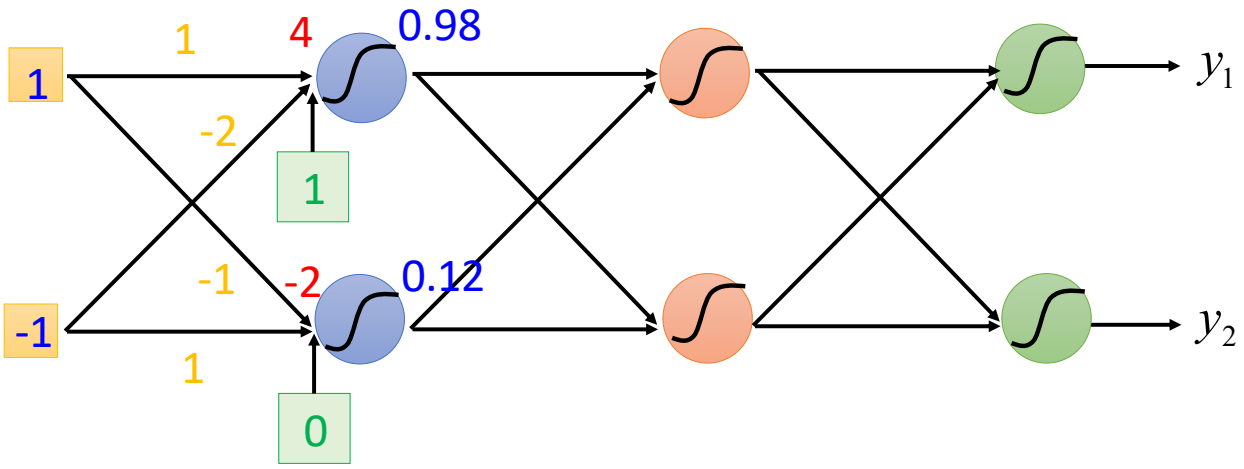
Ref: https://www.youtube.com/watch?v=dxB6299gpvI



He, K., Zhang, X., Ren, S. and Sun, J., 2016. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 770-778).

Cited by 235134

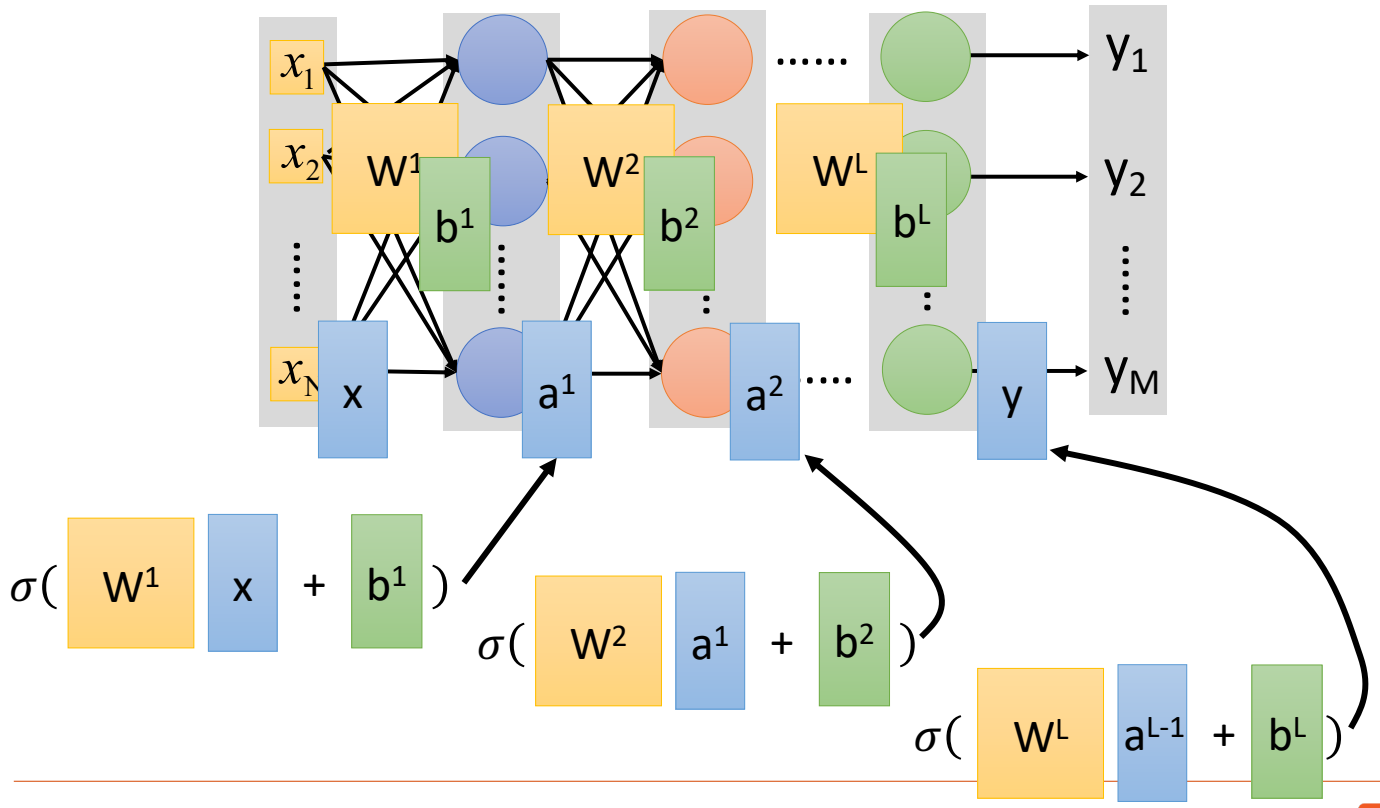
Matrix Operation



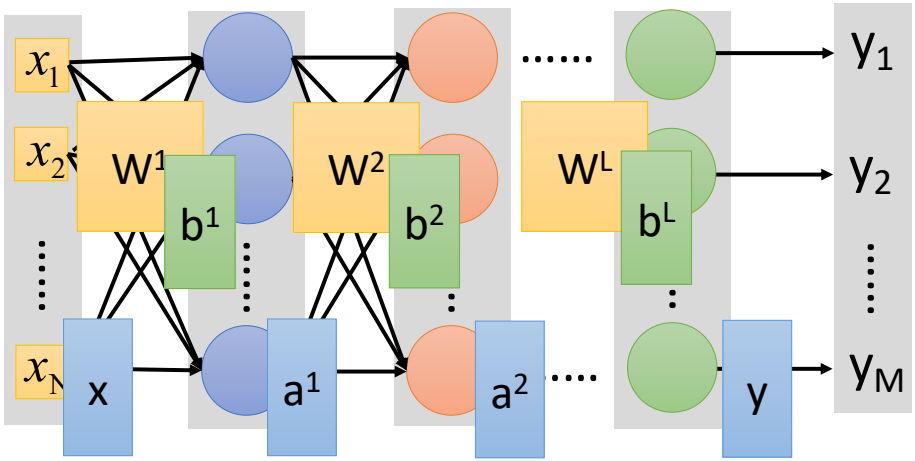
$$\sigma\left(\begin{bmatrix} 1 & -2 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) = \begin{bmatrix} 0.98 \\ 0.12 \end{bmatrix}$$

$$\begin{bmatrix} 4 \\ -2 \end{bmatrix}$$

Neural Network



Neural Network

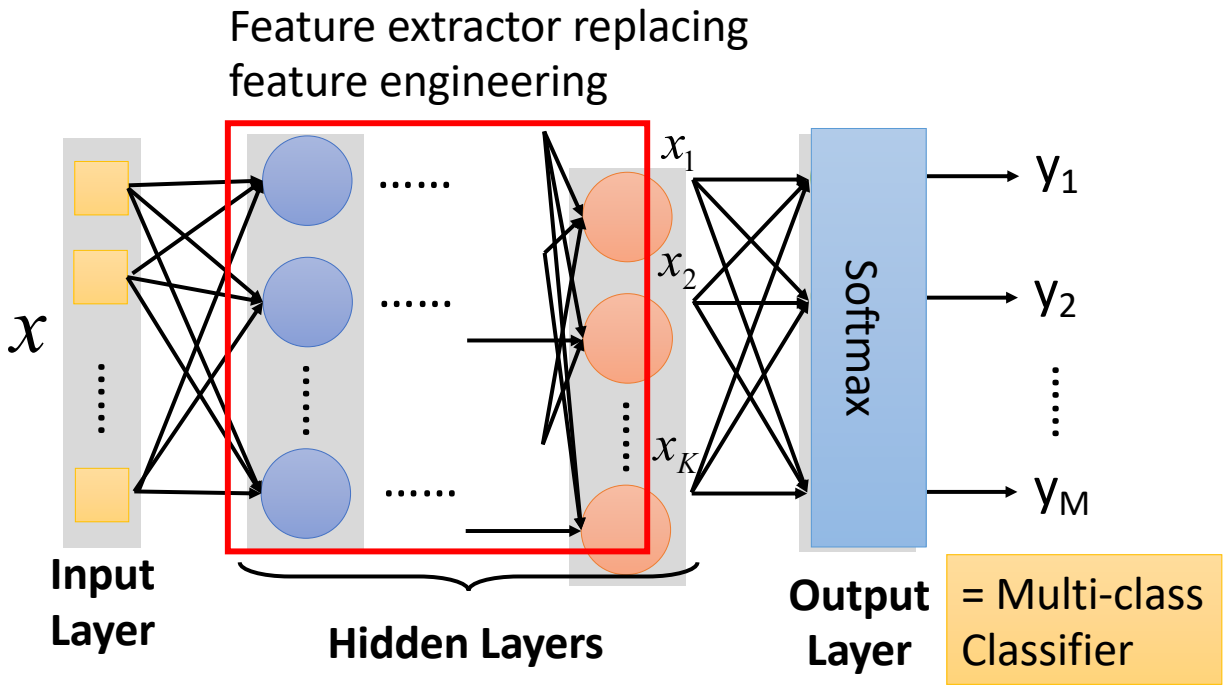


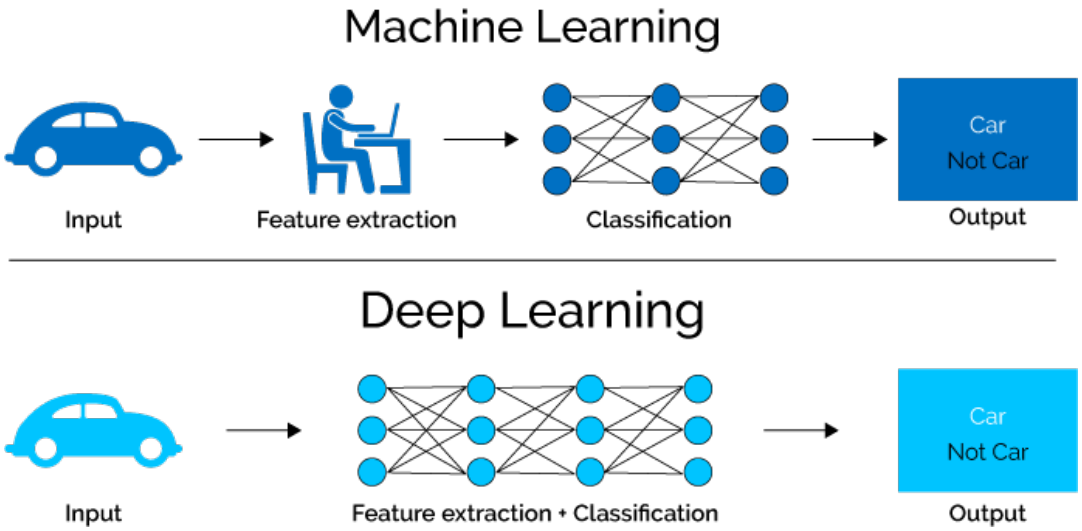
$$y = f(x)$$

Using parallel computing techniques to speed up matrix operation

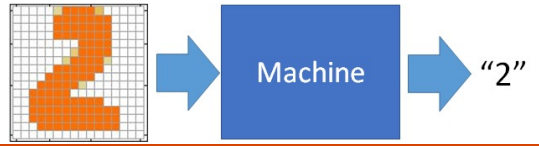
$$= \sigma(W^L \cdots \sigma(W^2 \sigma(W^1 x + b^1) + b^2) \cdots + b^L)$$

Output Layer as Multi-Class Classifier

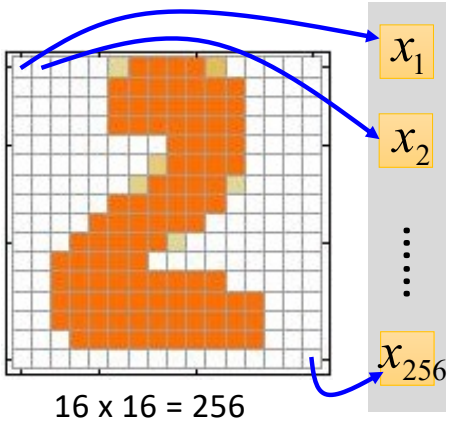



Machine Learning
Input
Feature extraction
Classification
Car
Not Car
Output
Deep Learning
Input
Feature extraction + Classification
Car
Not Car
Output

Example Application



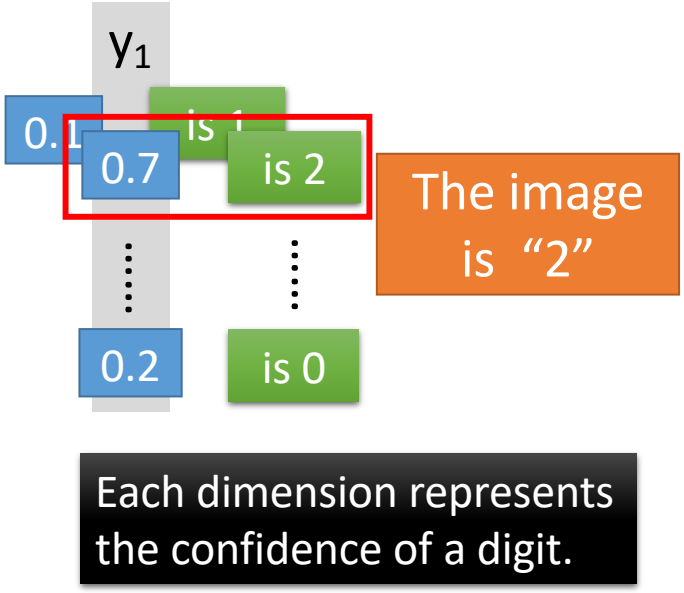
- Input



Ink → 1

No ink → 0

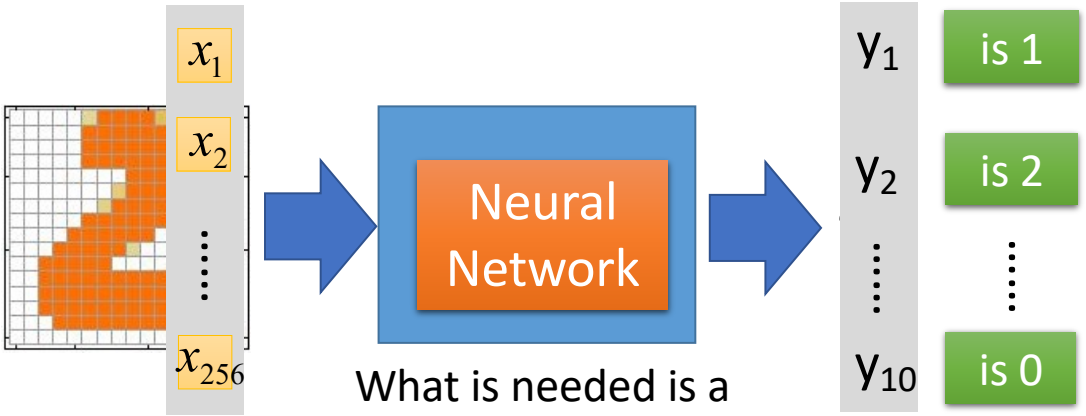
- Output



Each dimension represents the confidence of a digit.

Example Application

- Handwriting Digit Recognition

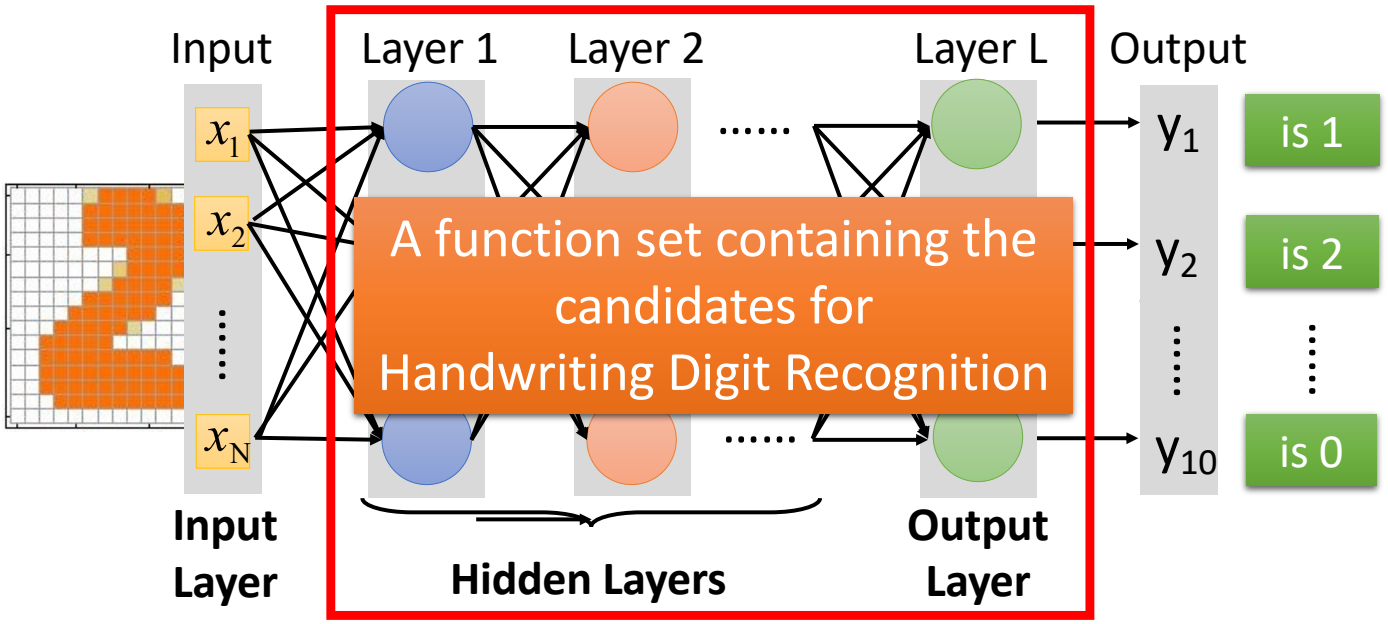


What is needed is a function ……

Input:
256-dim vector

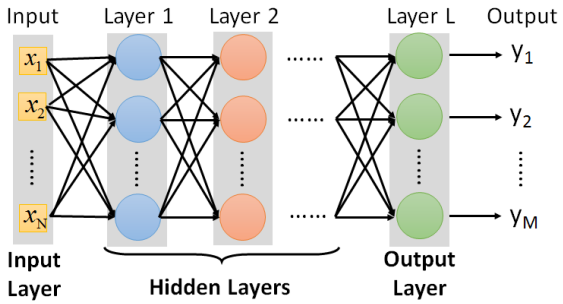
output:
10-dim vector

Example Application



You need to decide the network structure to let a good function in your function set.

FAQ



- Q: How many layers? How many neurons for each layer?

Trial and Error + Intuition

- Q: Can the structure be automatically determined?
  - E.g. Evolutionary Artificial Neural Networks
- Q: Can we design the network structure?

Convolutional Neural Network (CNN)

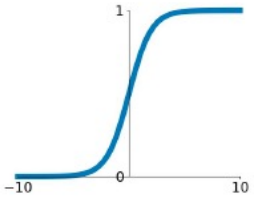
Activation Functions

(borrow some slides are from Stanford University)

Activation Functions

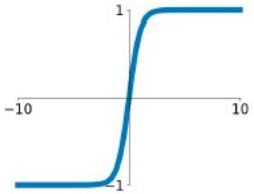
Sigmoid

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



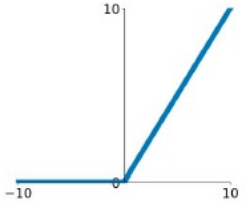
tanh

$$\tanh(x)$$



ReLU

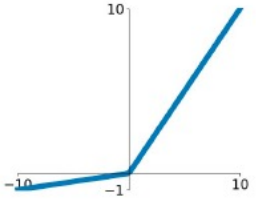
$$\max(0, x)$$



Rectified Linear Unit

Leaky ReLU

$$\max(0.1x, x)$$

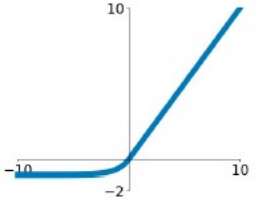


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

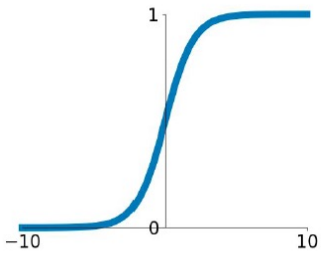
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Exponential Linear Units

Activation Functions



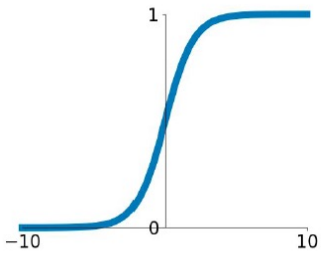
Sigmoid

$$\sigma(x) = 1/(1 + e^{-x})$$

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

Activation Functions



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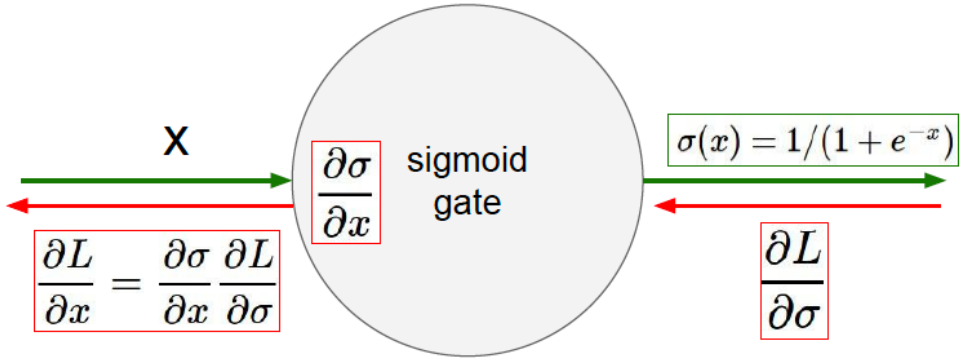
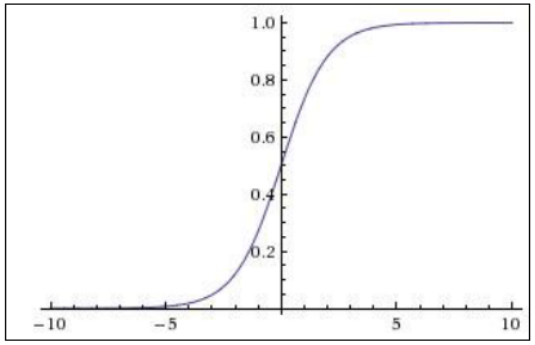
3 problems:

1. Saturated neurons “kill” the gradients

Activation Functions

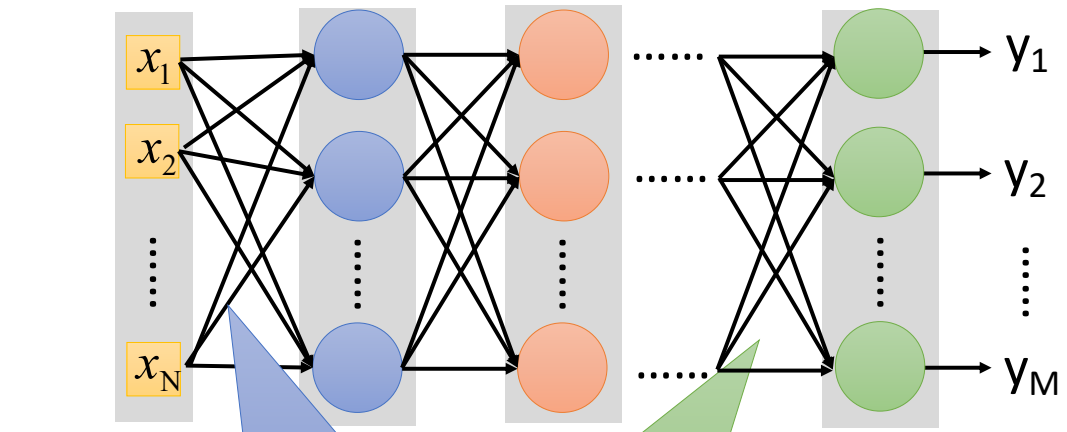




What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

Vanishing Gradient Problem



Smaller gradients

Learn very slow

Almost random

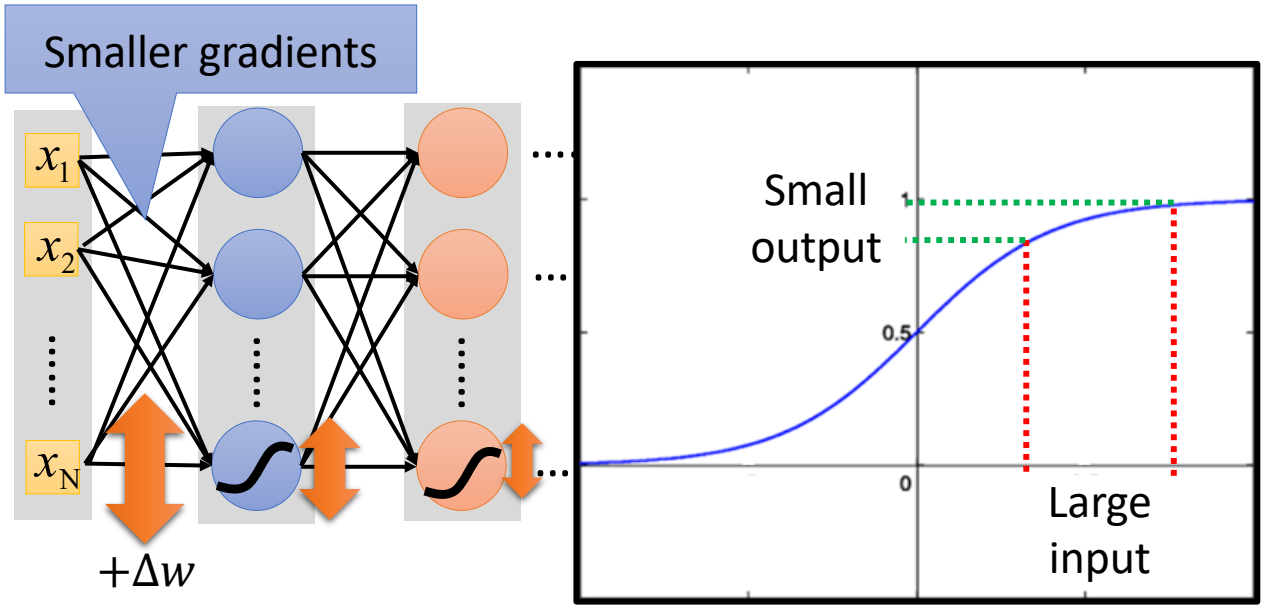
Larger gradients

Learn very fast

Already converge

based on random!?

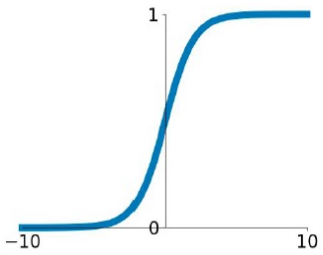
Vanishing Gradient Problem



Intuitive way to compute the derivatives …

$$\frac{\partial l}{\partial w} =? \frac{\Delta l}{\Delta w}$$

Activation Functions



Sigmoid

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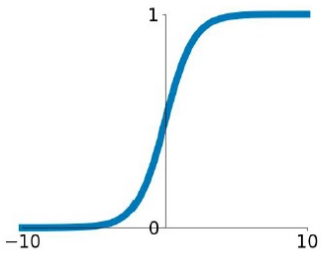
3 problems:

1. Saturated neurons "kill" the gradients
2. Sigmoid outputs are not zero-centered

Activation Functions



Sigmoid

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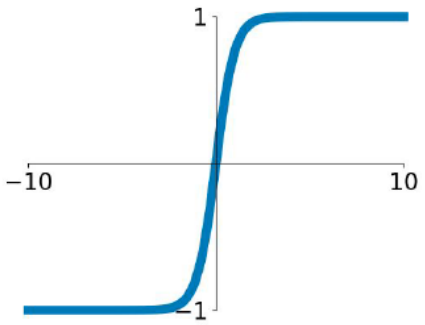
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered
3. exp() is a bit compute expensive

Activation Functions

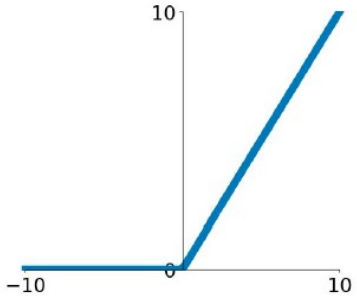


tanh(x)

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

Activation Functions



ReLU
(Rectified Linear Unit)

- Computes **f(x) = max(0,x)**

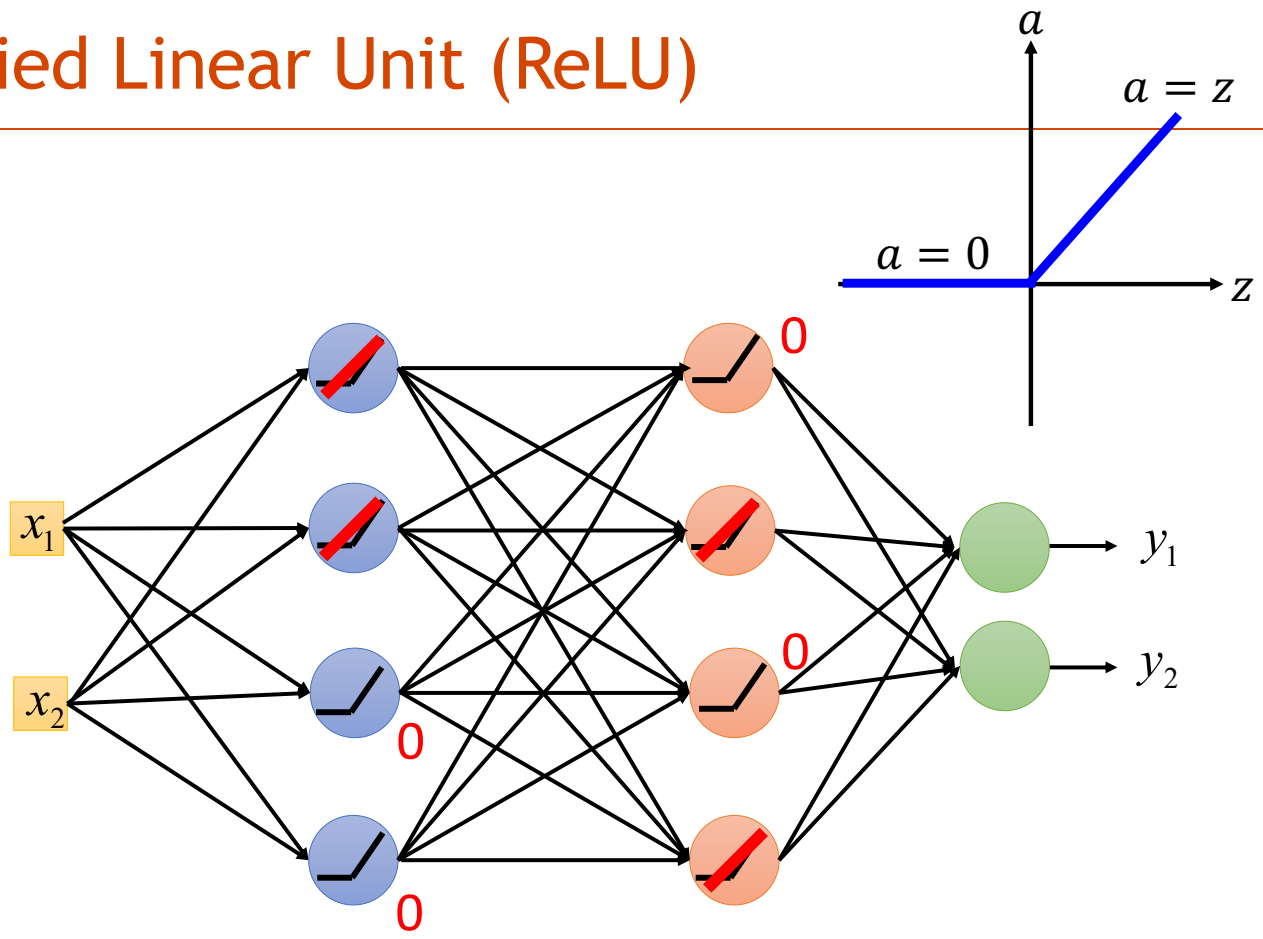
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

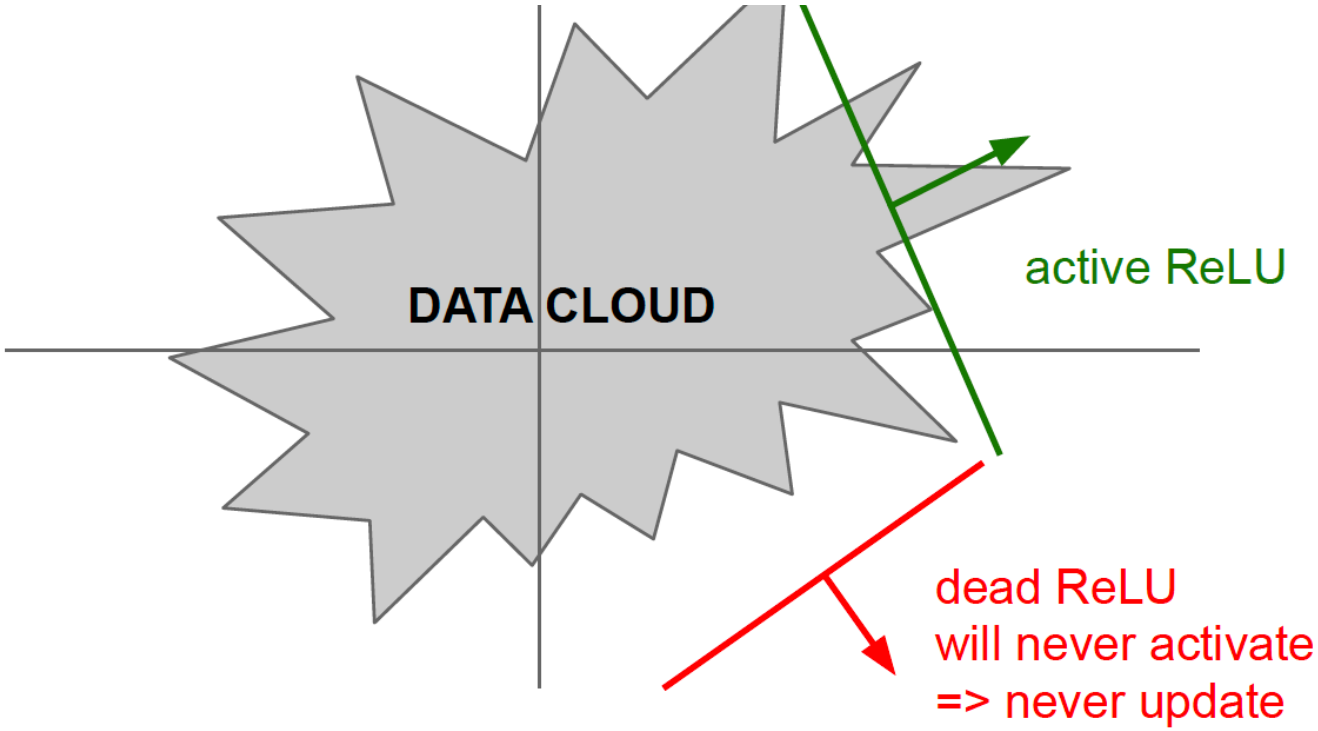
Problems

1. Not zero-centered output
2. Non-differentiable at zero; however, it is differentiable anywhere else.

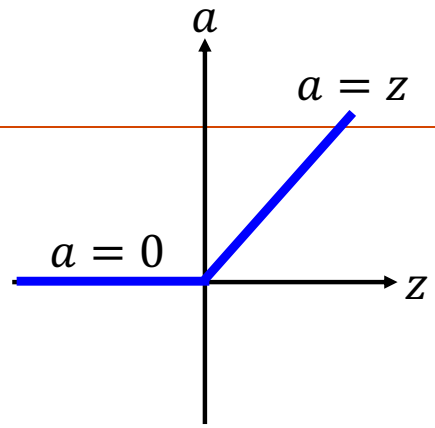
[Krizhevsky et al., 2012]

Rectified Linear Unit (ReLU)

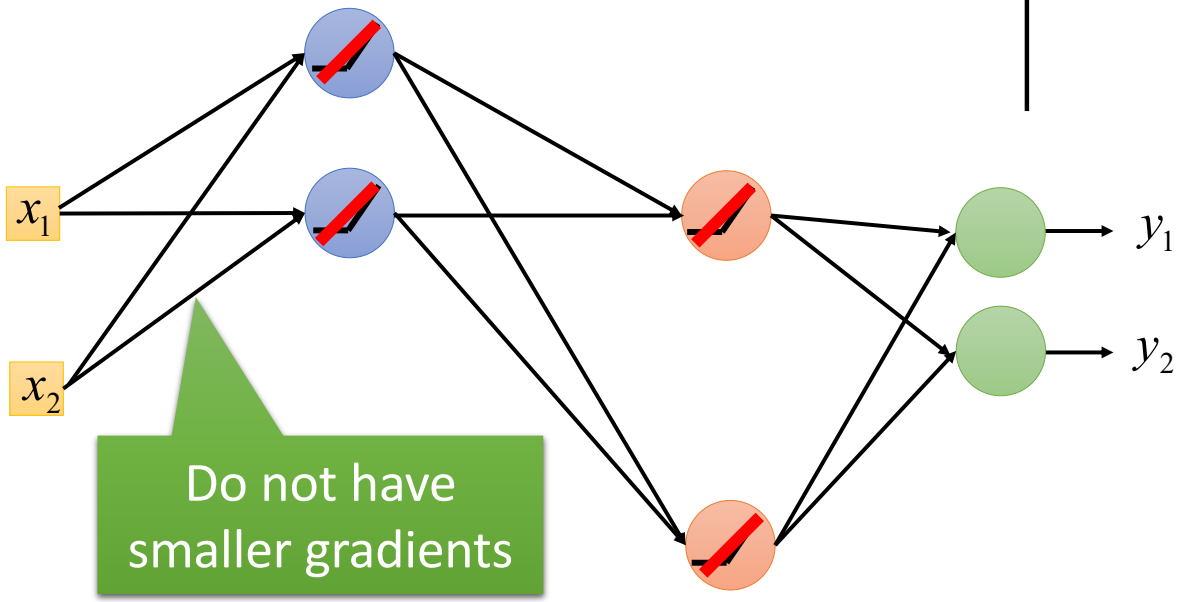



DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update

Rectified Linear Unit (ReLU)



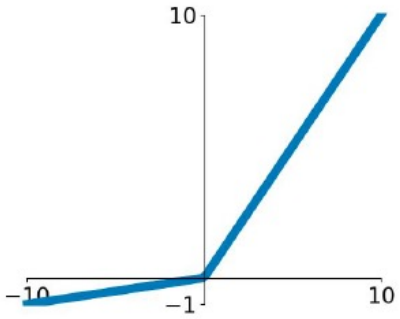
A Thinner linear network



Do not have smaller gradients

Activation Functions

[Mass et al., 2013]
[He et al., 2015]



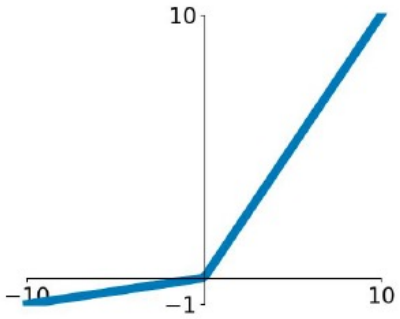
Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Activation Functions

[Mass et al., 2013]
[He et al., 2015]



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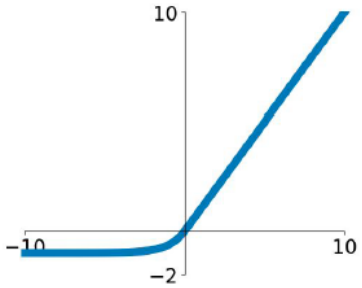
Parametric Rectifier (PReLU)

$$f(x) = \max(\alpha x, x)$$

backprop into \alpha (parameter)

Activation Functions

Exponential Linear Units (ELU)



- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

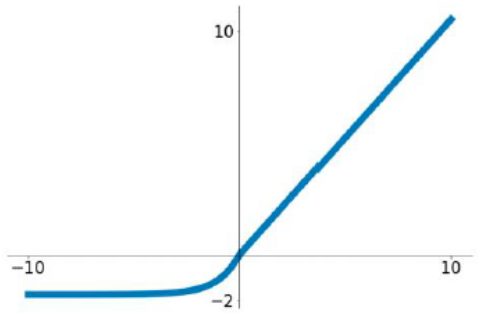
(Alpha default = 1)

- Computation requires exp()

[Clevert et al., 2015]

Activation Functions

Scaled Exponential Linear Units (SELU)



- Scaled versionof ELU that works better for deep networks
- "Self-normalizing" property;
- Can train deep SELU networks without BatchNorm
  - (will discuss more later)

$$f(x) = \begin{cases} \lambda x & \text{if } x > 0 \\ \lambda\alpha(e^x - 1) & \text{otherwise} \end{cases}$$

α = 1.6733, λ = 1.0507

[Klambauer et al. ICLR 2017]

Maxout "Neuron"

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

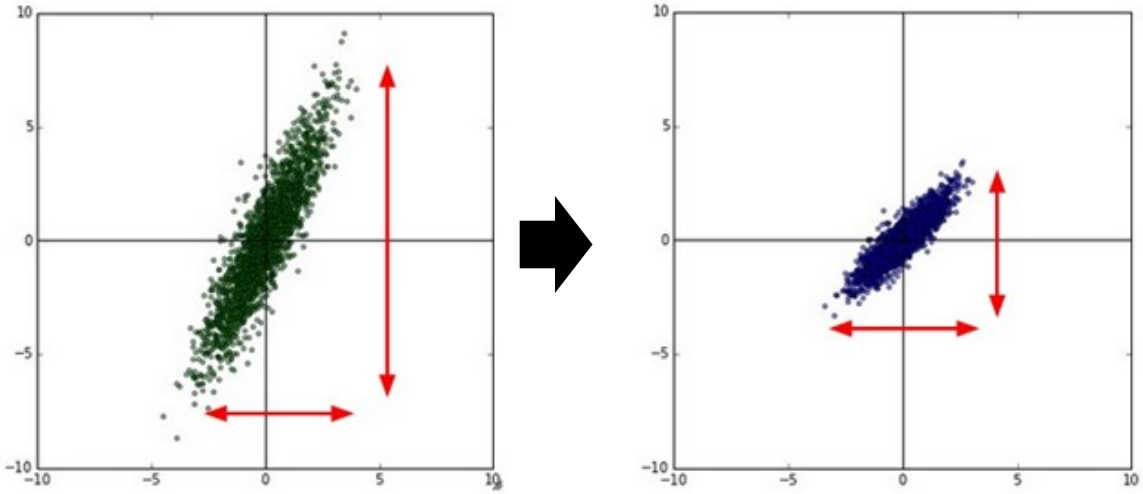
Problem: doubles the number of parameters/neuron :(

In Practice

- Use ReLU
- Don’t use sigmoid or tanh

Data Preprocessing-Feature Scaling

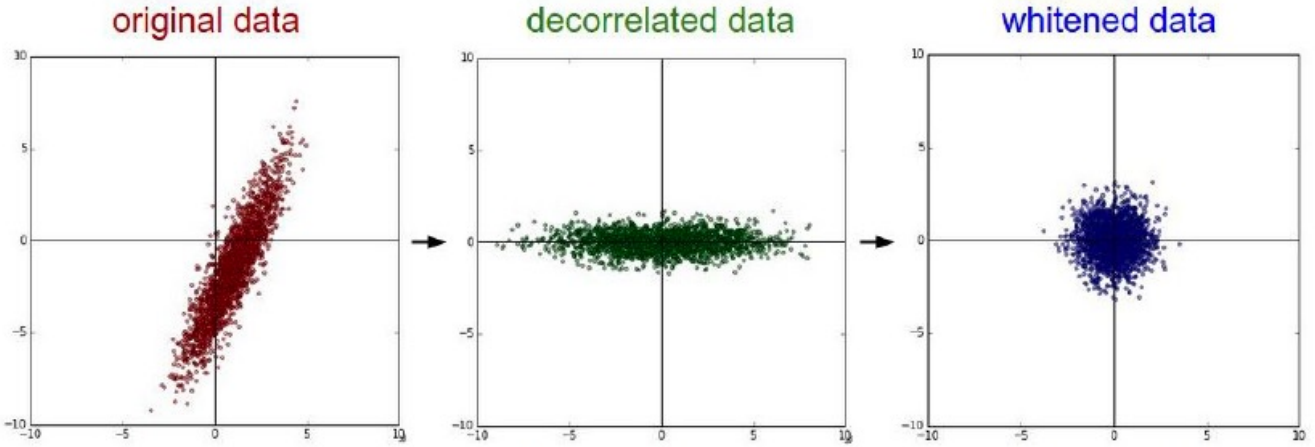
$$y = b + w_1 x_1 + w_2 x_2$$



Make different features have the same scaling

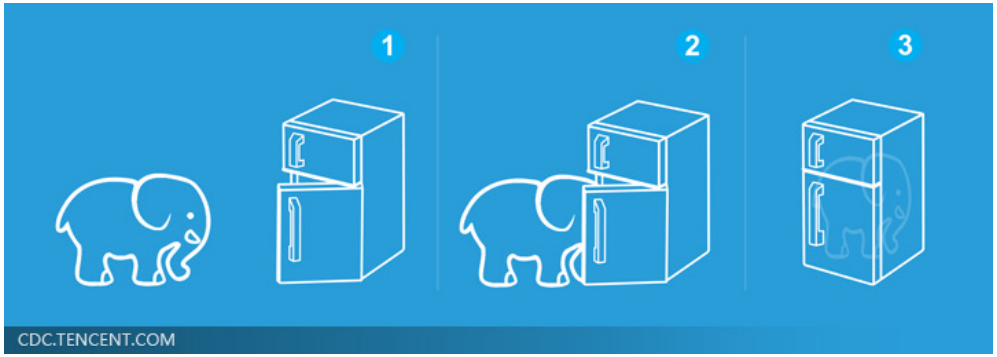
Data Preprocessing-Feature Scaling

In practice, you may also see **PCA** and **Whitening** of the data

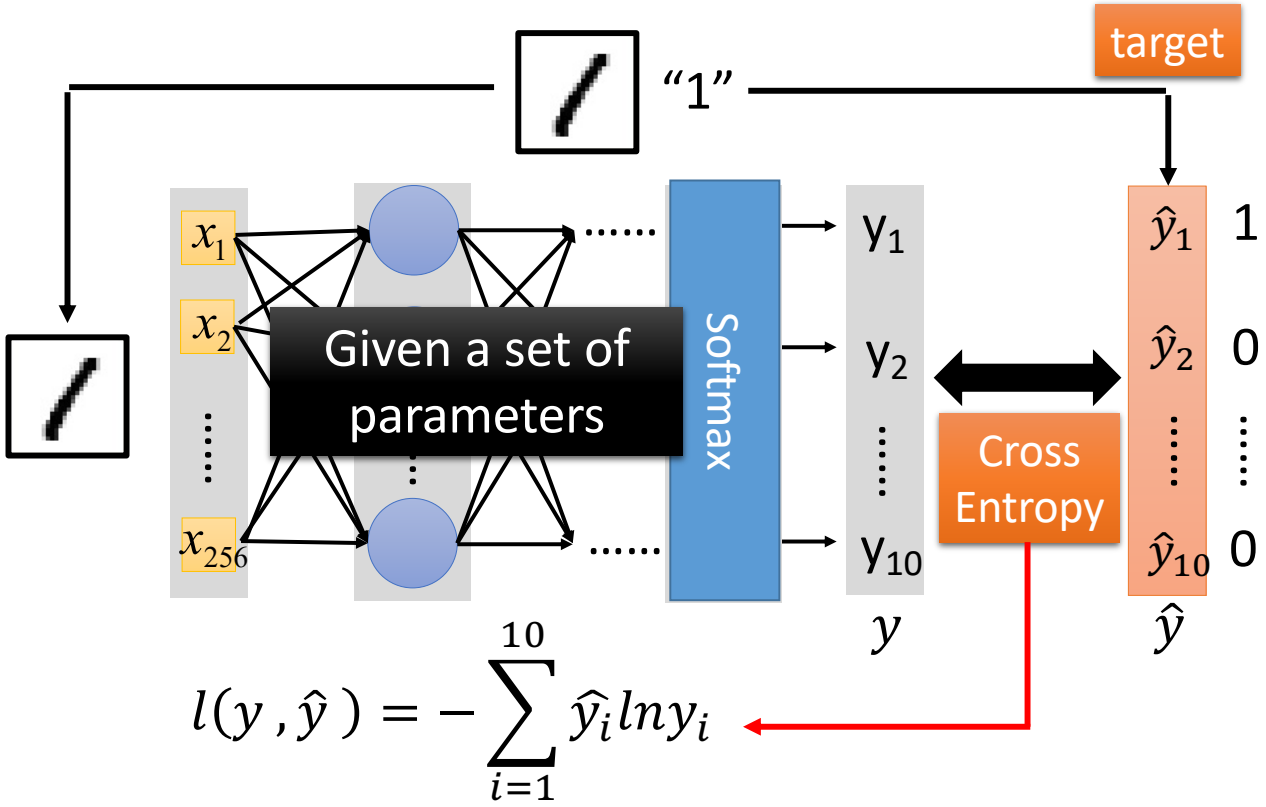


Three steps for deep learning

Deep Learning is so simple ……

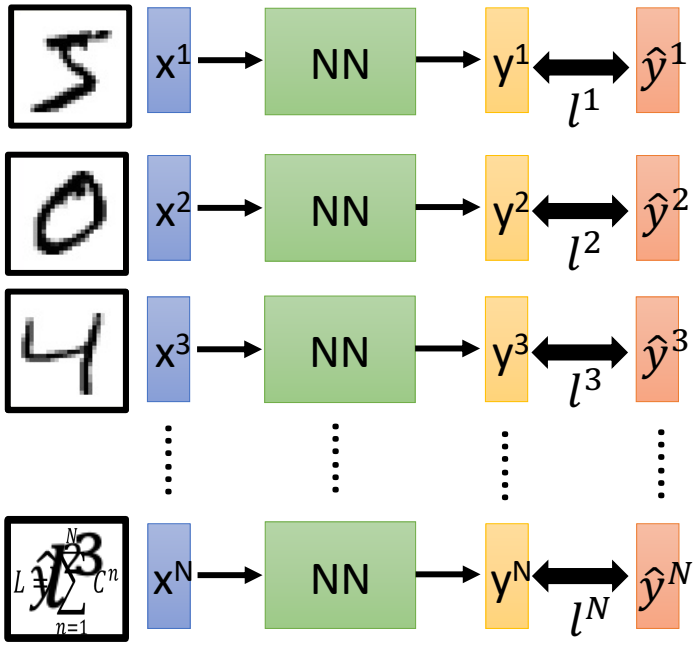


Loss for an Example



Total Loss

For all training data …



Total Loss:

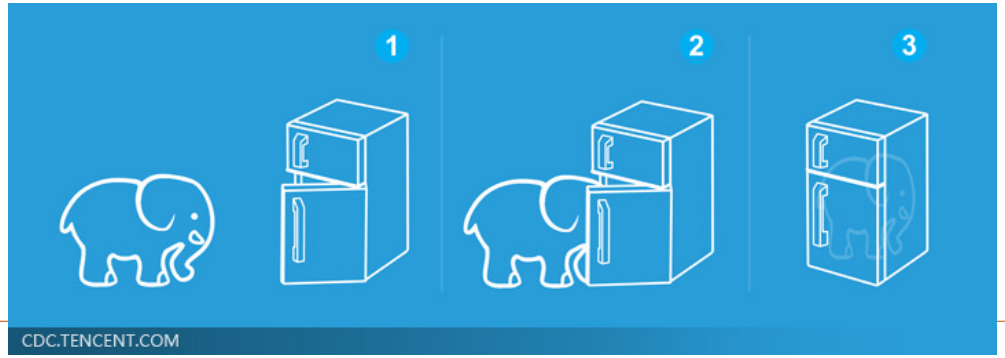
$$L = \sum_{n=1}^{N} l^n$$

Find ***a function in function set*** that minimizes total loss L

Find ***the network parameters*** θ^* that minimize total loss L

Three Steps for Deep Learning

Deep Learning is so simple ……



Gradient Descent

Gradient Descent

- In step 3, we have to solve the following optimization problem:

$\theta^* = \arg\min_{\theta} L(\theta)$ L: loss function θ: parameters

Suppose that θ has two variables $\{\theta_1, \theta_2\}$

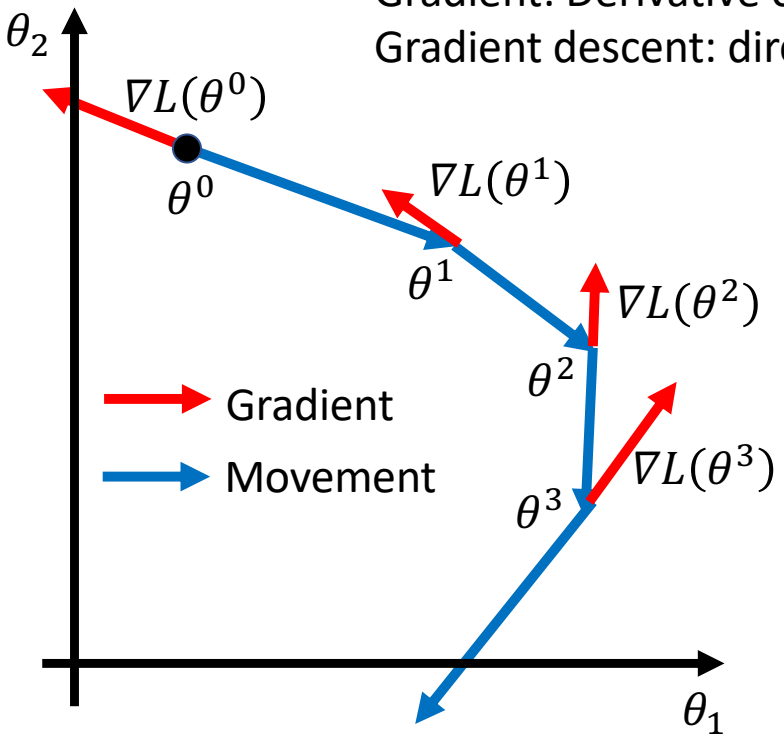
Randomly start at $\theta^0 = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix}$

$$\nabla L(\theta) = \begin{bmatrix} \partial L(\theta_1)/\partial\theta_1 \\ \partial L(\theta_2)/\partial\theta_2 \end{bmatrix}$$

$$\begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} = \begin{bmatrix} \theta_1^0 \\ \theta_2^0 \end{bmatrix} - \eta \begin{bmatrix} \partial L(\theta_1^0)/\partial\theta_1 \\ \partial L(\theta_2^0)/\partial\theta_2 \end{bmatrix} \Rightarrow \theta^1 = \theta^0 - \eta\nabla L(\theta^0)$$

$$\begin{bmatrix} \theta_1^2 \\ \theta_2^2 \end{bmatrix} = \begin{bmatrix} \theta_1^1 \\ \theta_2^1 \end{bmatrix} - \eta \begin{bmatrix} \partial L(\theta_1^1)/\partial\theta_1 \\ \partial L(\theta_2^1)/\partial\theta_2 \end{bmatrix} \Rightarrow \theta^2 = \theta^1 - \eta\nabla L(\theta^1)$$

Gradient Descent



Gradient: Derivative of the Loss function

Gradient descent: direction of negative gradient

Start at position θ^0

Compute gradient at θ^0

Move to $\theta^1 = \theta^0 - \eta\nabla L(\theta^0)$

Compute gradient at θ^1

Move to $\theta^2 = \theta^1 - \eta\nabla L(\theta^1)$

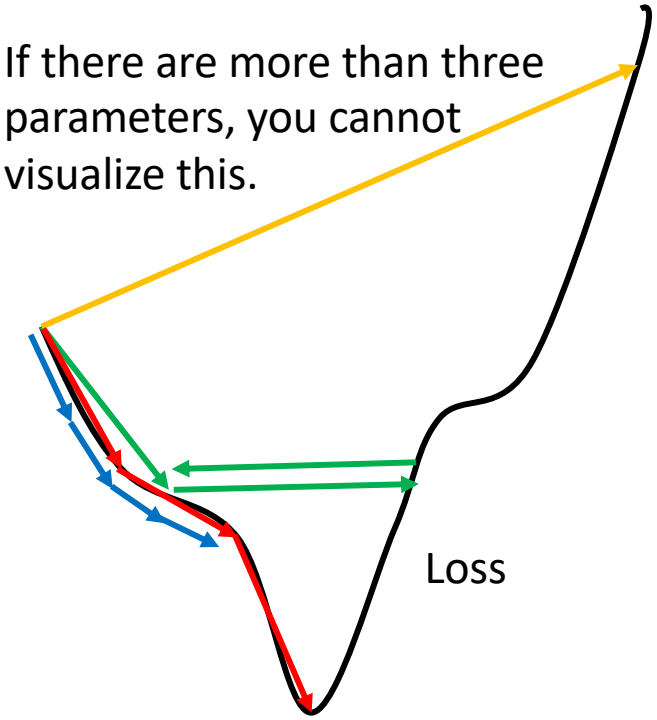
⋮

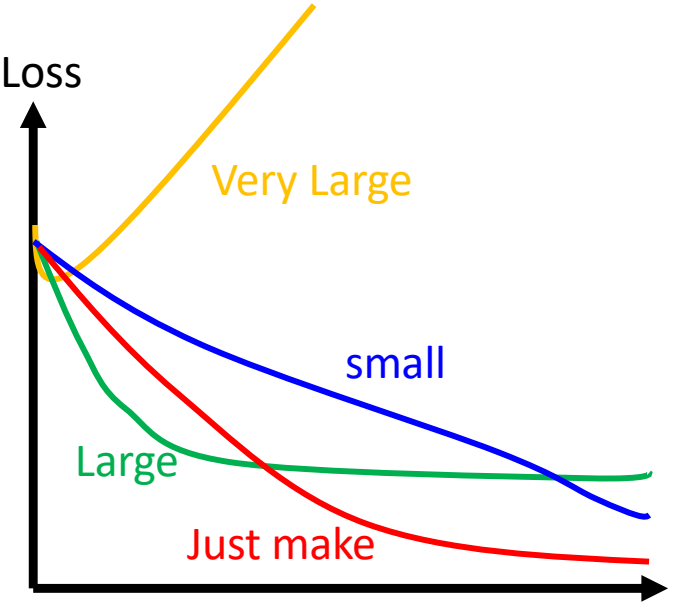
Tip 1: Tuning your learning rates

$$\theta^i = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$$

Set the **learning rate η** carefully

If there are more than three parameters, you cannot visualize this.





But you can always visualize this.

Adaptive Learning Rates

- Popular & Simple Idea: Reduce the learning rate by some factor every few epochs.
  - At the beginning, we are far from the destination, so we use larger learning rate
  - After several epochs, we are close to the destination, so we reduce the learning rate
  - E.g. 1/t decay: $\eta^t = \eta/\sqrt{t+1}$
- Learning rate cannot be one-size-fits-all
  - Giving different parameters different learning rates

Adaptive Learning Rates (Adagrad)

$$\eta^t = \frac{\eta}{\sqrt{t+1}} \qquad g^t = \frac{\partial L(\theta^t)}{\partial w}$$

- Divide the learning rate of each parameter by the ***root mean square of its previous derivatives***

Vanilla Gradient descent (a.k.a. batch gradient descent)

$$w^{t+1} \leftarrow w^t - \eta^t g^t$$

w is one parameter

Adagrad

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t$$

σ^t: ***root mean square*** of the previous derivatives of parameter w

$$\theta^{t+1} = \theta^t - \eta \nabla L(\theta^t)$$

Parameter dependent

Adagrad

σ^t: ***root mean square*** of the previous derivatives of parameter w

$$w^1 \leftarrow w^0 - \frac{\eta^0}{\sigma^0} g^0 \qquad \sigma^0 = \sqrt{(g^0)^2}$$

$$w^2 \leftarrow w^1 - \frac{\eta^1}{\sigma^1} g^1 \qquad \sigma^1 = \sqrt{\frac{1}{2}\left[(g^0)^2 + (g^1)^2\right]}$$

$$w^3 \leftarrow w^2 - \frac{\eta^2}{\sigma^2} g^2 \qquad \sigma^2 = \sqrt{\frac{1}{3}\left[(g^0)^2 + (g^1)^2 + (g^2)^2\right]}$$

$$\vdots$$

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t \qquad \sigma^t = \sqrt{\frac{1}{t+1}\sum_{i=0}^{t} (g^i)^2}$$

Adagrad

- Divide the learning rate of each parameter by the ***root mean square of its previous derivatives***

$$w^{t+1} \leftarrow w^t - \frac{\eta^t}{\sigma^t} g^t$$

$$\eta^t = \frac{\eta}{\sqrt{t+1}}$$ 1/t decay

$$\sigma^t = \sqrt{\frac{1}{t+1}\sum_{i=0}^{t}(g^i)^2}$$

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\sum_{i=0}^{t}(g^i)^2}} g^t$$

Stochastic Gradient Descent

Stochastic Gradient Descent

$$L = \sum_n \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2$$

Loss is the summation over all training examples

◆***Gradient Descent*** $\theta^i = \theta^{i-1} - \eta \nabla L\left(\theta^{i-1}\right)$

◆***Stochastic Gradient Descent*** Faster!

Pick an example x^n

Drawn uniform at random from {1,...,n}

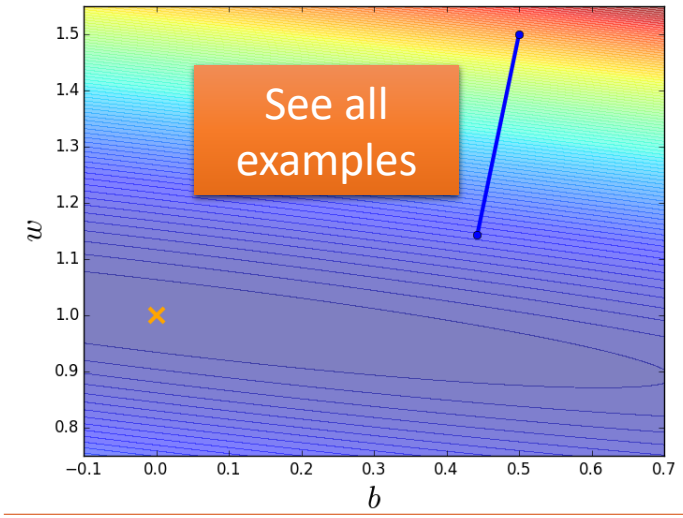
$$L^n = \left(\hat{y}^n - \left(b + \sum w_i x_i^n \right) \right)^2 \qquad \theta^i = \theta^{i-1} - \eta \nabla L^n\left(\theta^{i-1}\right)$$

Loss for only one example, NO summing

SGD: An Illustration

Gradient Descent

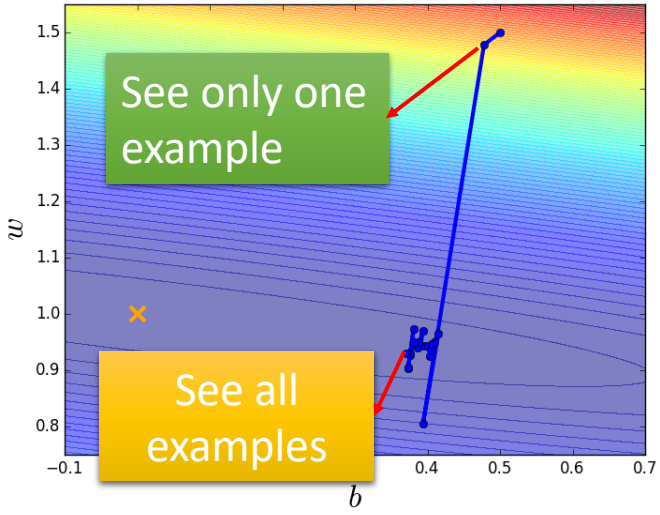
Update after seeing all examples



Stochastic Gradient Descent

Update for each example

If there are 20 examples, 20 times faster.

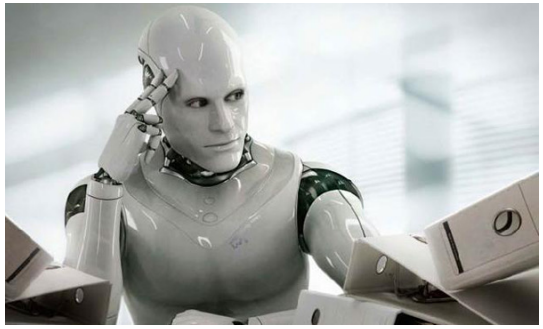


Gradient Descent

This is the “learning” of machines in deep learning ……

➡ Even alpha go using this approach.

People image ……



Actually …..

Gradient Descent

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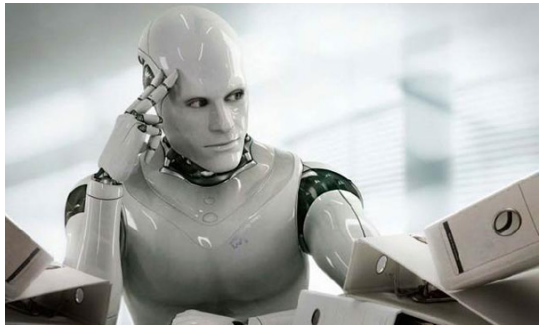
People image ……



Actually …..

I hope you are not too disappointed :p

Backpropagation

- Backpropagation: an efficient way to compute $\partial L/\partial w$ in neural network

theano

Caffe

Microsoft CNTK

PyTorch

Deep Learning library produced by Amazon
DSSTNE

mxnet

Any Questions?

bidong@syr.edu