Neural Networks (NN)

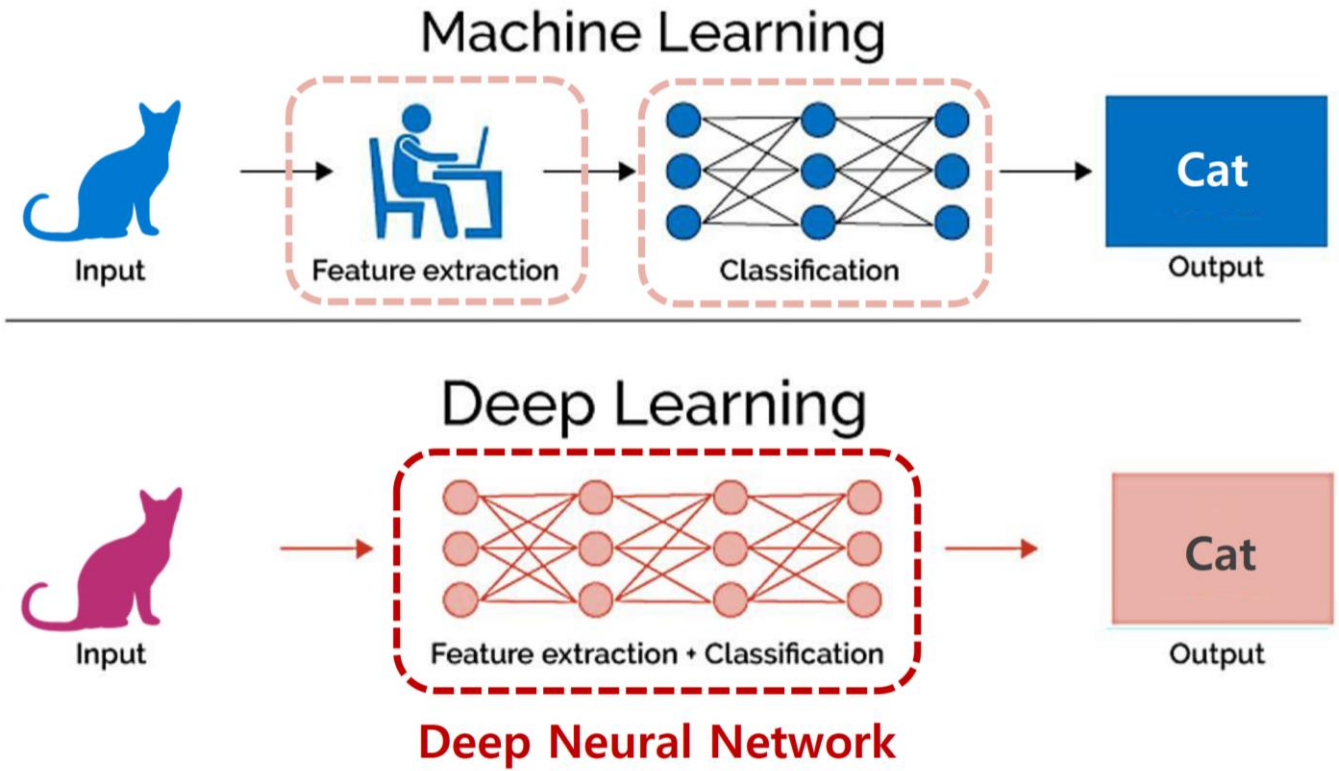
Jongbin Ryu

Contents

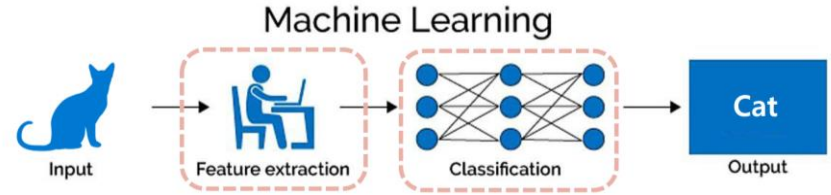
- Traditional ML Approaches
- Introduction to Neural Networks
- Activation Functions (Nonlinearity)
  - Sigmoid
  - ReLU
  - Leaky ReLU, ELU, SELU, and Maxout

Slides are adopted from cs231n
http://cs231n.stanford.edu/

Machine Learning vs Deep Learning



Pixel Features



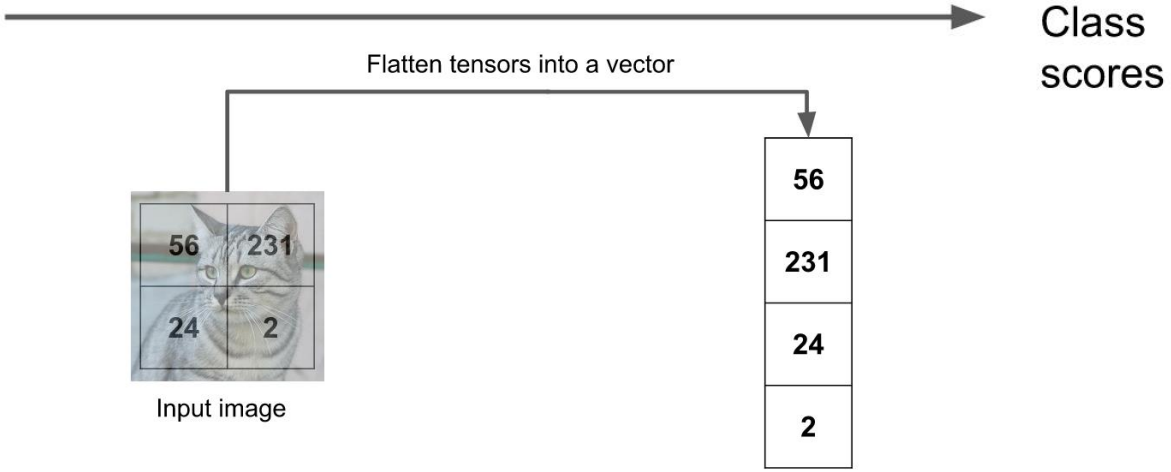
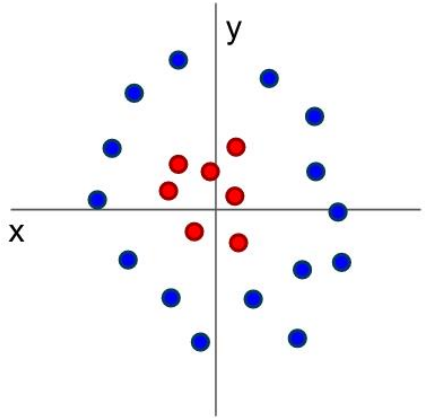
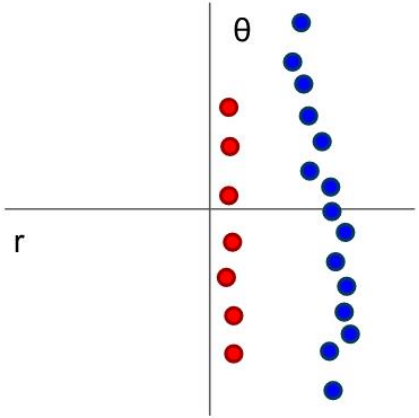


Image Features: Motivation



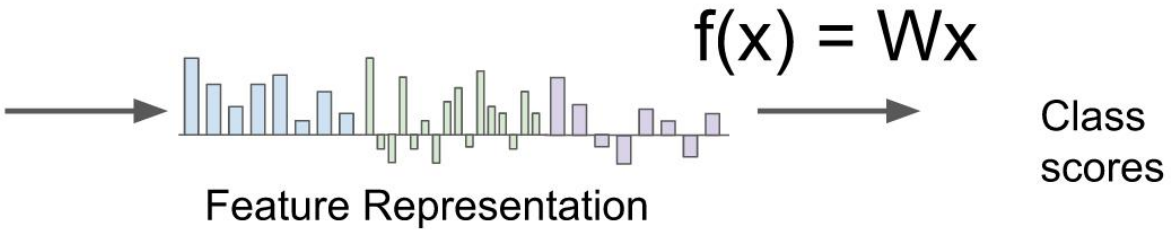
Cannot separate red and blue points with linear classifier

$$f(x, y) = (r(x, y), \theta(x, y))$$

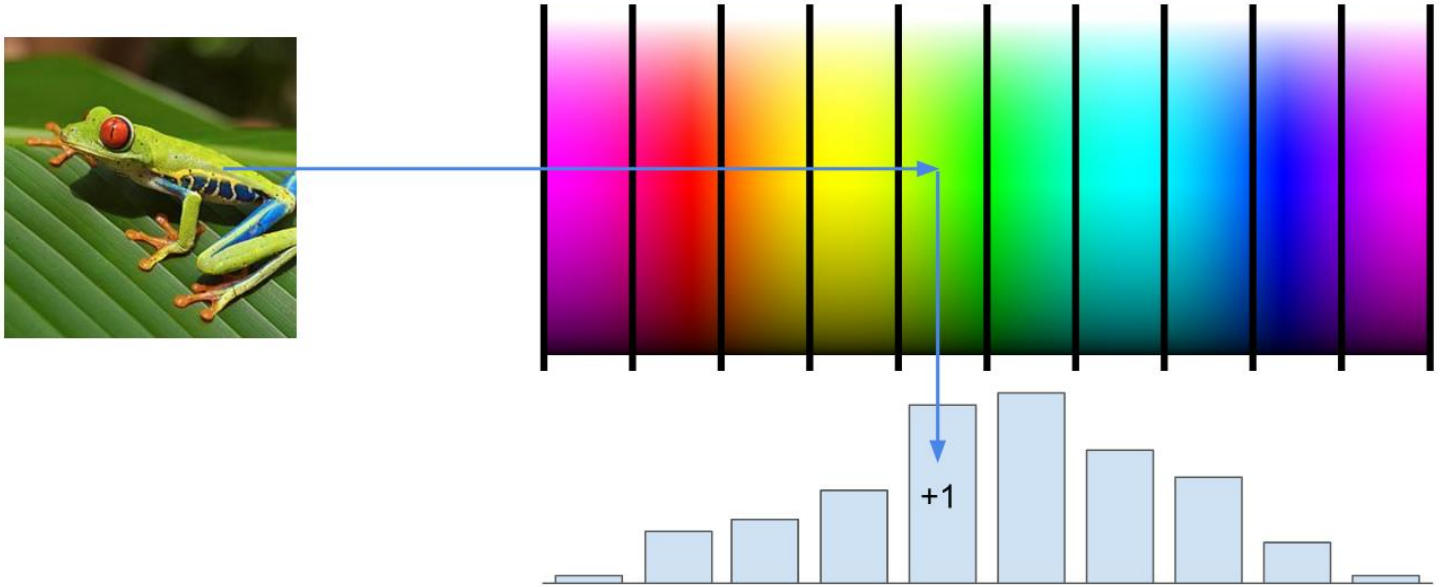


After applying feature transform, points can be separated by linear classifier

Image Features

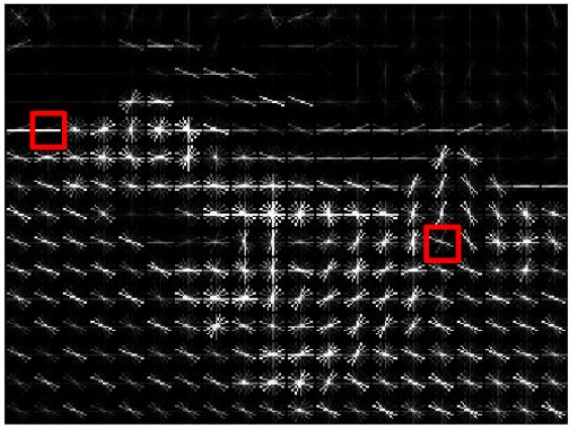


Example: Color Histogram



Example: Histogram of Oriented Gradients (HoG)

Divide image into 8x8 pixel regions
Within each region quantize edge direction into 9 bins



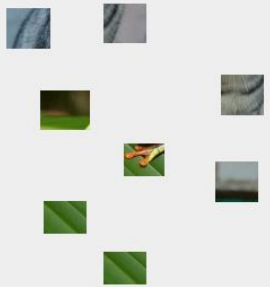
Example: 320x240 image gets divided into 40x30 bins; in each bin there are 9 numbers so feature vector has 30*40*9 = 10,800 numbers

Lowe, “Object recognition from local scale-invariant features”, ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Example: Bag of Words

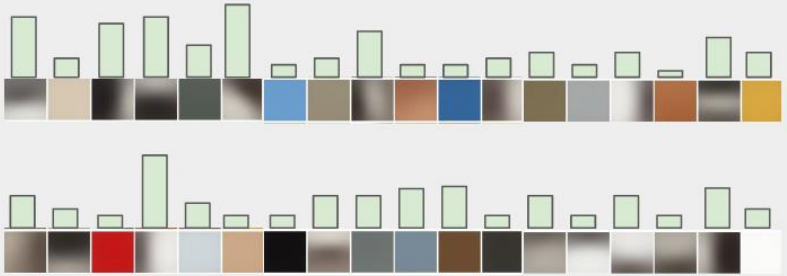
Step 1: Build codebook

Extract random patches



Cluster patches to form “codebook” of “visual words”

Step 2: Encode images



Fei-Fei and Perona, “A bayesian hierarchical model for learning natural scene categories”, CVPR 2005

Image Features

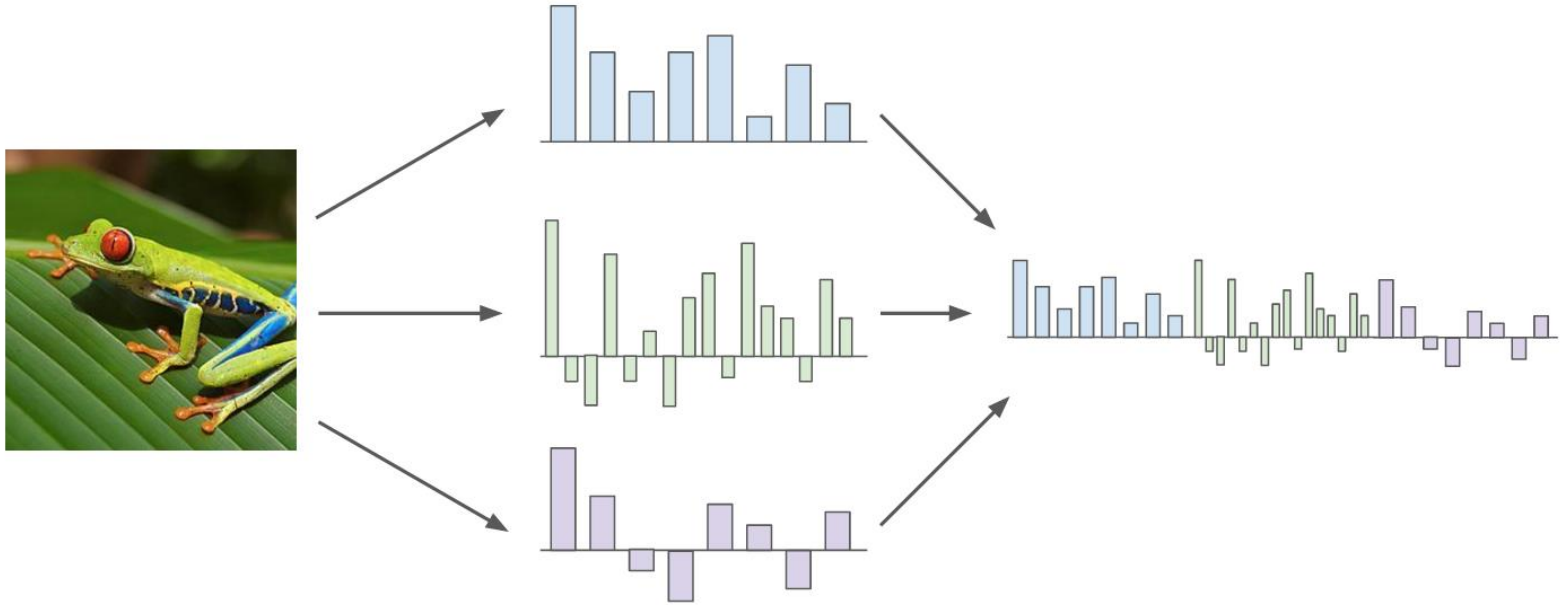
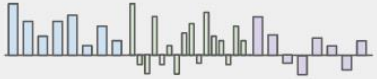


Image features vs ConvNets

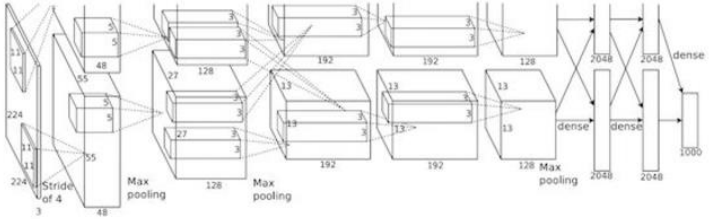
Feature Extraction



f

10 numbers giving scores for classes

training



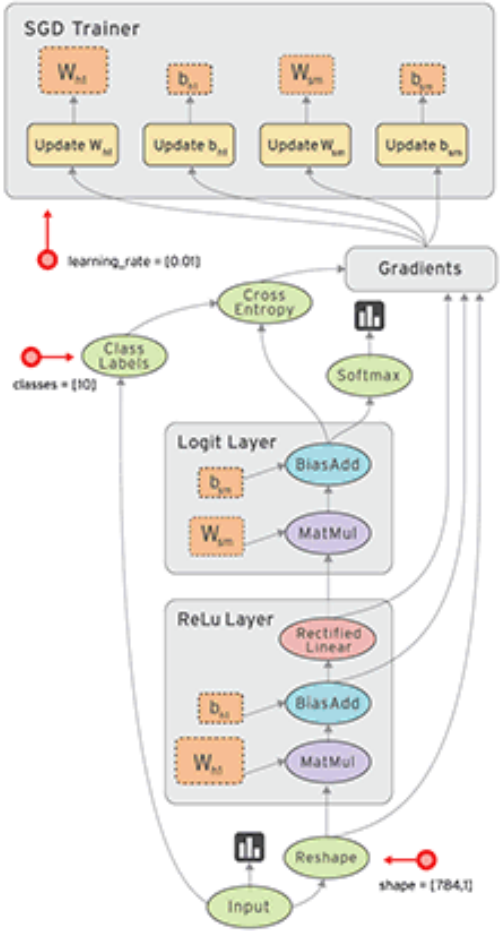
Krizhevsky, Sutskever, and Hinton, "Imagenet classification with deep convolutional neural networks", NIPS 2012. Figure copyright Krizhevsky, Sutskever, and Hinton, 2012. Reproduced with permission.

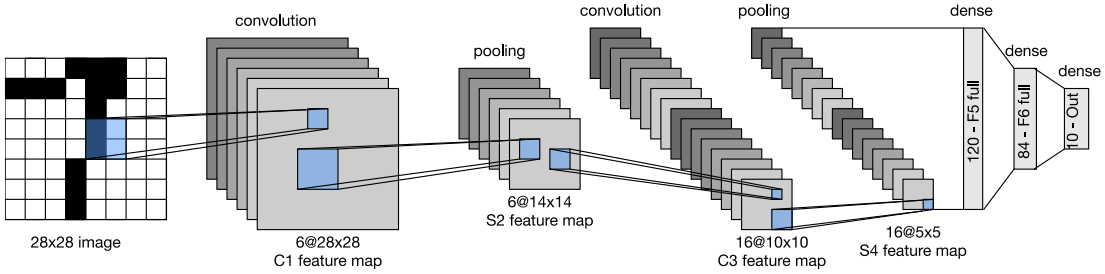
10 numbers giving scores for classes

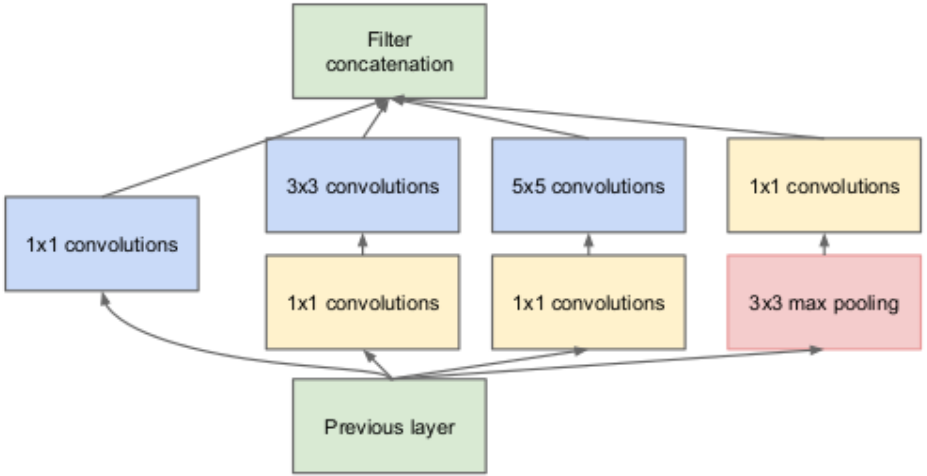
training

Contents

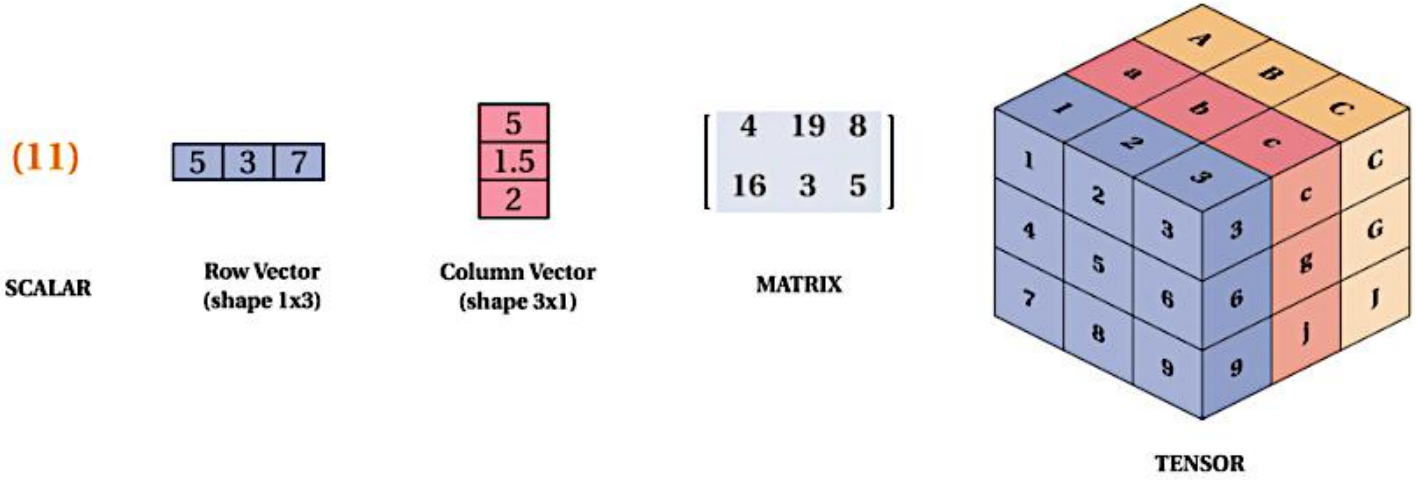
- Traditional ML Approaches
- Introduction to Neural Networks
- Activation Functions (Nonlinearity)
  - Sigmoid
  - ReLU
  - Leaky ReLU, ELU, SELU, and Maxout


SGD Trainer
Update W_h1
Update b_h1
Update W_sm
Update b_sm
learning_rate = [0.01]
Gradients
Cross Entropy
Class Labels
classes = [10]
Softmax
Logit Layer
BiasAdd
MatMul
ReLu Layer
Rectified Linear
BiasAdd
MatMul
Reshape
shape = [784,1]
Input

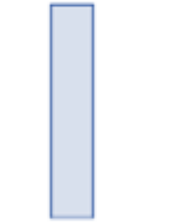

convolution
pooling
convolution
pooling
dense
dense
dense
120 - F5 full
84 - F6 full
10 - Out
28x28 image
6@28x28
C1 feature map
6@14x14
S2 feature map
16@10x10
C3 feature map
16@5x5
S4 feature map


Filter concatenation
1x1 convolutions
3x3 convolutions
5x5 convolutions
1x1 convolutions
1x1 convolutions
1x1 convolutions
1x1 convolutions
3x3 max pooling
Previous layer

From Scalar to Tensor

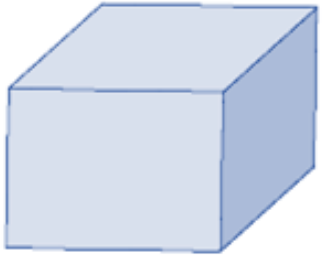


From Scalar to Tensor



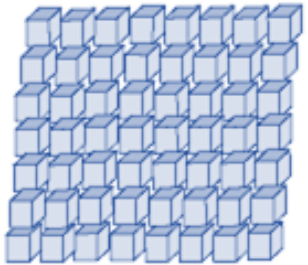
1 d - Tensor

2 d - Tensor

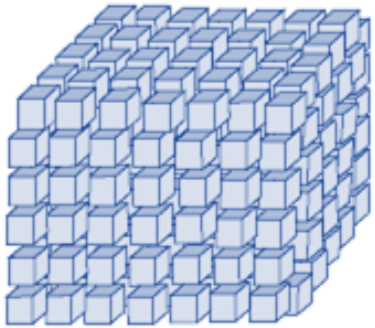


3 d -Tensor

4 d -Tensor



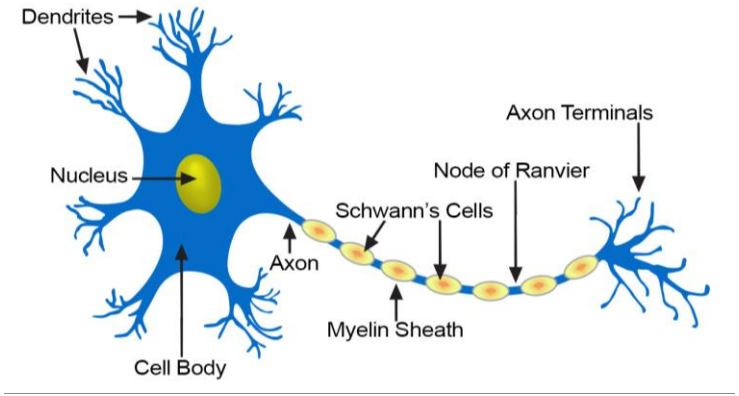
5 d -Tensor

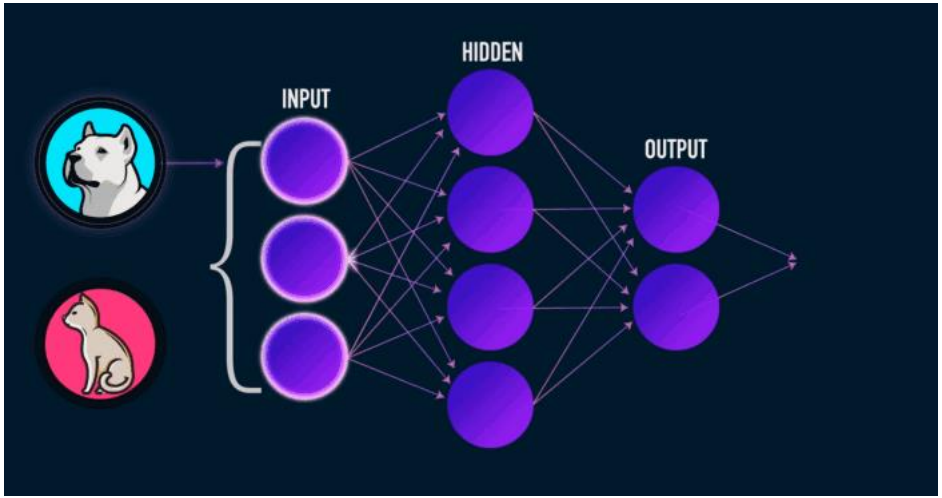


6 d -Tensor

Neural Networks (NN)

Artificial neural networks (**ANNs**), usually simply called **neural networks** (**NNs**) are computing systems inspired by the [biological neural networks]





Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

"Neural Network" is a very broad term; these are more accurately called "fully-connected networks" or sometimes "multi-layer perceptrons" (MLP)

(In practice we will usually add a learnable bias at each layer as well)

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

or 3-layer Neural Network

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

(In practice we will usually add a learnable bias at each layer as well)

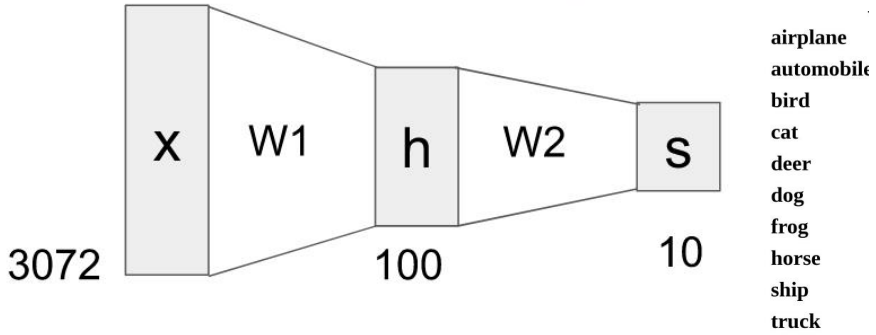
Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

Image

Array of **32x32x3** numbers
(3072 numbers total)



$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

The function $\max(0, z)$ is called the **activation function.**

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

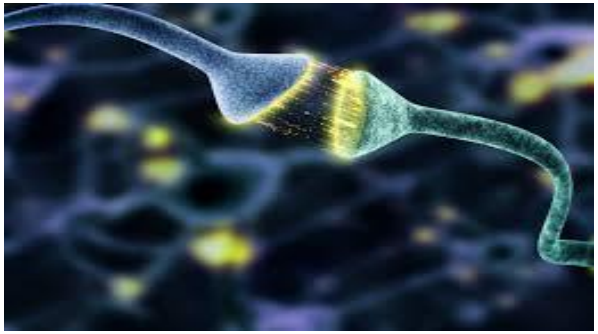
(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

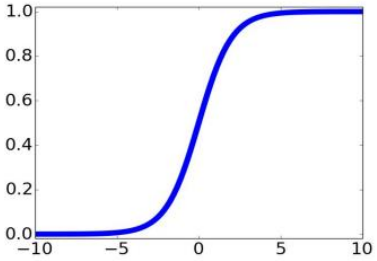
The function $\max(0, z)$ is called the **activation function.**

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x \qquad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

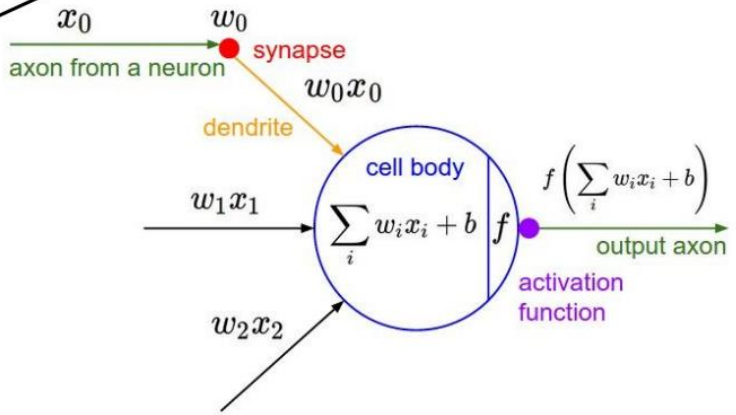
A: We end up with a linear classifier again!

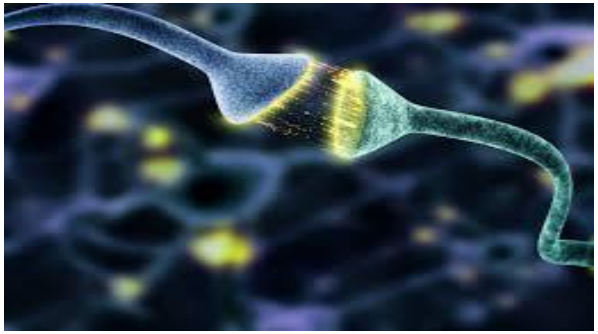




sigmoid activation function

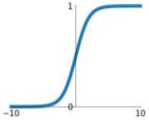
$$\frac{1}{1+e^{-x}}$$





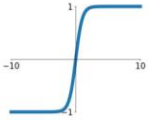
Sigmoid

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



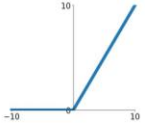
tanh

$\tanh(x)$



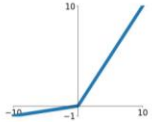
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

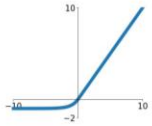


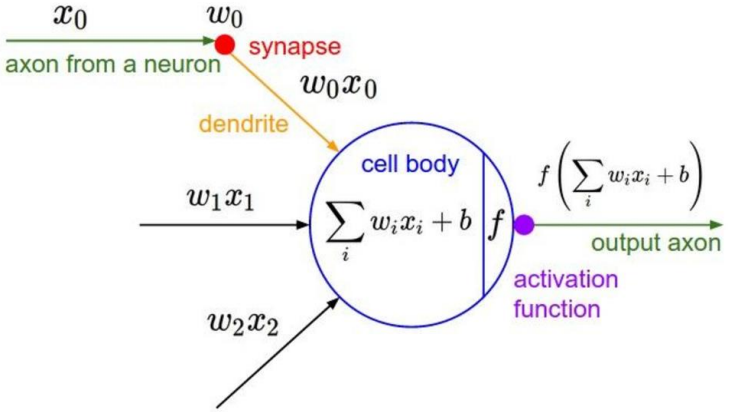
Maxout

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

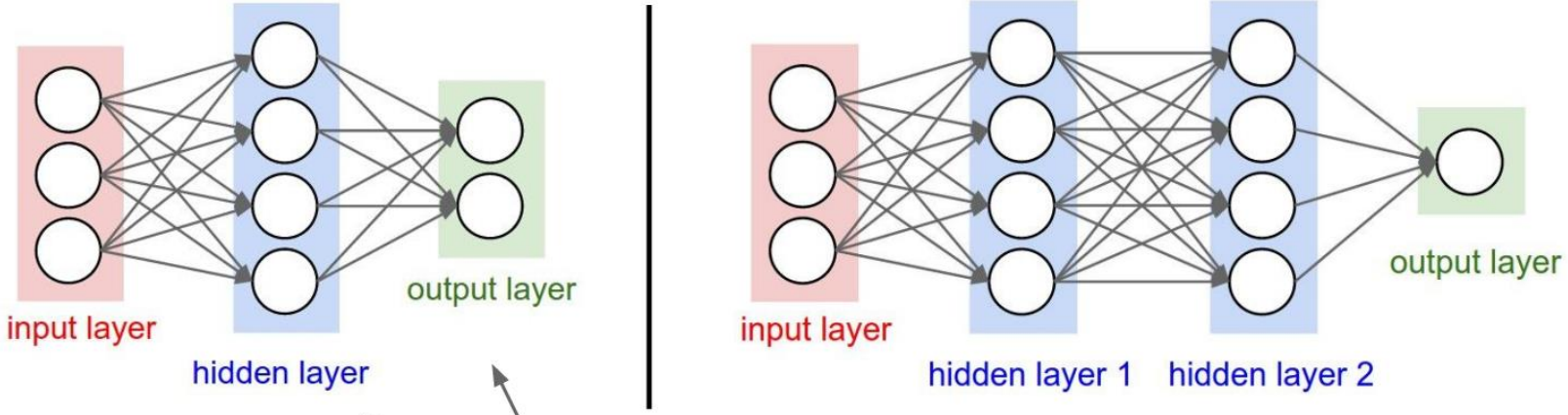
ELU

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





Neural networks: Architectures

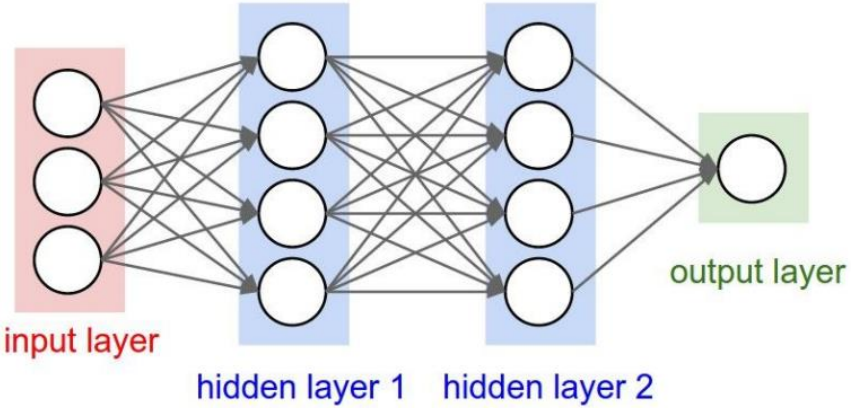


"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

"Fully-connected" layers

Example feed-forward computation of a neural network




```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Full implementation of training a 2-layer Neural Network needs ~20 lines:

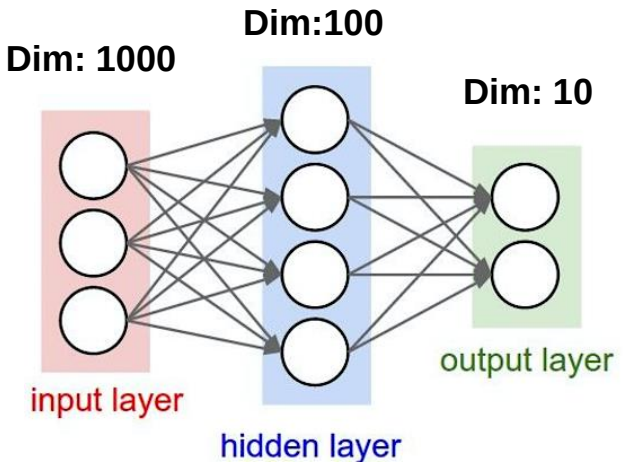
```python
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```



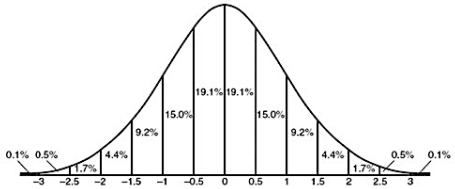
Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

Define the network

numpy.random.randn

numpy.random.**randn**(*d0*, *d1*, ..., *dn*)



Return a sample (or samples) from the “standard normal” distribution.

If positive, int_like or int-convertible arguments are provided, randn generates an array of shape `(d0, d1, ..., dn)`, filled with random floats sampled from a univariate “normal” (Gaussian) distribution of mean 0 and variance 1 (if any of the d_i are floats, they are first converted to integers by truncation). A single float randomly sampled from the distribution is returned if no argument is provided.

Full implementation of training a 2-layer Neural Network needs ~20 lines:

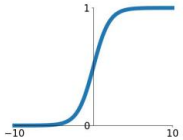
```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

Define the network

Forward pass

Sigmoid

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



$$\text{SSE} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

test set; predicted vaue; actual value

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

Define the network

Forward pass

Calculate the analytical gradients

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

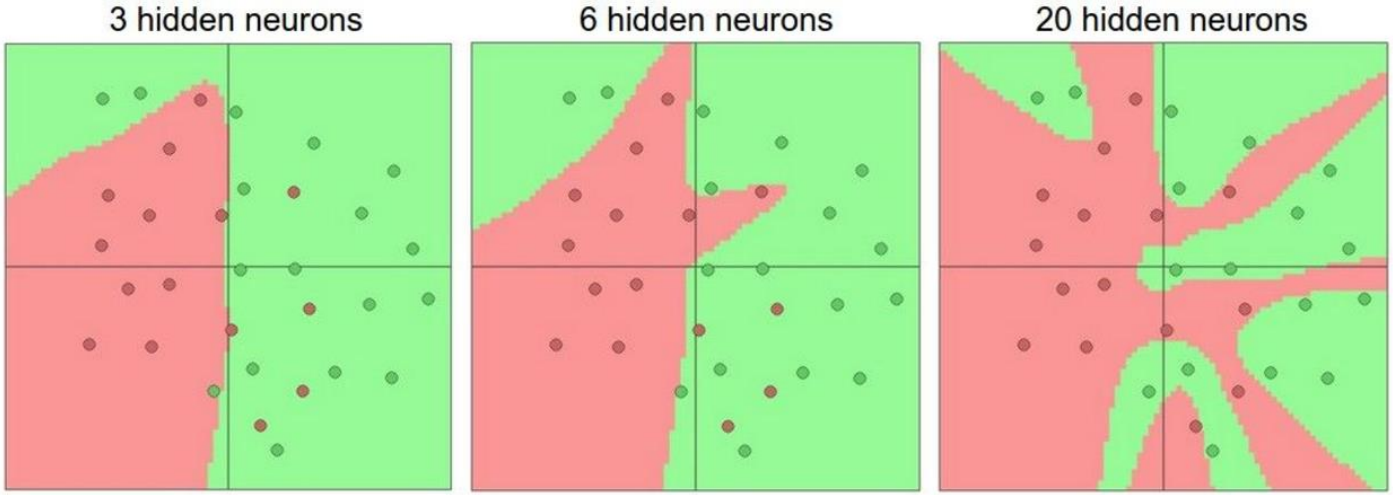
Define the network

Forward pass

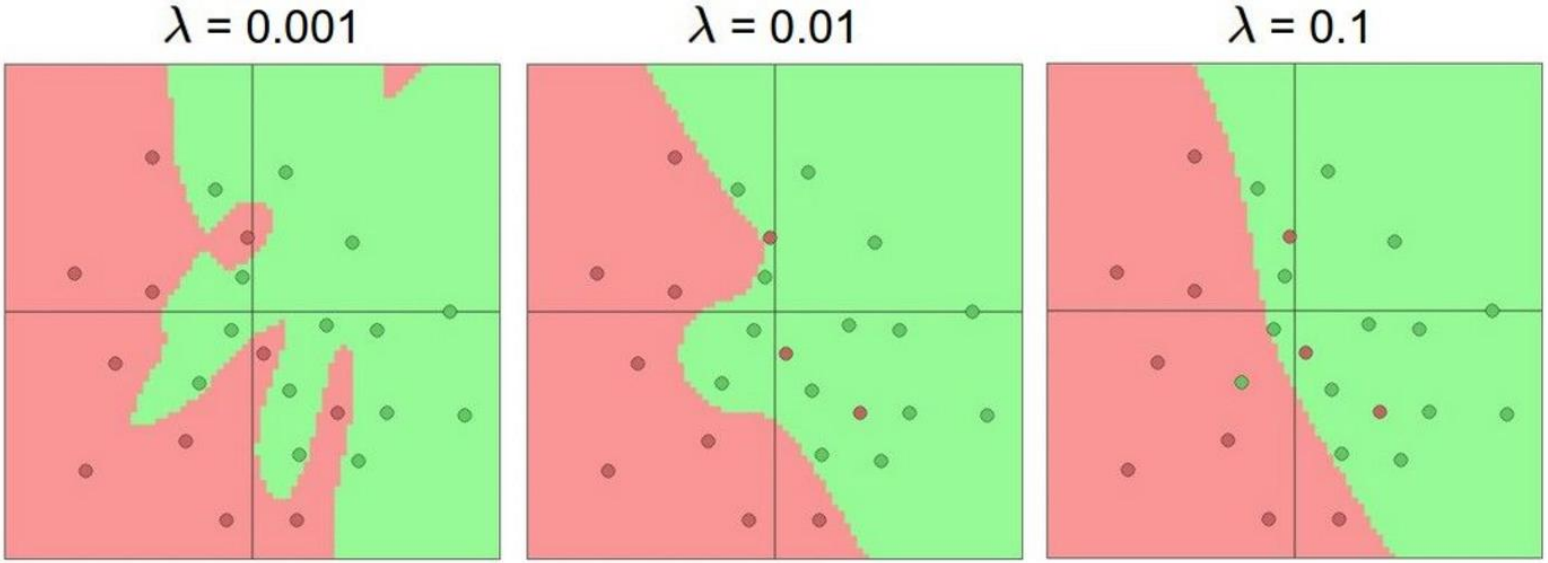
Calculate the analytical gradients

Gradient descent

Setting the number of layers and their sizes



Do not use size of neural network as a regularizer. Use stronger regularization instead:



(Web demo with ConvNetJS: http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

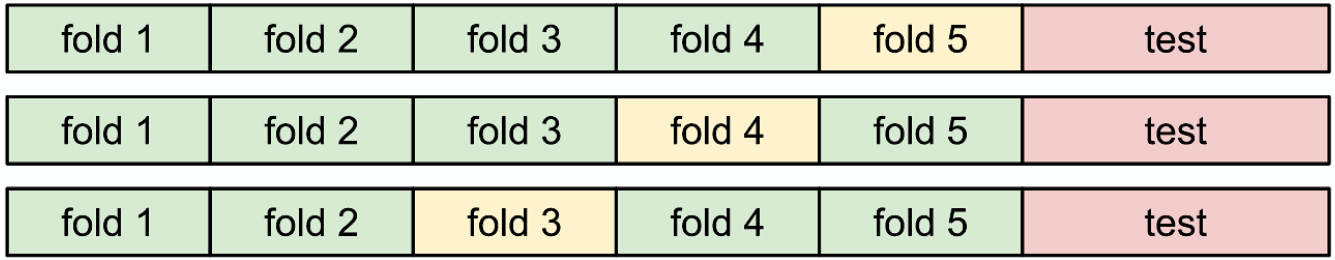
$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Setting Hyperparameters

Idea #3: Split data into **train**, **val**, and **test**; choose hyperparameters on val and evaluate on test

Better!

Idea #4: **Cross-Validation**: Split data into **folds**, try each fold as validation and average the results

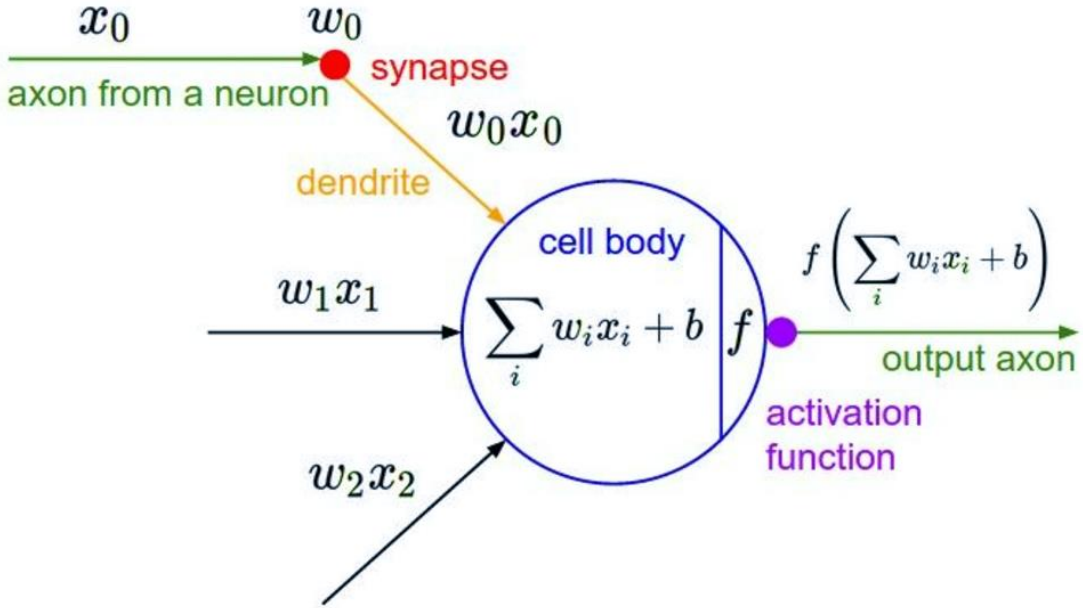


Useful for small datasets, but not used too frequently in deep learning

Contents

- Traditional ML Approaches
- Introduction to Neural Networks
- Activation Functions (Nonlinearity)
  - Sigmoid
  - ReLU
  - Leaky ReLU, ELU, SELU, and Maxout

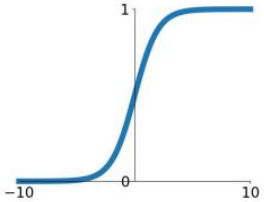
Activation Functions



Activation Functions

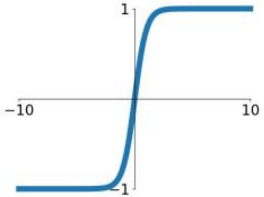
Sigmoid

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



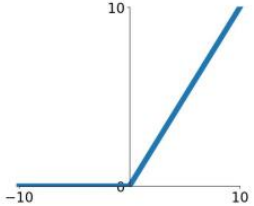
tanh

$$\tanh(x)$$



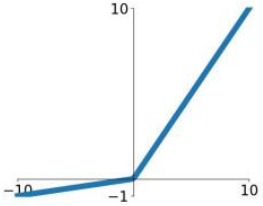
ReLU

$$\max(0, x)$$



Leaky ReLU

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

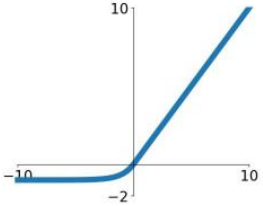


Maxout

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

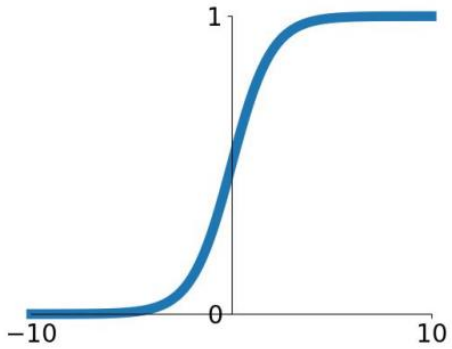
ELU

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



Activation Functions

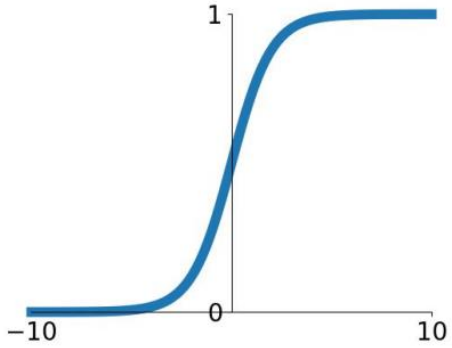
$$\sigma(x) = 1/(1 + e^{-x})$$



Sigmoid

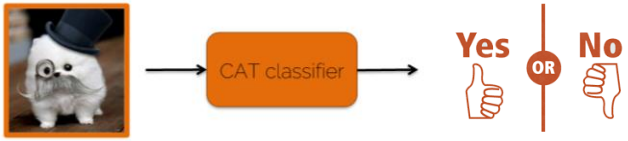
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

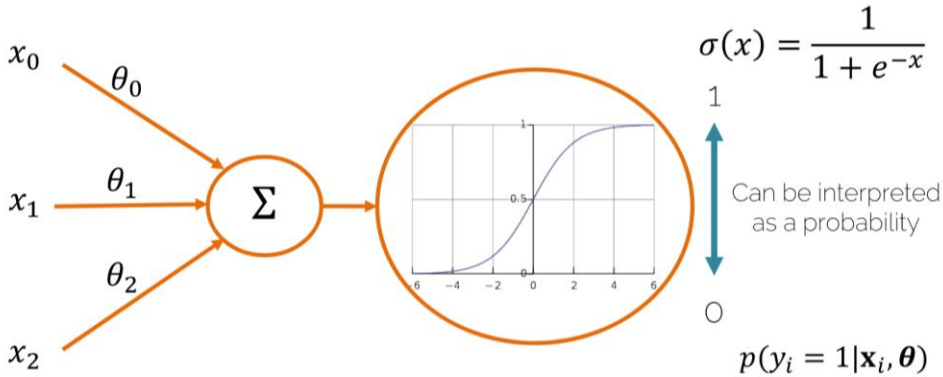
Activation Functions



Sigmoid

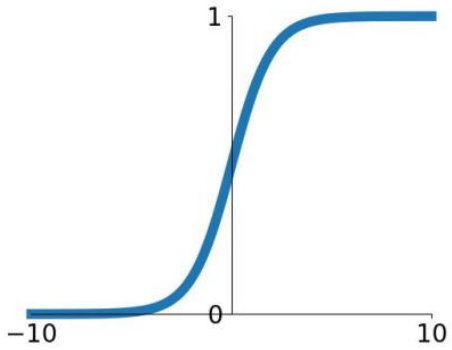
Logistic Regression





Activation Functions

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

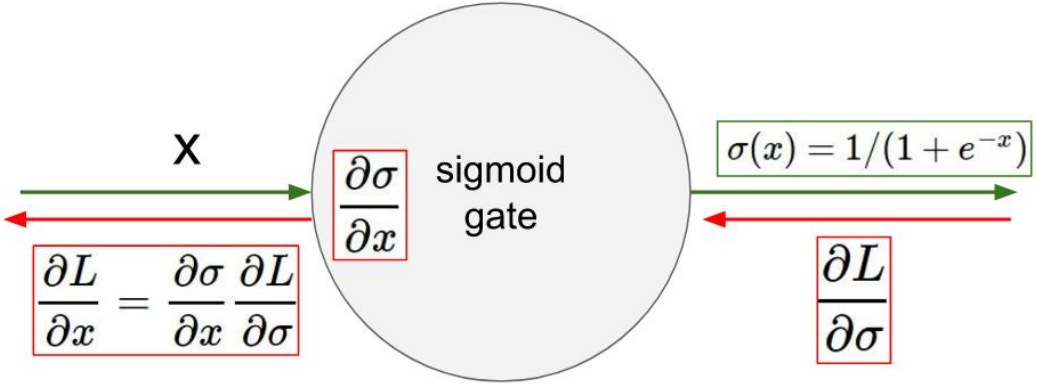


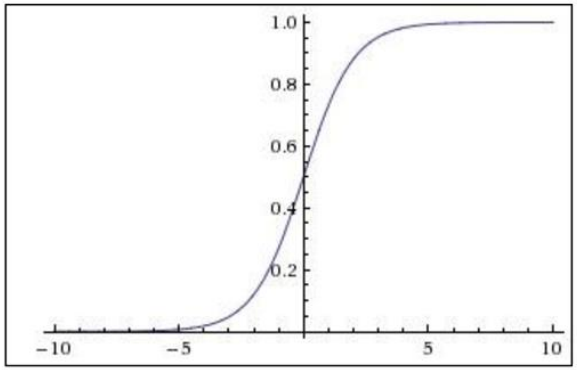
Sigmoid

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

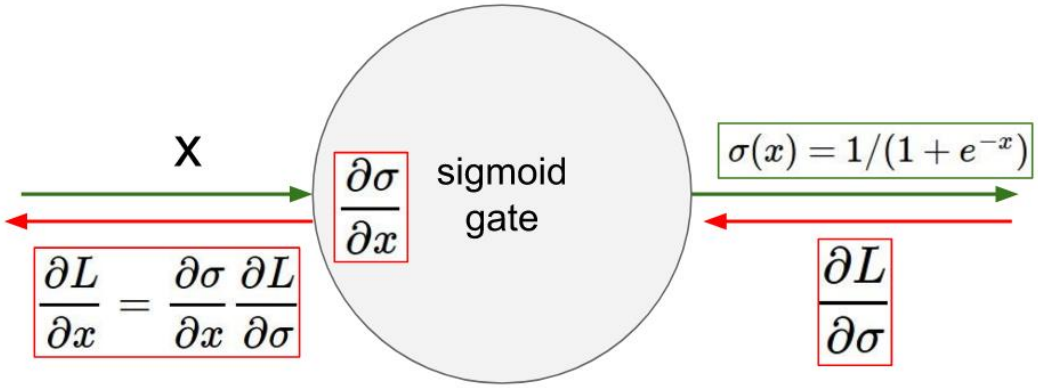
3 problems:

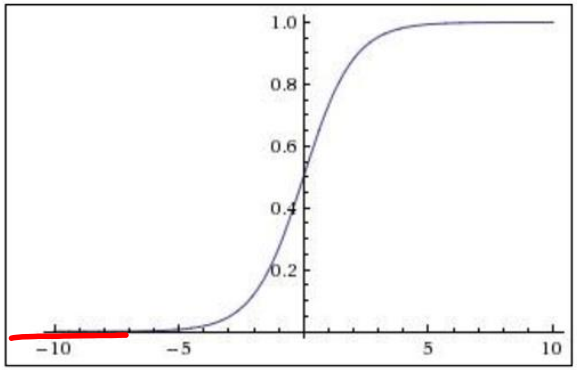
1. Saturated neurons “kill” the gradients





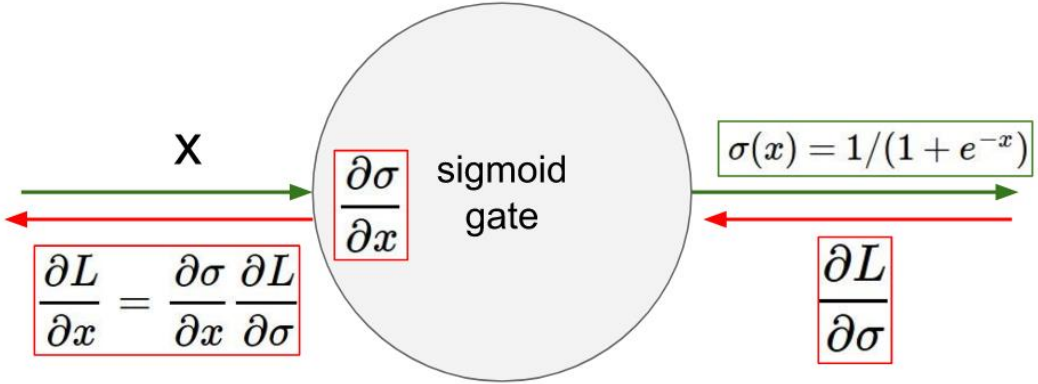
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

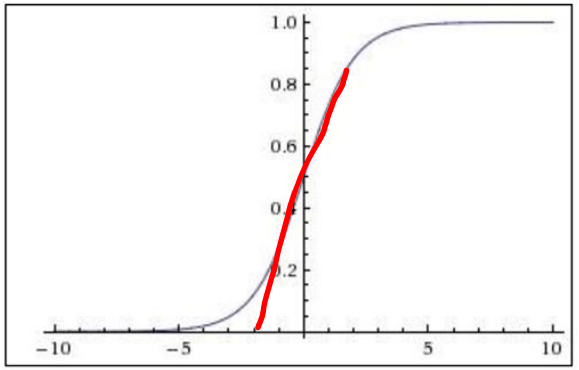




What happens when x = -10?

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

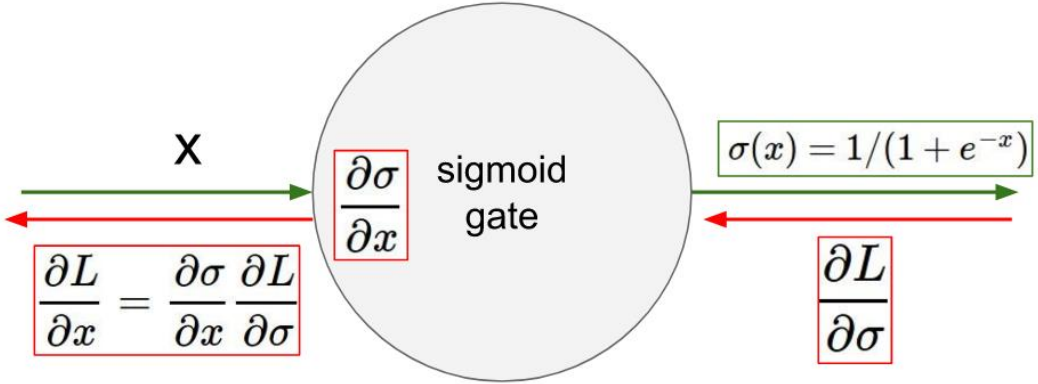


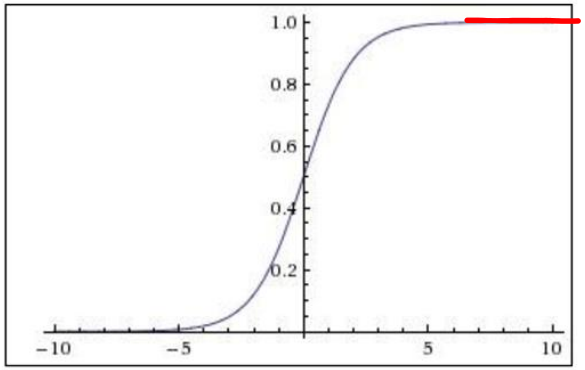


What happens when x = -10?

What happens when x = 0?

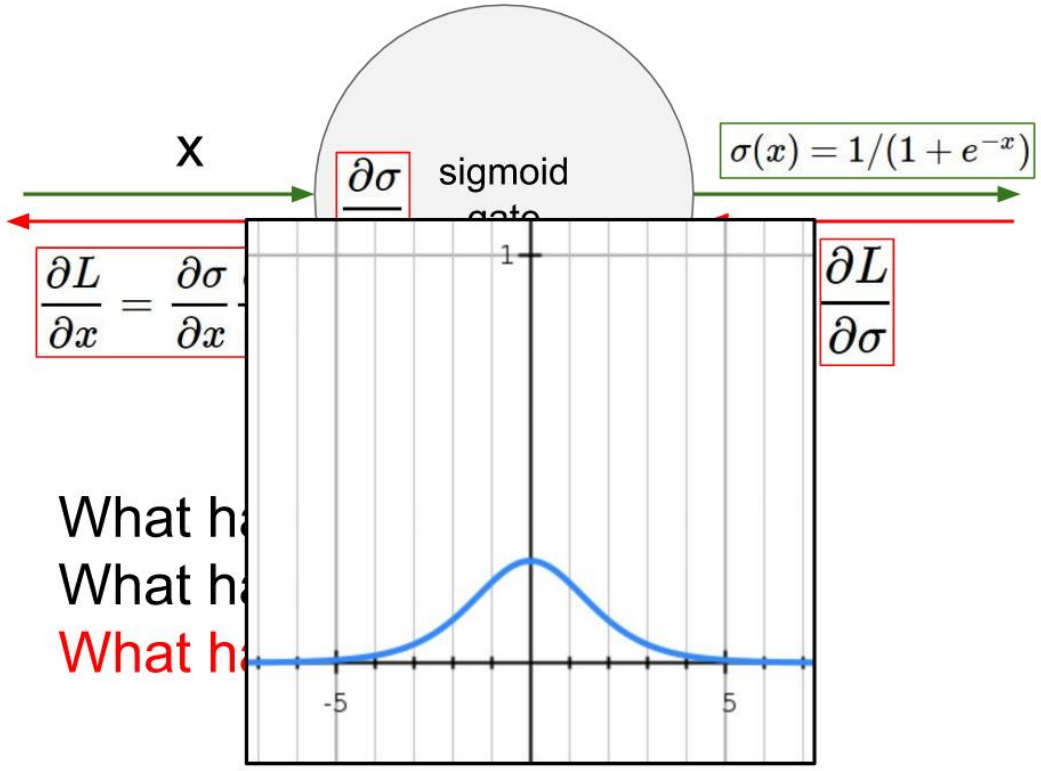
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

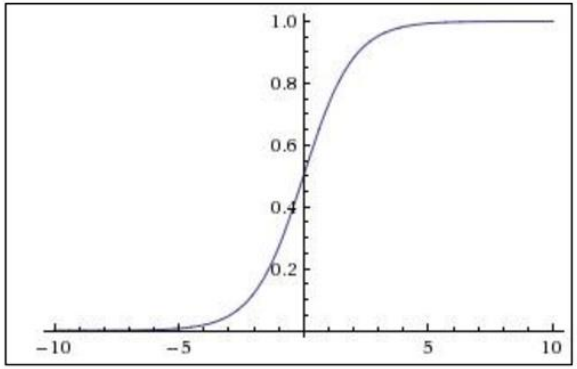




What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

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



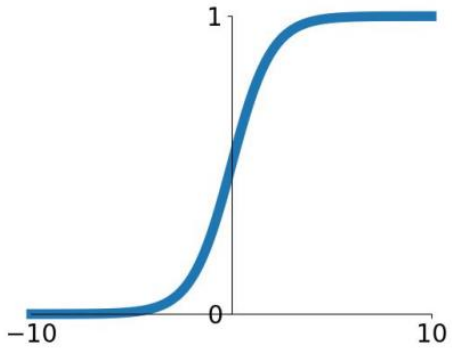


What ha
What ha
What ha

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

Activation Functions

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



Sigmoid

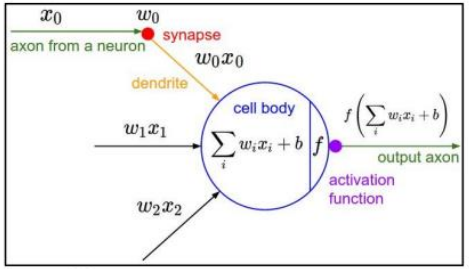
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

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

Consider what happens when the input to a neuron is always positive...

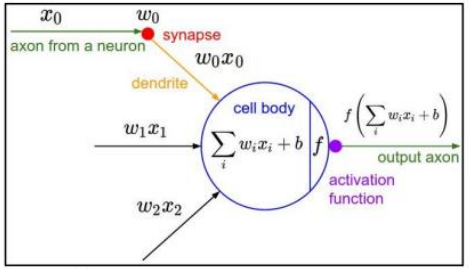
$$f\left(\sum_i w_i x_i + b\right)$$



What can we say about the gradients on **w**?

Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b\right)$$



What can we say about the gradients on **w**?

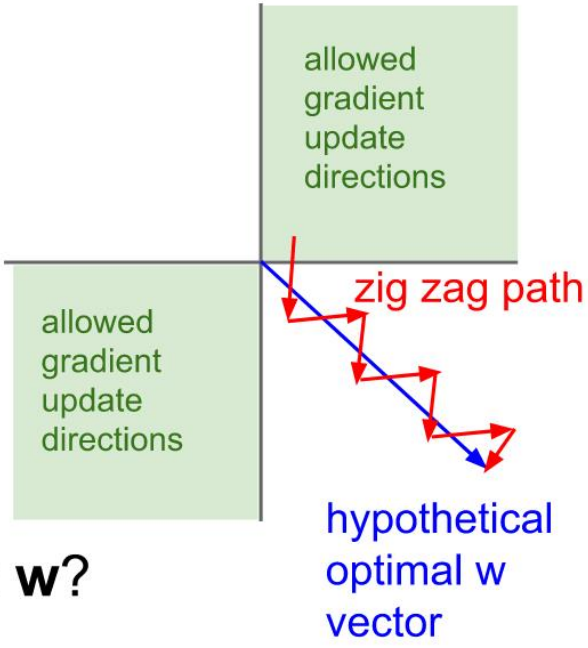
We know that local gradient of sigmoid is always positive
We are assuming x is always positive

So!! Sign of gradient **for all w_i** is the same as the sign of upstream scalar gradient!

$$\frac{\partial L}{\partial w} = \sigma\left(\sum_i w_i x_i + b\right)\left(1 - \sigma\left(\sum_i w_i x_i + b\right)\right) x \times upstream\_gradient$$

Consider what happens when the input to a neuron is always positive...

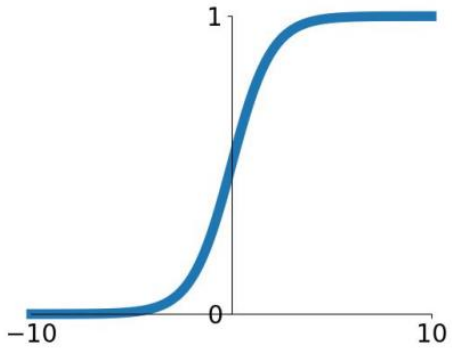
$$f\left(\sum_i w_i x_i + b\right)$$



What can we say about the gradients on **w**?
Always all positive or all negative :(

Activation Functions

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



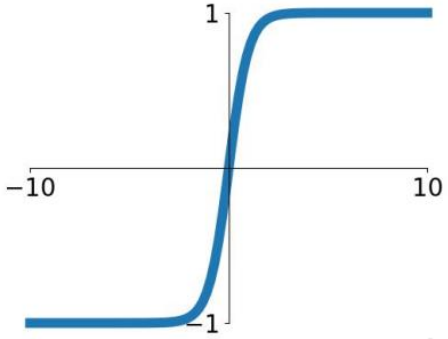
Sigmoid

- 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 :(

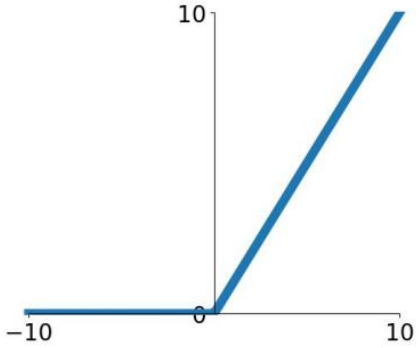
$$tanh(x) = 2\sigma(2x) - 1$$

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

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

[LeCun et al., 1991]

Activation Functions



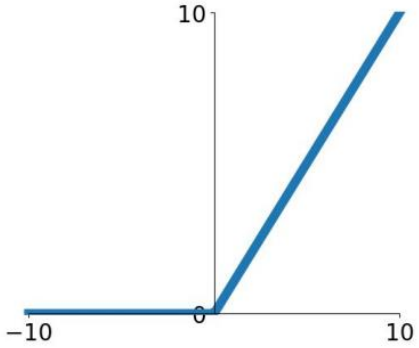
ReLU
(Rectified Linear Unit)

- 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)

[Krizhevsky et al., 2012]

Activation Functions



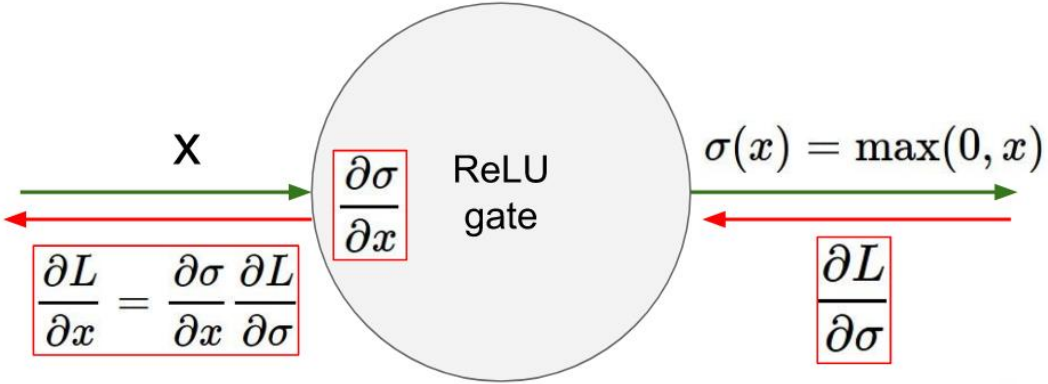
ReLU
(Rectified Linear Unit)

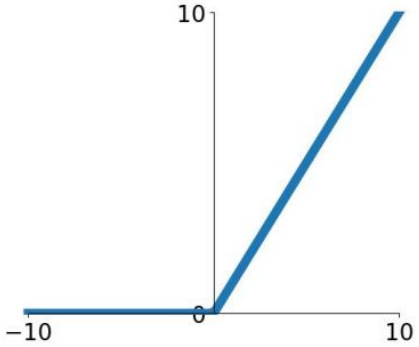
- Computes **f(x) = max(0,x)**

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

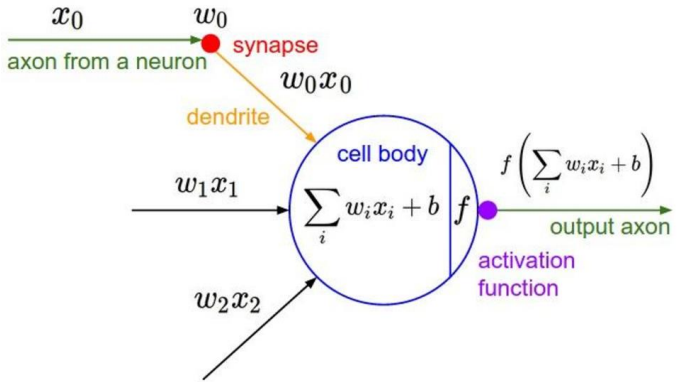
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?



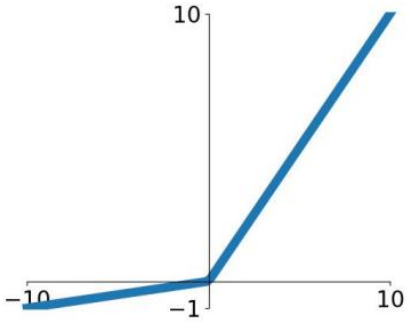


What happens when x = -10?
What happens when x = 0?
What happens when x = 10?



Activation Functions

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



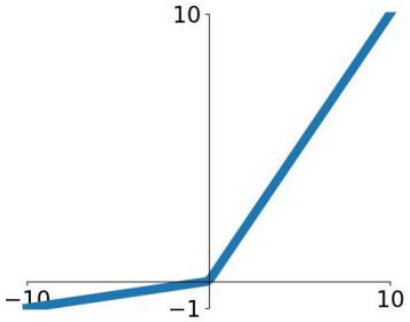
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

Leaky ReLU

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

Activation Functions

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



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

Leaky ReLU

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

Parametric Rectifier (PReLU)

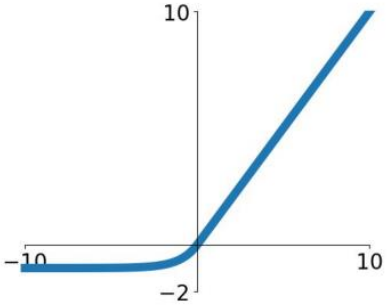
$$f(x) = \max(\alpha x, x)$$

backprop into \alpha (parameter) learnable

Activation Functions

[Clevert et al., 2015]

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

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

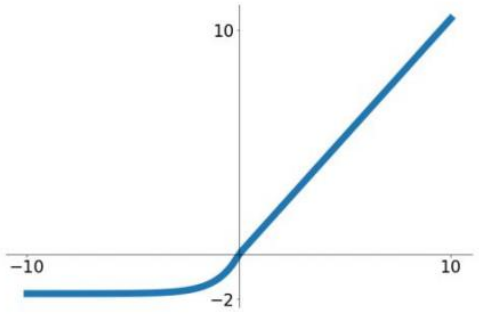
(Alpha default = 1)

- Computation requires exp()

Activation Functions

[Klambauer et al. ICLR 2017]

Scaled Exponential Linear Units (SELU)



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

α = 1.6733, λ = 1.0507

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

Maxout "Neuron"

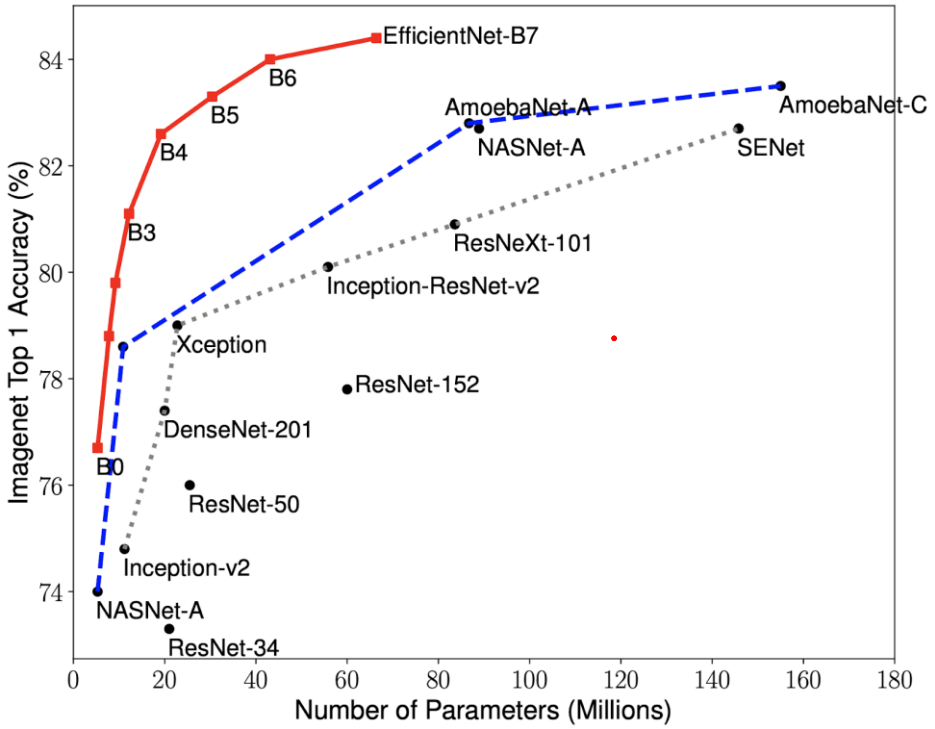
[Goodfellow et al., 2013]

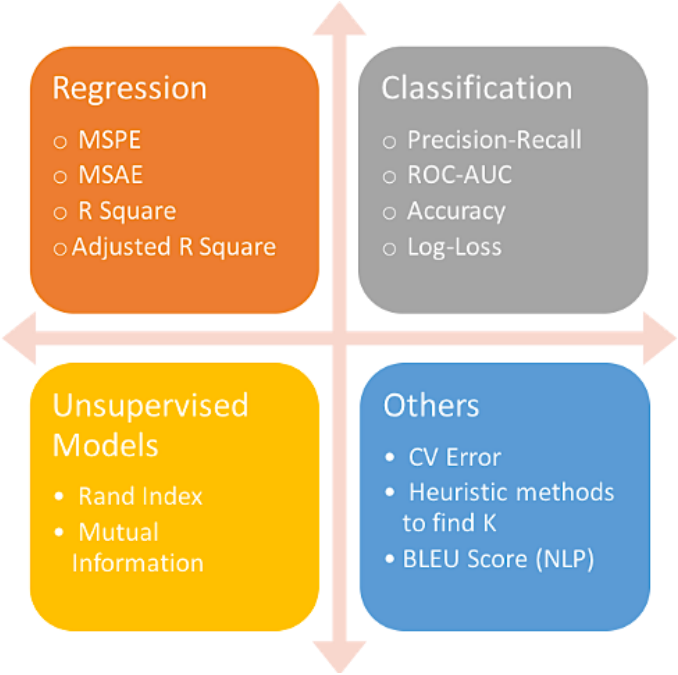
- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

Problem: doubles the number of parameters/neuron :(

of Parameters/FLOPs vs Evaluation Metric





TLDR: In practice:

- Use ReLU. Be careful about Dead ReLU Units
- Try out Leaky ReLU / Maxout / ELU / SELU
  - To squeeze out some marginal gains
- Don’t use sigmoid or tanh