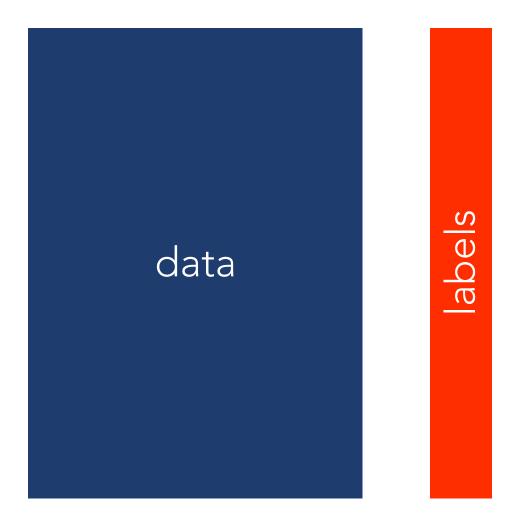
# DEEP LEARNING

#### **PART ONE - INTRODUCTION**

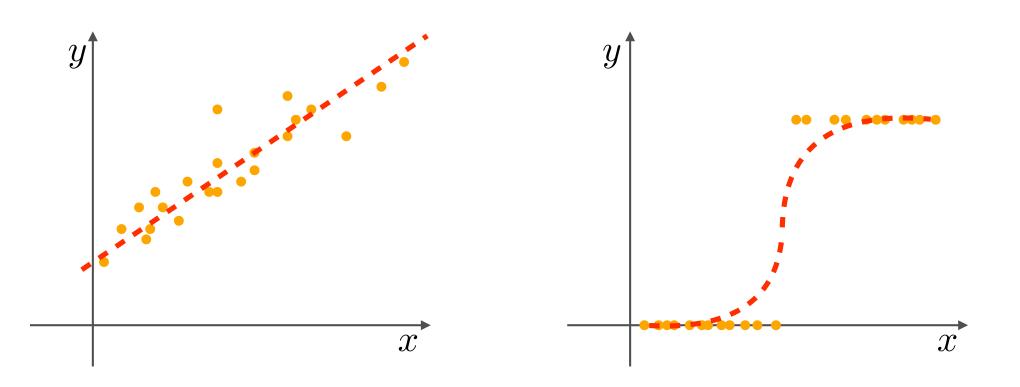
CS/CNS/EE 155 - MACHINE LEARNING & DATA MINING

# INTRODUCTION & MOTIVATION



### y is continuous

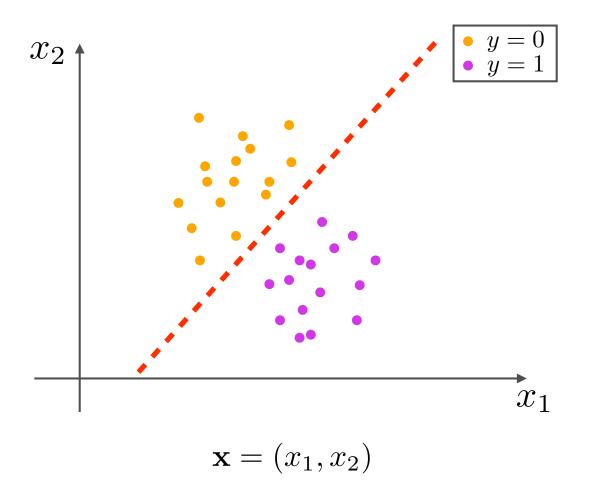
#### y is binary or categorical



regression

classification

## classification example



#### logistic regression

regress to the logistic transform

*linear* decision boundary

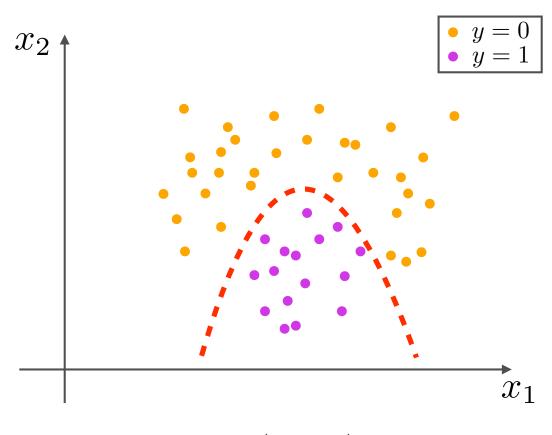
$$\log \frac{p(y=1|\mathbf{x})}{1-p(y=1|\mathbf{x})} = \mathbf{w}^{\mathsf{T}}\mathbf{x} + b$$

$$\rightarrow \quad p(y=1|\mathbf{x}) = \frac{1}{1+e^{-(\mathbf{w}^{\mathsf{T}}\mathbf{x}+b)}}$$

minimize the binary cross entropy loss function  $\mathcal{L}$  to find the optimal  $\mathbf{w}$  and b.

 $\begin{array}{l} \underline{\text{gradient descent}}\\ \mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} \mathcal{L}\\ b \leftarrow b - \alpha \frac{\partial \mathcal{L}}{\partial b} \end{array}$ 

### classification example

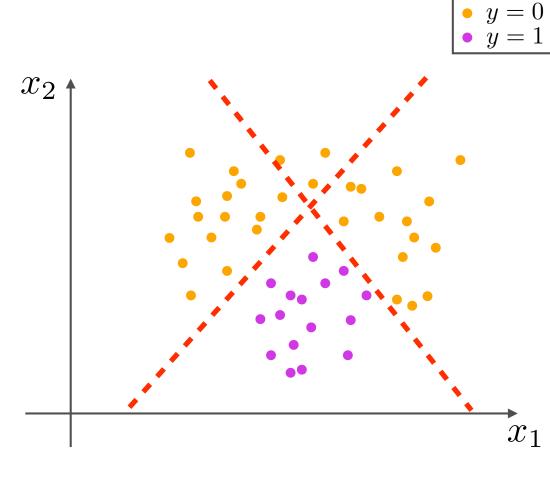


we need a <u>non-linear</u> decision boundary

option 1: use non-linear terms,  
expand 
$$\mathbf{x}$$
 and  $\mathbf{w}$   
 $(x_1, x_2) \rightarrow (x_1^2, x_2^2, x_1 x_2, x_1, x_2)$ 

 $\mathbf{x} = (x_1, x_2)$ 

## classification example



$$\mathbf{x} = (x_1, x_2)$$

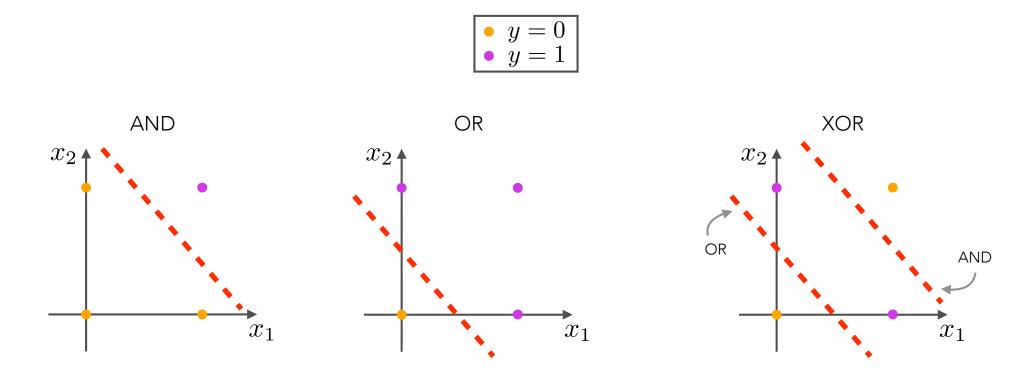
we need a <u>non-linear</u> decision boundary

option 1: use non-linear terms, expand  $\mathbf{x}$  and  $\mathbf{w}$  $(x_1, x_2) \rightarrow (x_1^2, x_2^2, x_1 x_2, x_1, x_2)$ 

**option 2:** use multiple linear decision boundaries to compose a non-linear boundary

in both cases, transform the data into a representation that is linearly separable

### boolean operations

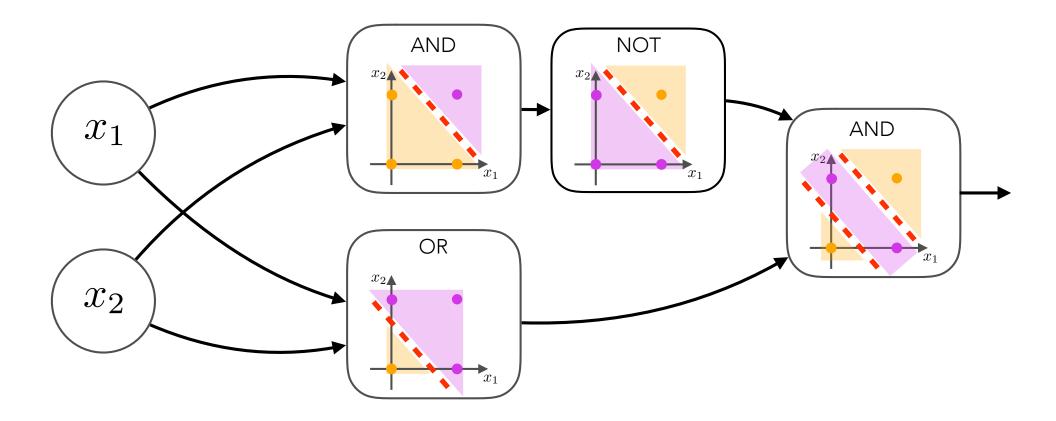


AND and OR are both linearly separable

XOR is not linearly separable, but can be separated using AND and OR

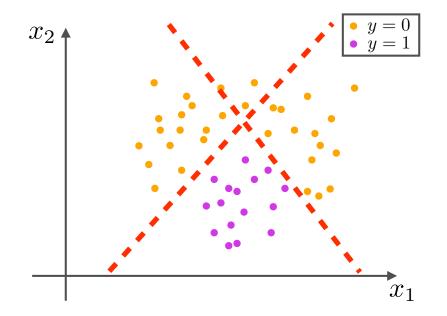
### boolean operations

#### building XOR from AND and OR composing **non-linear** boundaries from **linear** boundaries



### recapitulation

to fit more complex data, we need more expressive **non-linear** functions



we can form non-linear functions by composing stages of processing

depth: the number of stages of processing

deep learning: learning functions with multiple stages of processing

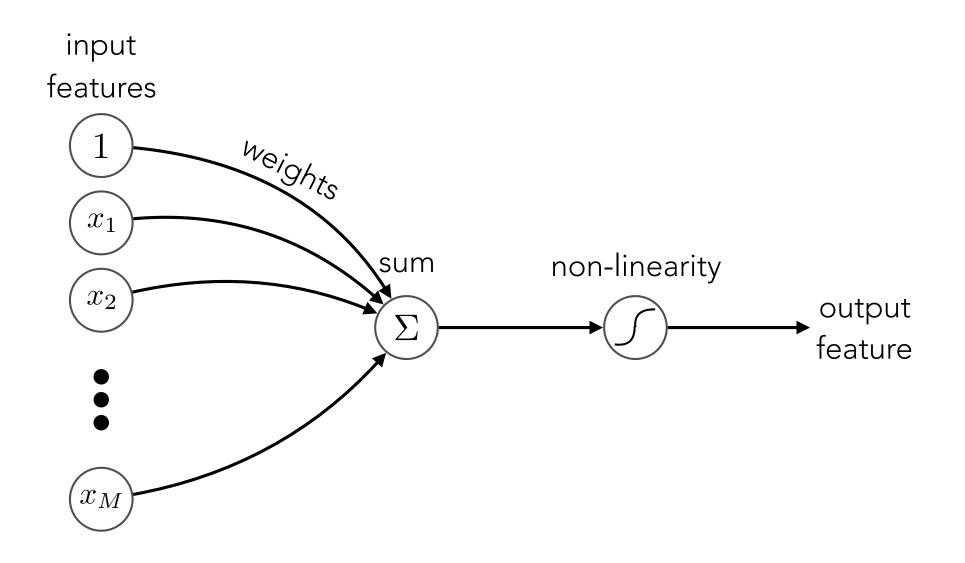
wait...why not just use non-linear terms?  $(x_1, x_2) \to (x_1^2, x_2^2, x_1 x_2, x_1, x_2)$ y = 0 $x_2 \bullet$  $\tilde{y} = 1$  $x_1$ 

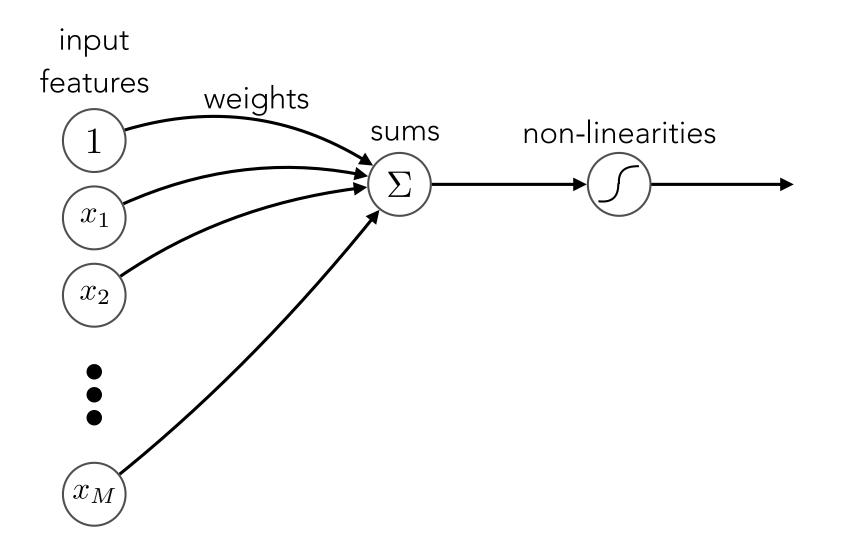
you certainly can!

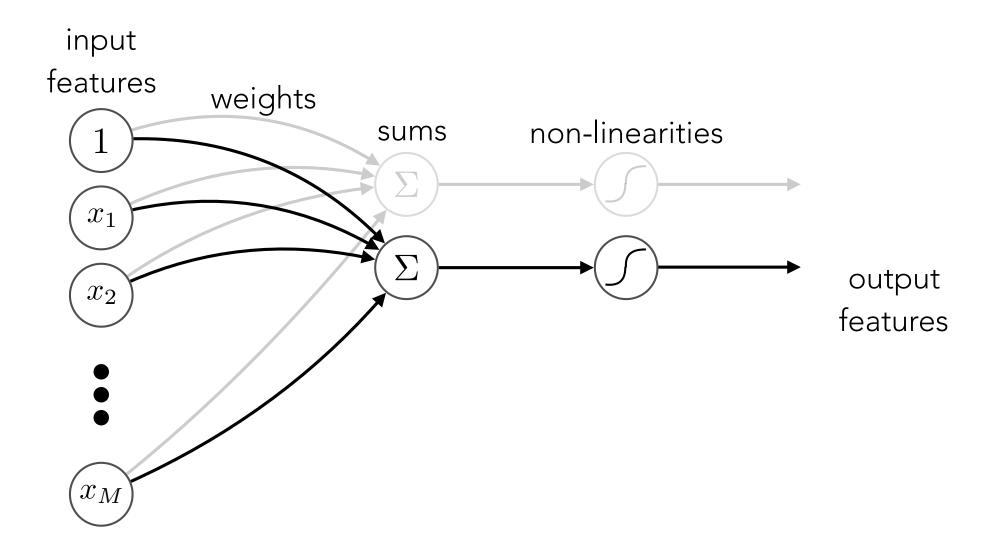
but we will see that with enough stages of linear boundaries, we can approximate any non-linear function

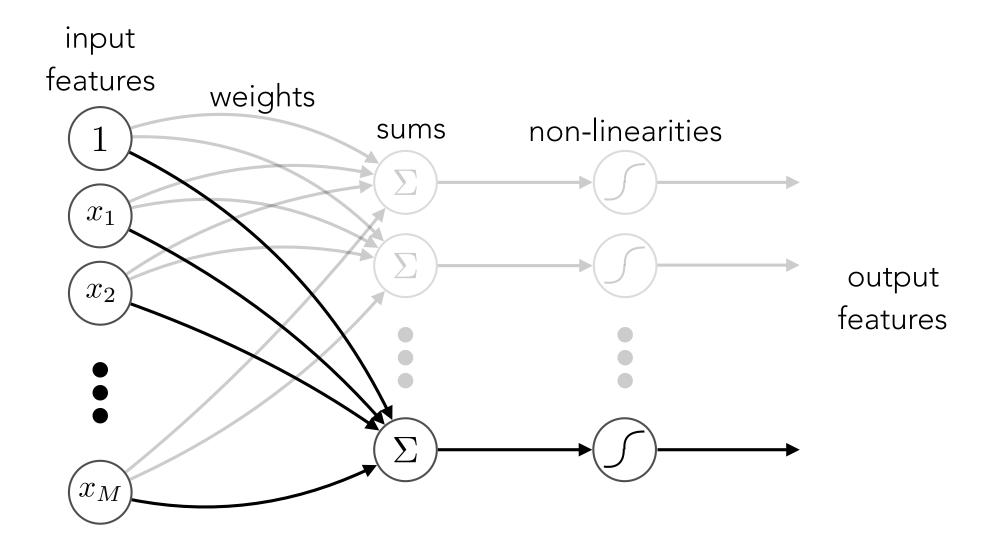
# DEEP NEURAL NETWORKS

## artificial **neuron**

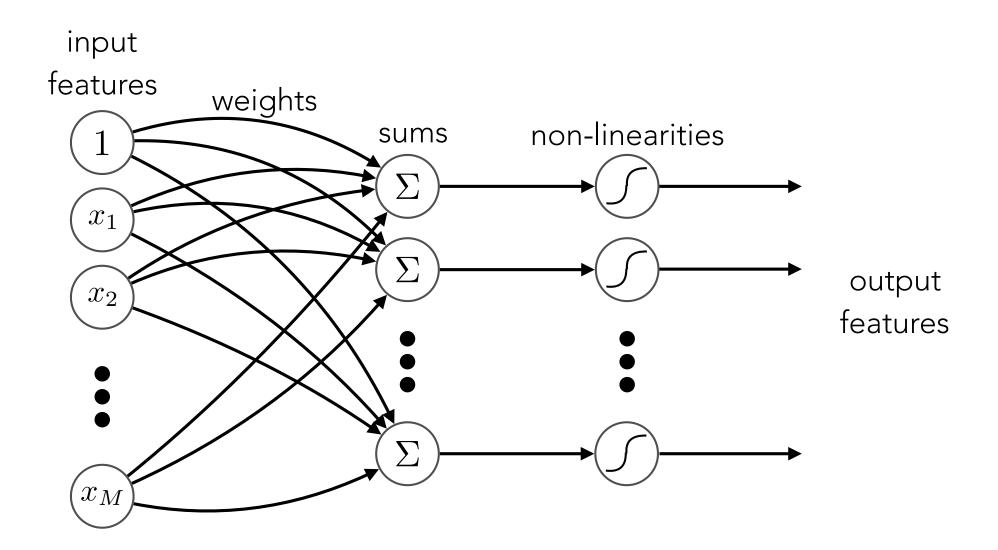


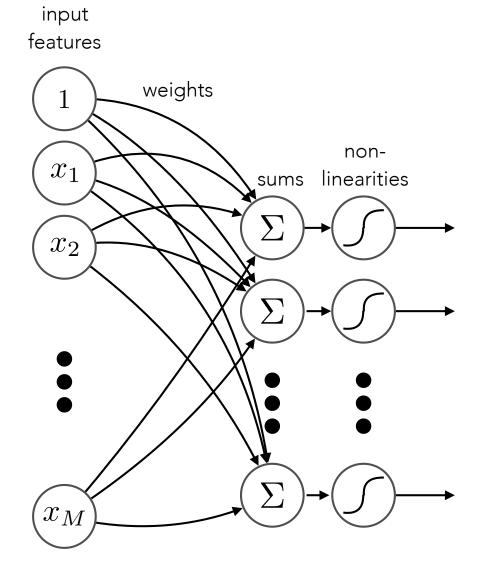


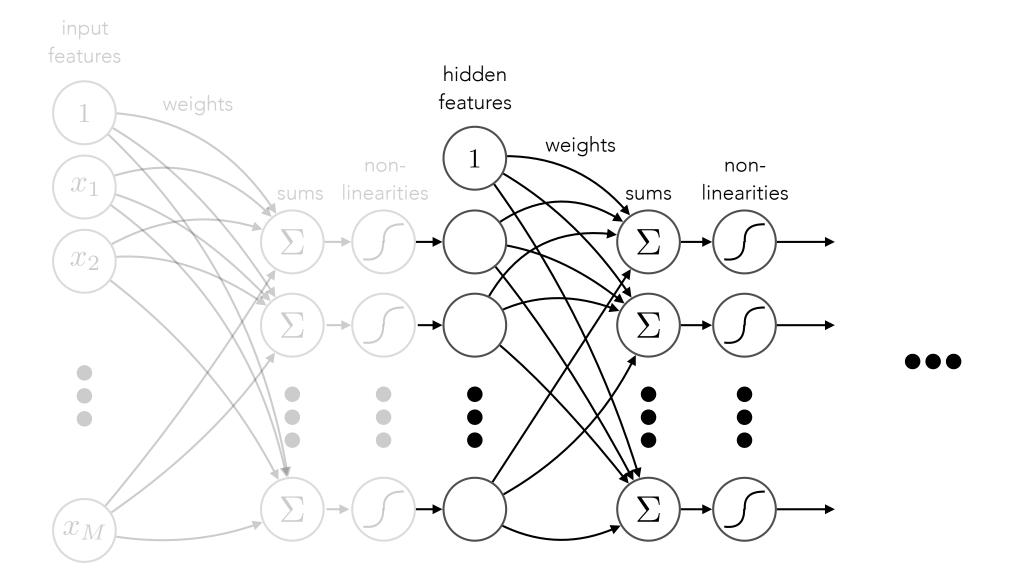




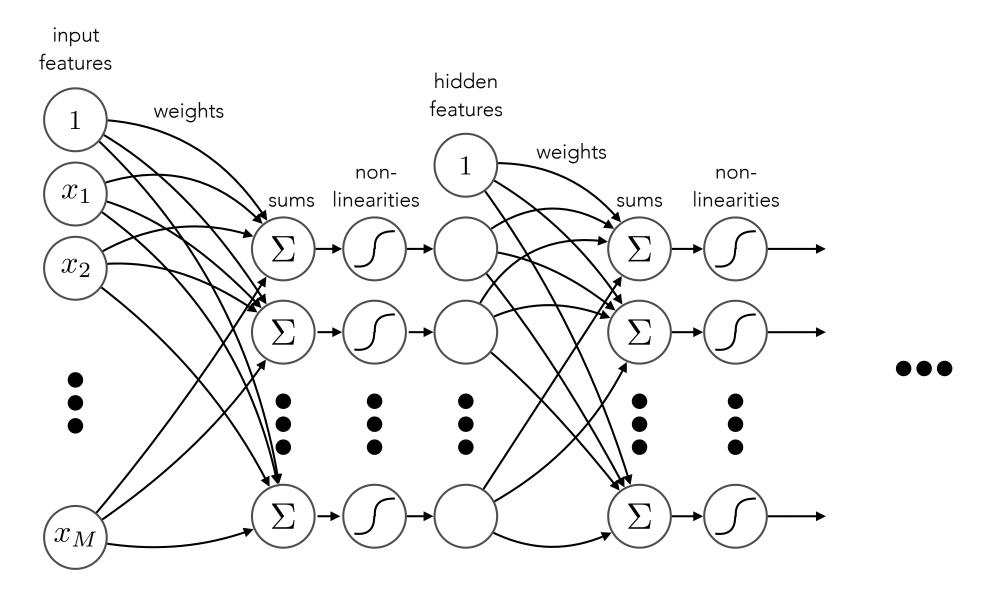
### multiple neurons form a layer

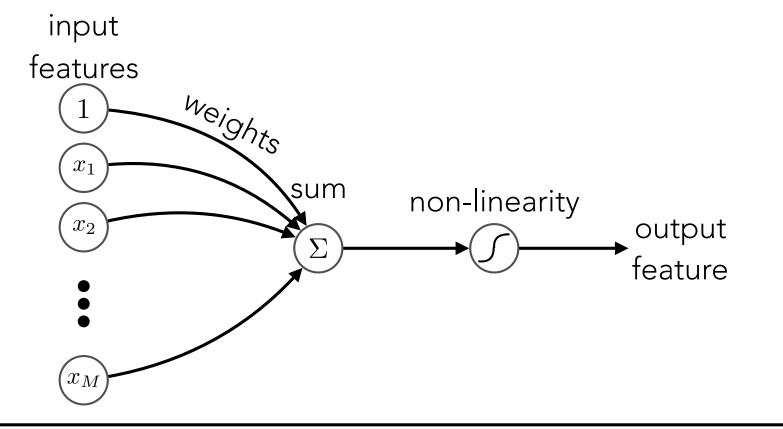


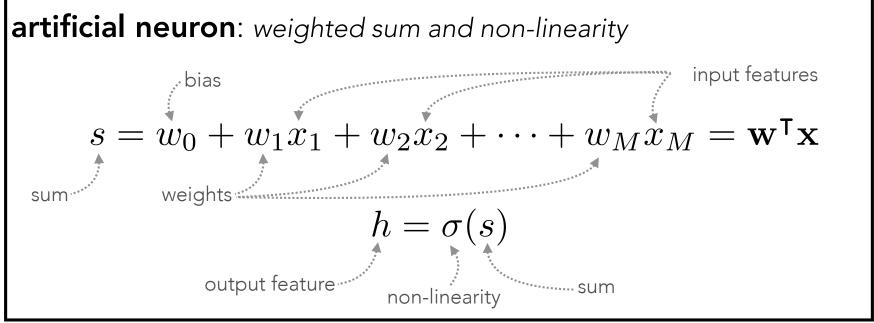


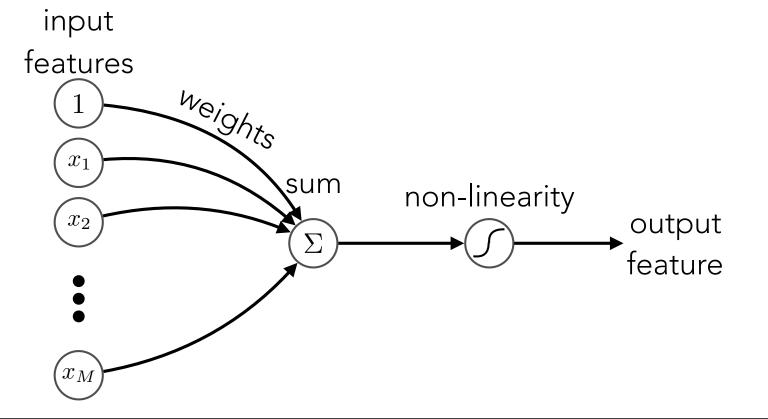


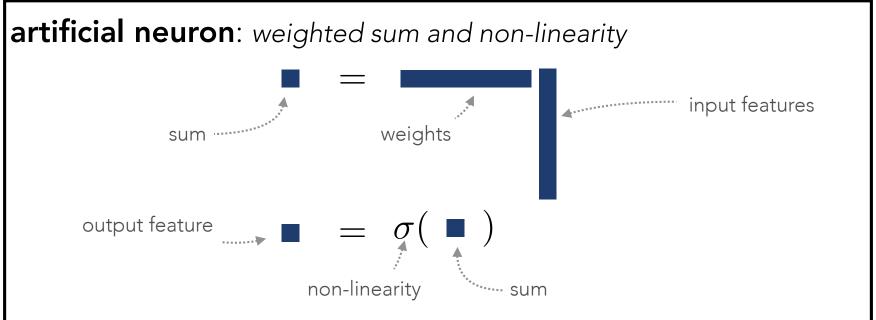
## multiple layers form a **network**

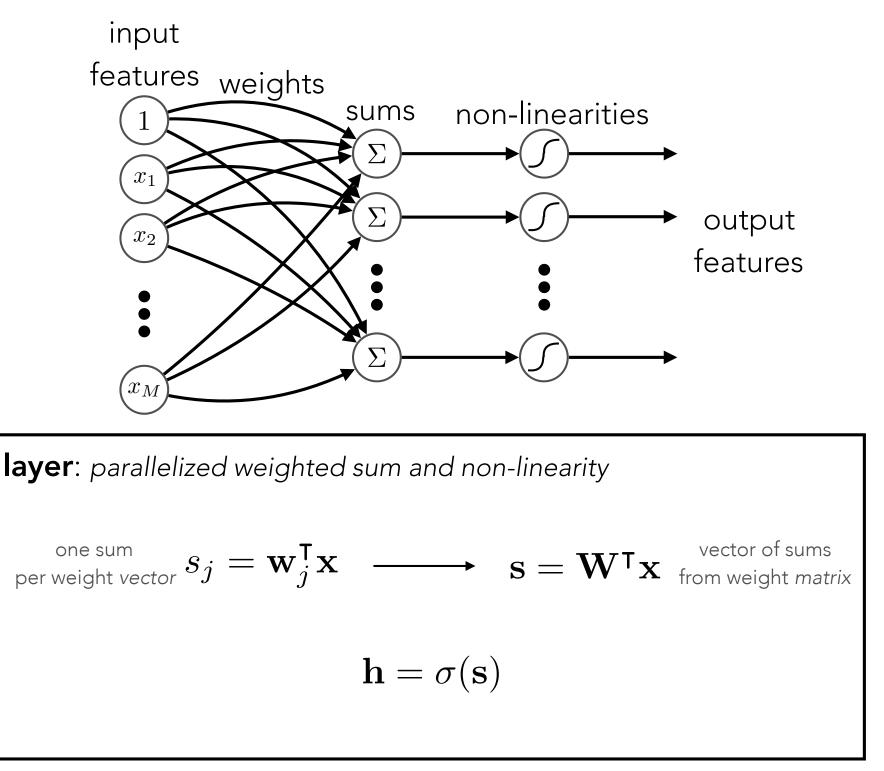


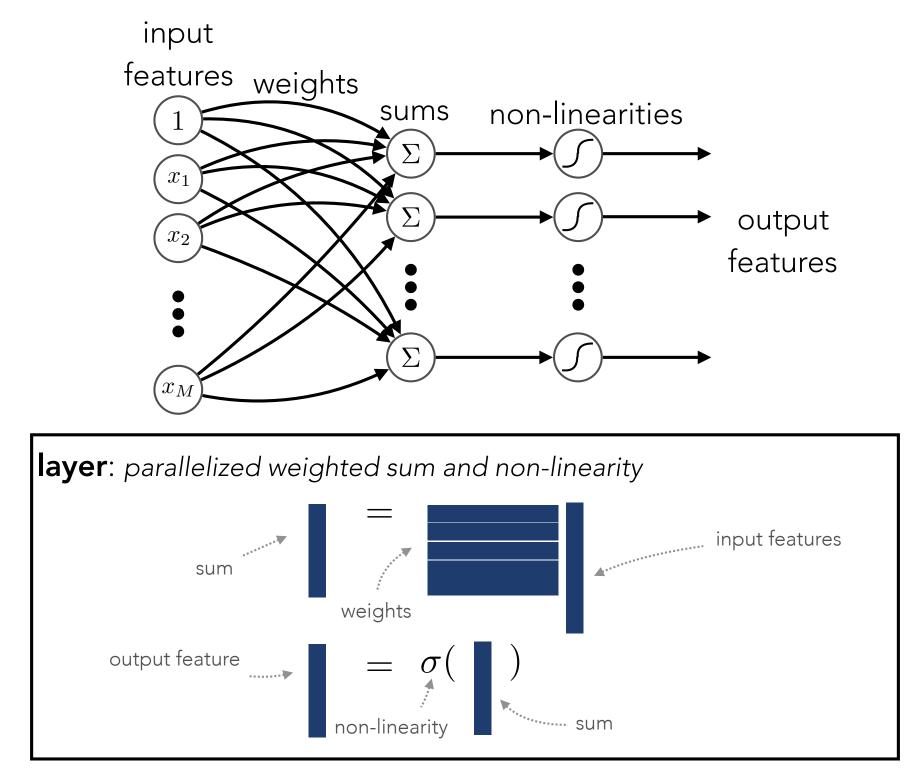


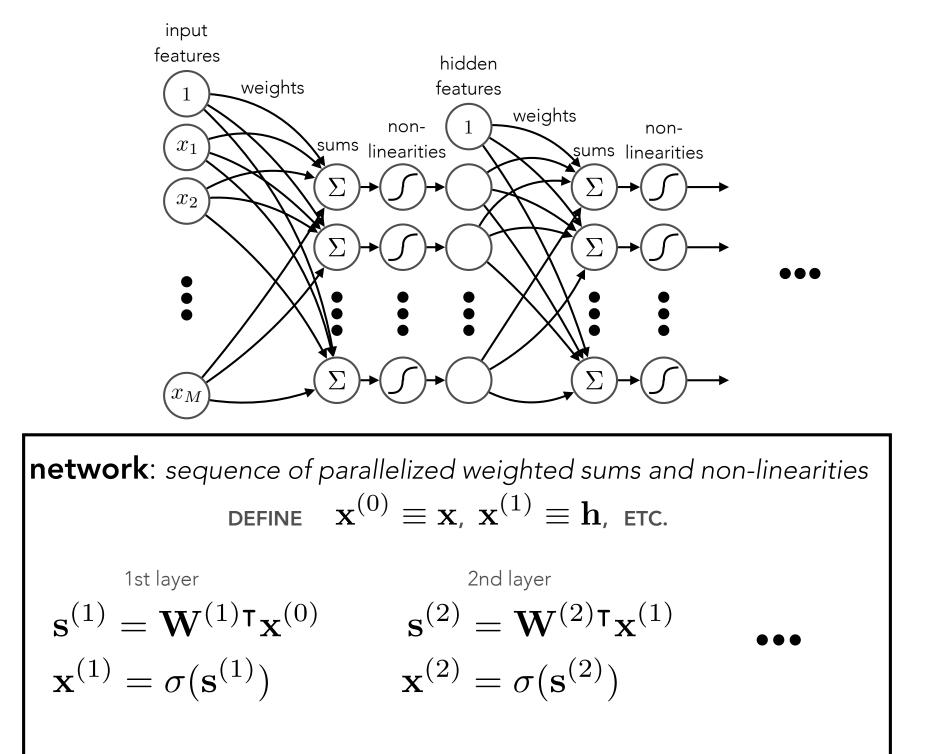


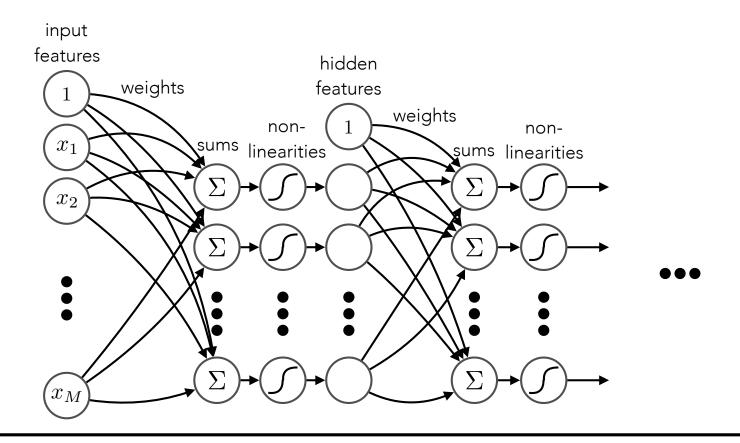


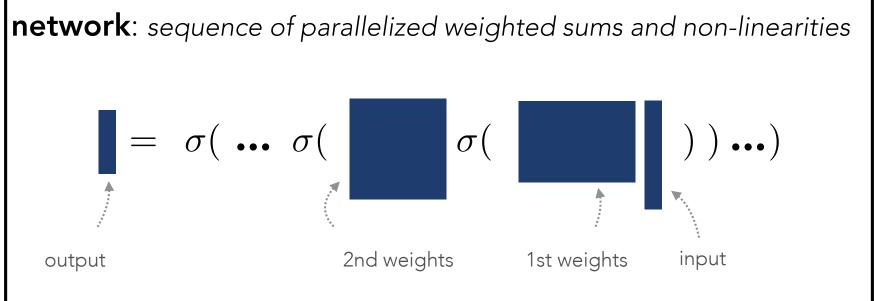




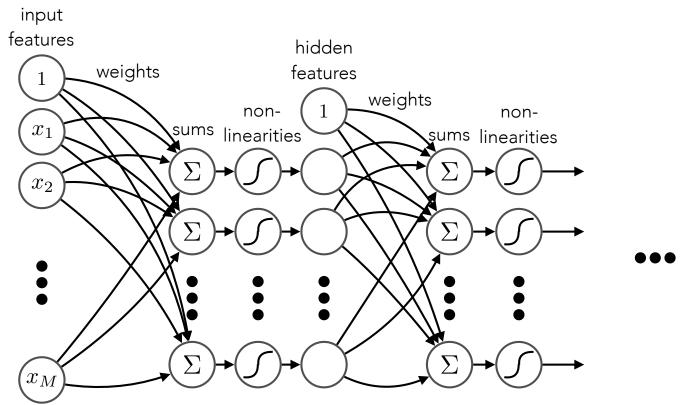








## recapitulation



we have a method for building *expressive* non-linear functions

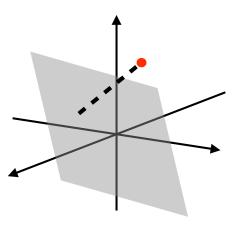
deep networks are *universal function approximators* (Hornik, 1991) → with enough units & layers, can approximate <u>any</u> function

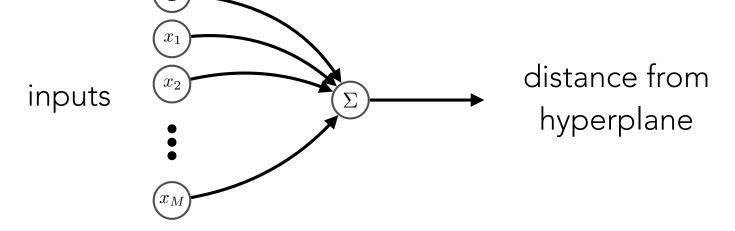
### reinterpretation

the dot product is the distance between a point and a plane

each artificial neuron defines a (hyper)plane:

$$0 = w_0 + w_1 x_1 + w_2 x_2 + \dots + w_M x_M$$

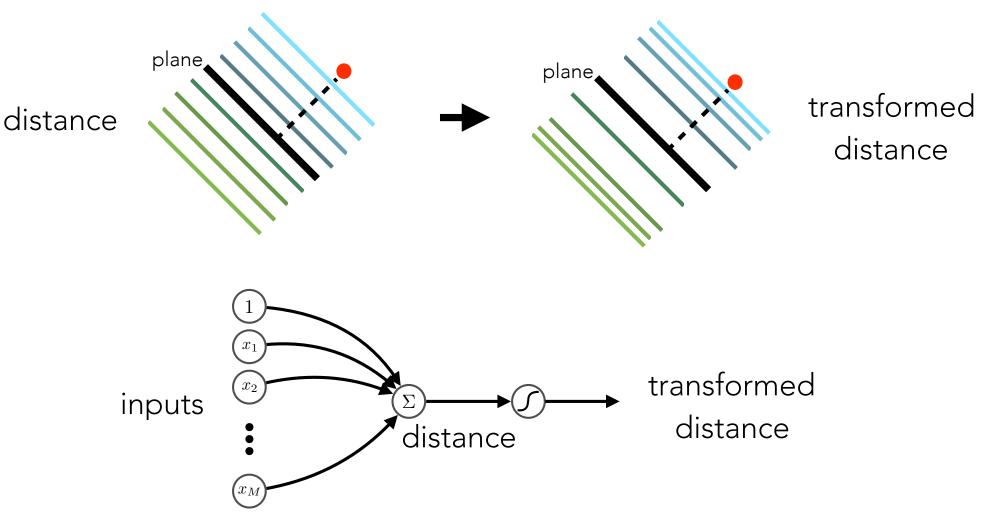




<u>calculating the weighted sum</u> corresponds to finding the shortest distance between the input point and the weight hyperplane

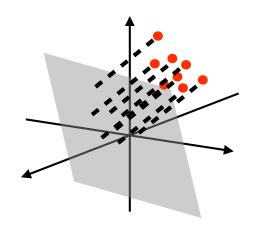
### reinterpretation

<u>the non-linearity</u> transforms this distance, creating a field that changes non-linearly with distance

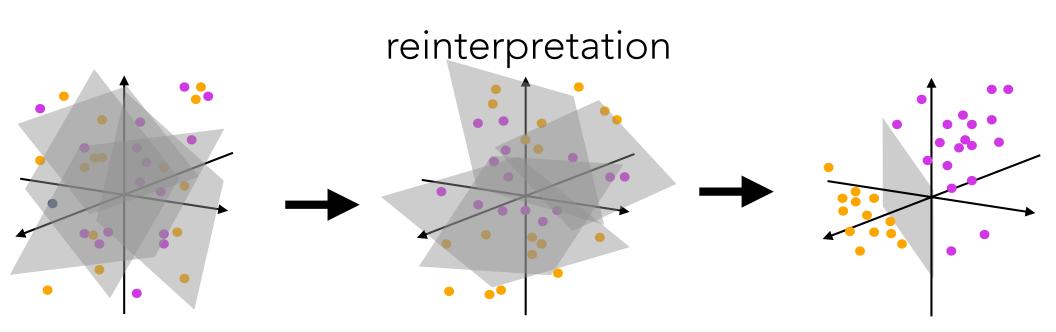


### reinterpretation

a weight vector therefore becomes a *filter* if its hyperplane faces a cluster of points within a region or subregion



the unit selects for the abstract feature shared by the cluster of points



at each stage,

- 1. cut the space up with hyperplanes
- 2. evaluate distance of each point to each hyperplane
- 3. transform these distances according to non-linear function
- 4. transformed distances become points in new space

repeat until the data are sufficiently *linearized* → can separate clusters with hyperplanes

## big picture

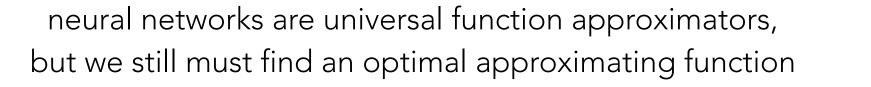
### neural networks are functions / function approximators

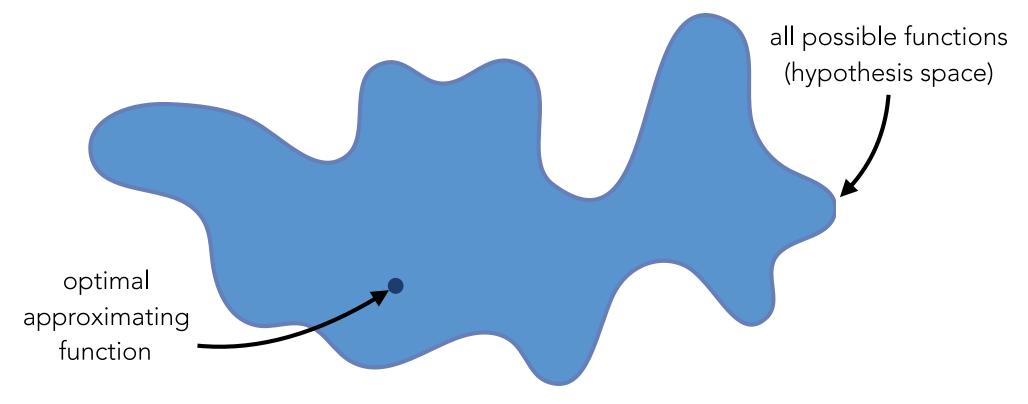
their nested (deep) structure enables a broader set of functions

- output = NN(inputs)
  - $= \operatorname{Layer}_{L}(\operatorname{Layer}_{L-1}(\dots \operatorname{Layer}_{1}(\operatorname{inputs})\dots))$

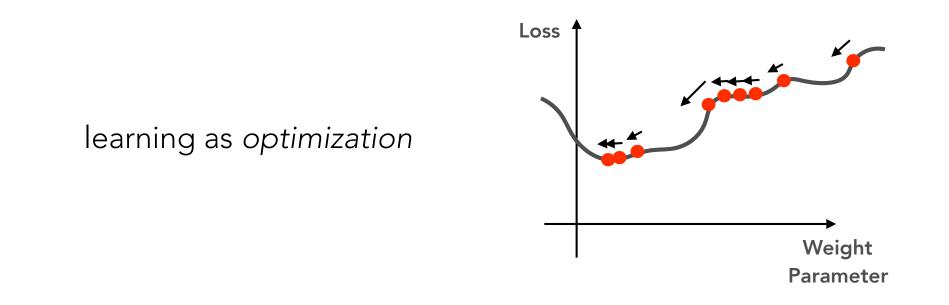
can approximate a variety of functions, particularly **conditional probability distributions** 

# BACKPROPAGATION





we do so by <u>adjusting the weights</u>



to learn the weights, we need the **derivative** of the loss w.r.t. the weight i.e. "*how should the weight be updated to decrease the loss?*"

$$w = w - \alpha \frac{\partial \mathcal{L}}{\partial w}$$

with multiple weights, we need the gradient of the loss w.r.t. the weights

$$\mathbf{w} = \mathbf{w} - \alpha \nabla_{\mathbf{w}} \mathcal{L}$$

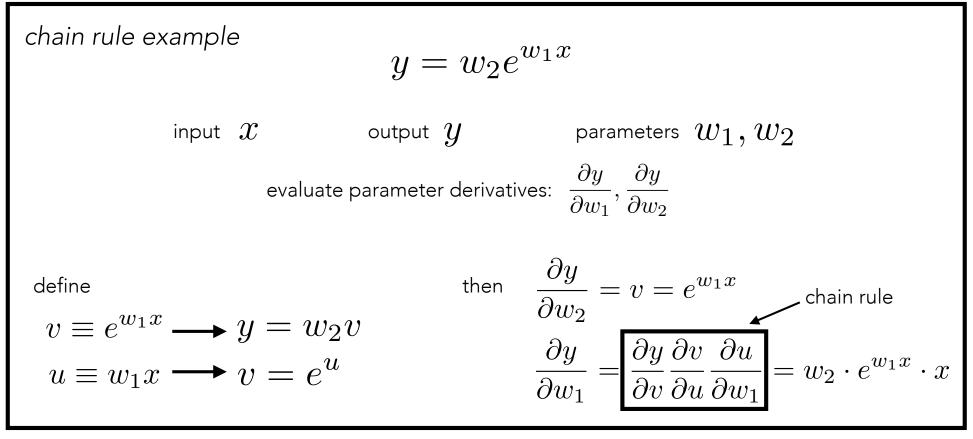
## backpropagation

a neural network defines a function of composed operations

$$f_L(\mathbf{w}_L, f_{L-1}(\mathbf{w}_{L-1}, \dots, f_1(\mathbf{w}_1, \mathbf{x}) \dots))$$

and the loss  ${\cal L}$  is a function of the network output

→ use <u>chain rule</u> to calculate gradients

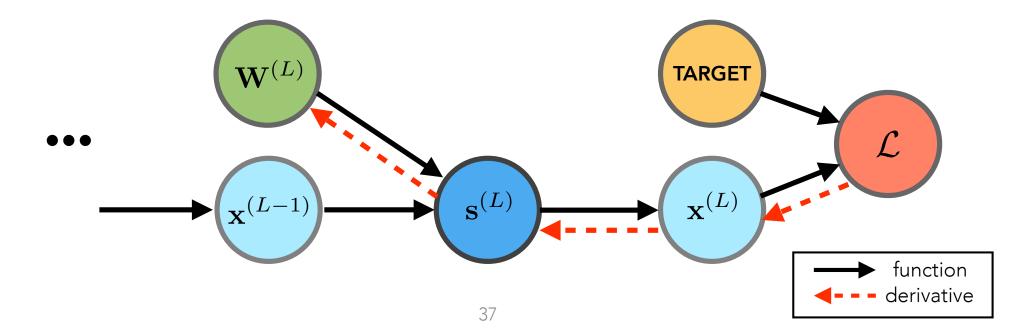


recall

1st layer2nd layerLoss
$$\mathbf{s}^{(1)} = \mathbf{W}^{(1)\intercal} \mathbf{x}^{(0)}$$
 $\mathbf{s}^{(2)} = \mathbf{W}^{(2)\intercal} \mathbf{x}^{(1)}$  $\bullet \bullet \bullet$  $\mathcal{L}$  $\mathbf{x}^{(1)} = \sigma(\mathbf{s}^{(1)})$  $\mathbf{x}^{(2)} = \sigma(\mathbf{s}^{(2)})$  $\bullet \bullet \bullet$  $\mathcal{L}$ 

calculate  $\nabla_{W^{(1)}}\mathcal{L}, \nabla_{W^{(2)}}\mathcal{L}, \ldots$  let's start with the final layer:  $\nabla_{W^{(L)}}\mathcal{L}$ 

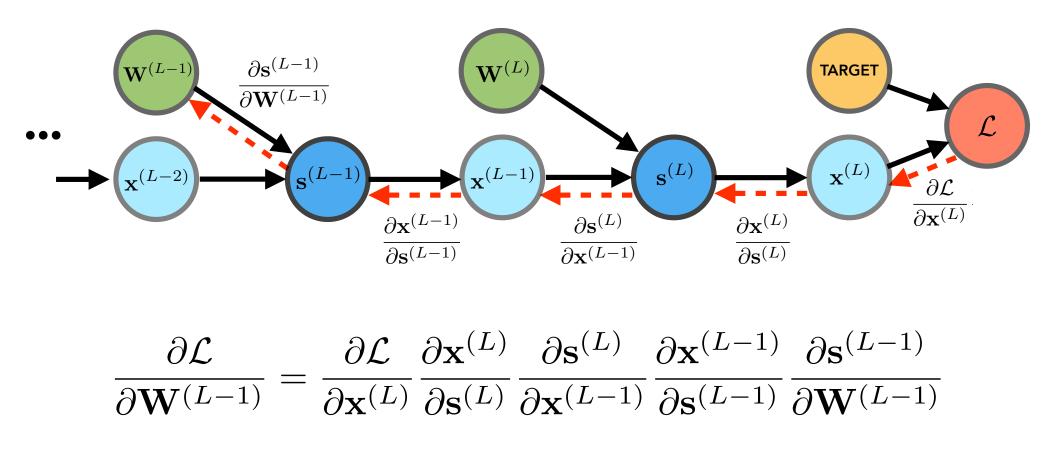
to determine the chain rule ordering, we'll draw the dependency graph

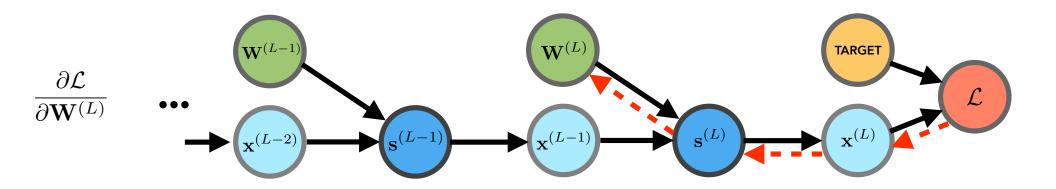


## backpropagation $\frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{W}^{(L)}}$ $\mathbf{W}^{(L)}$ TARGET $\mathcal{L}$ $\partial \mathbf{x}^{(L)}$ $\overline{\partial \mathbf{s}^{(L)}}$ $\mathbf{x}^{(L-1)}$ $\mathbf{s}^{(L)}$ $\mathbf{x}^{(L)}$ $rac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}}$ $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{W}^{(L)}}$ $\begin{aligned} \dot{\partial} \\ \frac{\partial}{\partial \mathbf{W}^{(L)}} (\mathbf{W}^{(L)\mathsf{T}} \mathbf{x}^{(L-1)}) \\ = \mathbf{x}^{(L-1)\mathsf{T}} \end{aligned}$ depends on the derivative of the form of the loss non-linearity note $\nabla_{\mathbf{W}^{(L)}} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$ is notational convention

now let's go back one more layer...

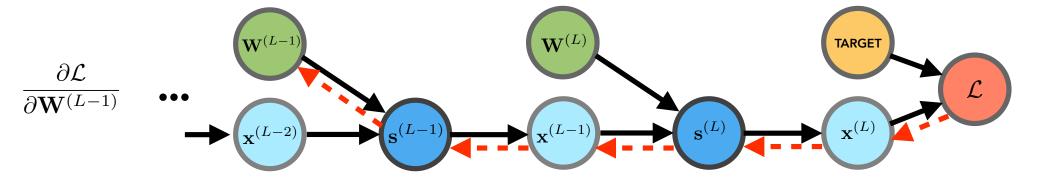
again we'll draw the dependency graph:

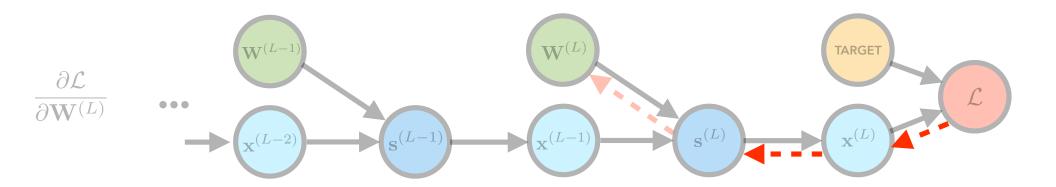




notice that some of the same terms appear in both gradients

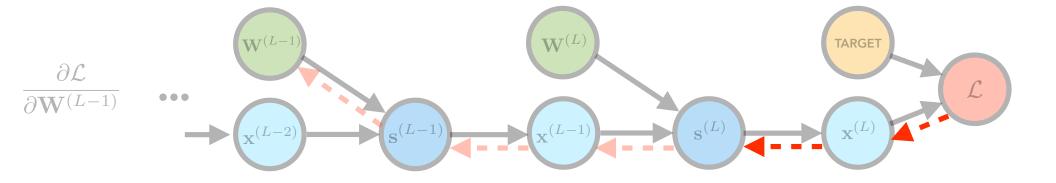
specifically, we can reuse  $\frac{\partial \mathcal{L}}{\partial \mathbf{s}^{(\ell)}}$  to calculate gradients in reverse order





notice that some of the same terms appear in both gradients

specifically, we can reuse  $\frac{\partial \mathcal{L}}{\partial s^{(\ell)}}~$  to calculate gradients in reverse order

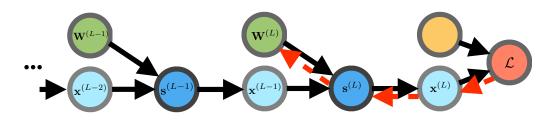




#### **BACKPROPAGATION ALGORITHM**

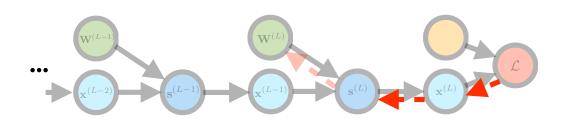
#### **BACKPROPAGATION ALGORITHM**

calculate  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$ 

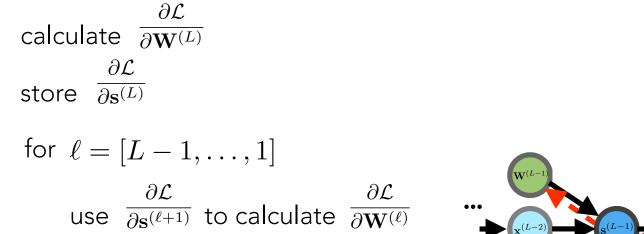


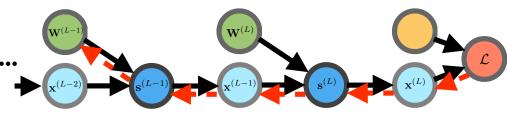
#### **BACKPROPAGATION ALGORITHM**

 $\begin{array}{ll} \text{calculate} & \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} \\ \text{store} & \frac{\partial \mathcal{L}}{\partial \mathbf{s}^{(L)}} \end{array}$ 

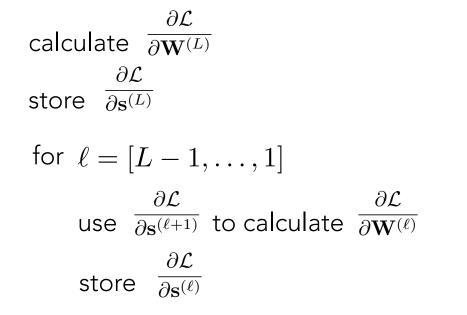


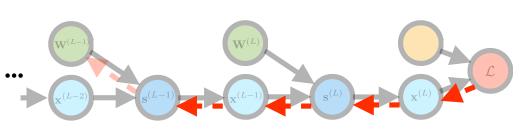
#### **BACKPROPAGATION ALGORITHM**





#### **BACKPROPAGATION ALGORITHM**



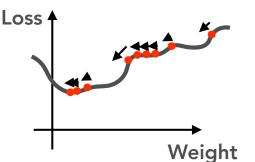


#### **BACKPROPAGATION ALGORITHM**

calculate  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$ store  $\frac{\partial \mathcal{L}}{\partial \mathbf{s}^{(L)}}$ for  $\ell = [L - 1, \dots, 1]$ use  $\frac{\partial \mathcal{L}}{\partial \mathbf{s}^{(\ell+1)}}$  to calculate  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(\ell)}}$ store  $\frac{\partial \mathcal{L}}{\partial \mathbf{s}^{(\ell)}}$ return  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(1)}}, \dots, \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$ 

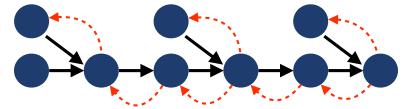
# recapitulation

update weights using gradient of loss



backpropagation calculates the loss gradients w.r.t. internal weights

gradient is propagated backward through the network



most deep learning software libraries automatically calculate gradients

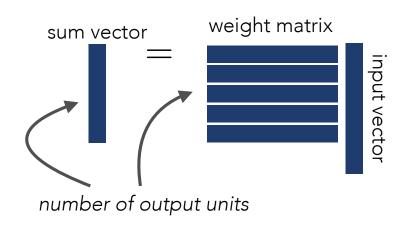
- → "automatic differentiation" or "auto-diff"
- can calculate gradients for any differentiable operation

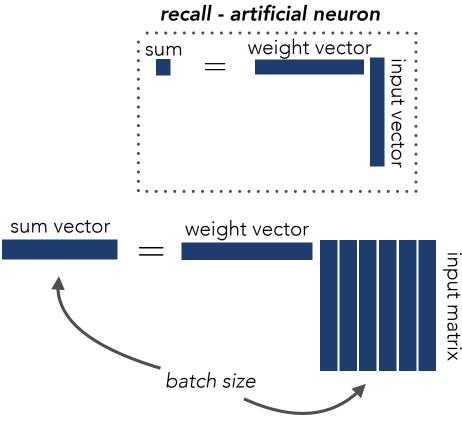
# IMPLEMENTATION

## parallelization

neural networks can be parallelized

- matrix multiplications
- point-wise operations





unit parallelization

perform all operations within a layer simultaneously

#### data parallelization process multiple data examples simultaneously

using parallel computing architectures, we can efficiently implement neural network operations

#### implementation

import numpy as np

```
def nn_layer(x, W):
    s = np.dot(W.T, x)
    return np.maximum(s, 0) # ReLU
```

#### implementation

```
import numpy as np
class nn_layer(object):
    def __init__(self, num_input, num_output):
        # initialize W from uniform(-0.25, 0.25)
        self.W = np.random.rand(num_input, num_output)
        self.W = 0.5 * (self.W - 0.5)
```

def \_\_call\_\_(self, x):
 s = np.dot(self.W.T, x)
 return np.maximum(s, 0) # ReLU

implementation

we need to manually implement backpropagation and weight updates
 → can be difficult for arbitrary, large computation graphs

most deep learning software libraries automatically handle this for you



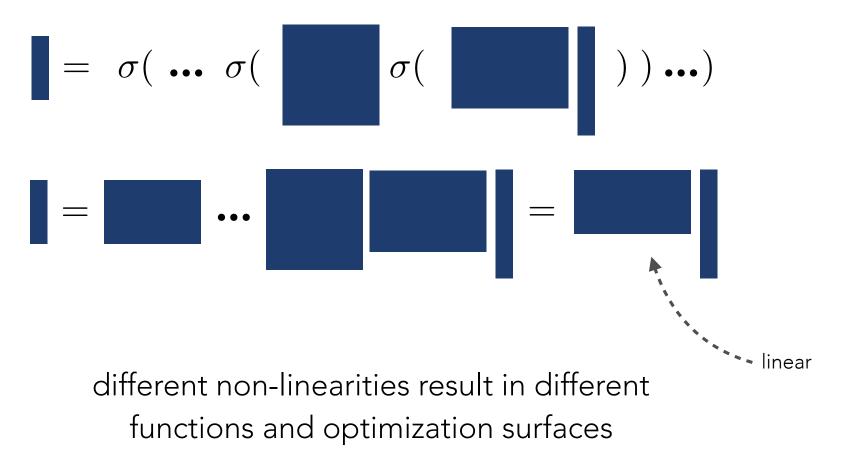
just build the computational graph and define the loss

# TIPS & TRICKS

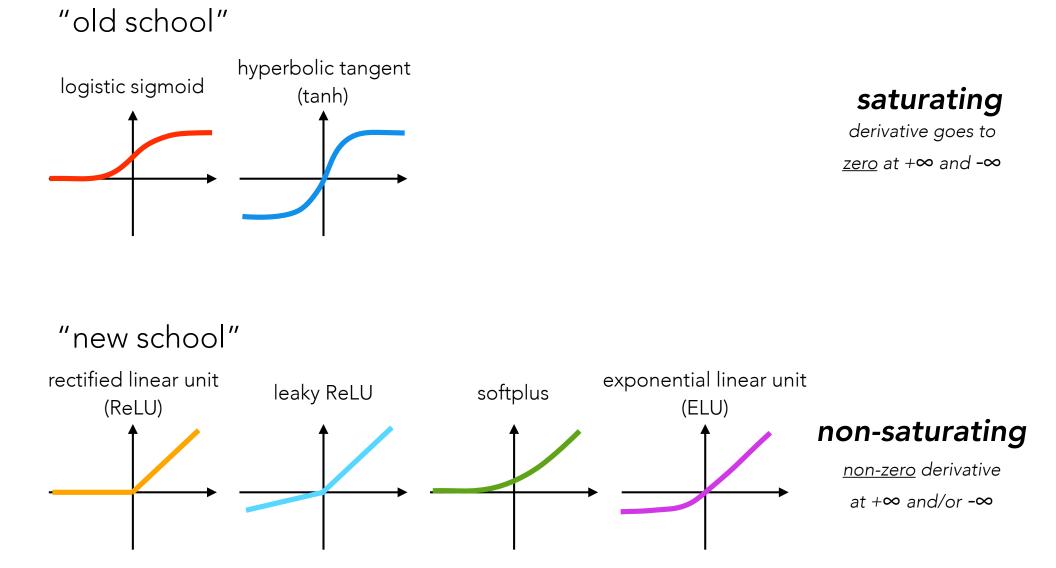
non-linearities

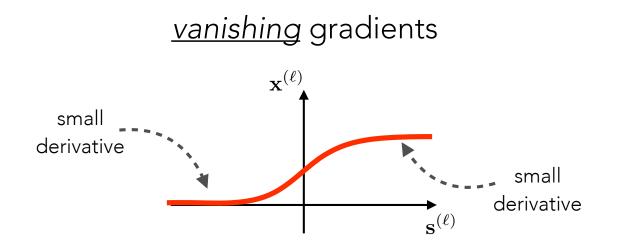
the non-linearities are *essential* 

without them, the network collapses to a linear function

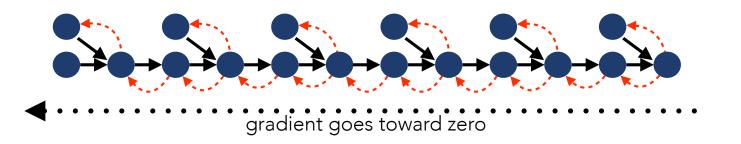


## non-linearities





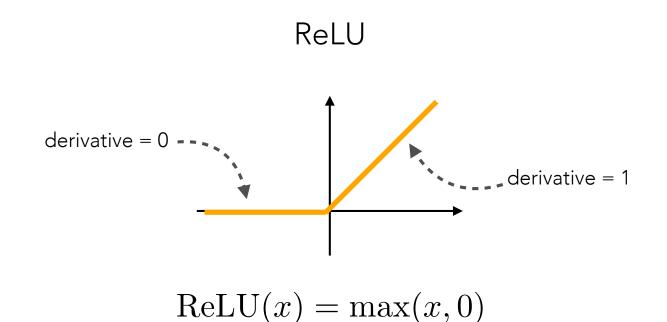
saturating non-linearities have *small* derivatives almost everywhere



in backprop, the product of many small terms (i.e.  $\frac{\partial \mathbf{x}^{(\ell)}}{\partial \mathbf{s}^{(\ell)}}$  ) goes to zero

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(\ell)}} = \dots \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \dots \frac{\partial \mathbf{x}^{(L-1)}}{\partial \mathbf{s}^{(L-1)}} \dots \frac{\partial \mathbf{x}^{(\ell+1)}}{\partial \mathbf{s}^{(\ell+1)}} \dots \frac{\partial \mathbf{x}^{(\ell)}}{\partial \mathbf{s}^{(\ell)}} \frac{\partial \mathbf{s}^{(\ell)}}{\partial \mathbf{W}^{(\ell)}}$$

difficult to train very deep networks with saturating non-linearities



in the positive region, ReLU does not saturate, preventing gradients from vanishing in deep networks

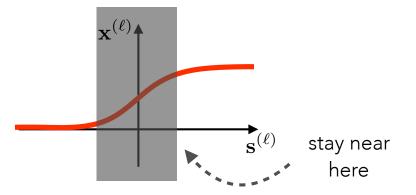
in the negative region, ReLU saturates at zero, resulting in 'dead units' where the gradient is zero

but in practice, this doesn't seem to be a significant problem

normalization

can we prevent the gradients from saturating non-linearities from becoming too small?

--> keep the inputs within the dynamic range of the non-linearity



we can *normalize* the activations before applying the non-linearity

$$\mathbf{s} \leftarrow \frac{\mathbf{s} - \mathrm{shift}}{\mathrm{scale}}$$

batch normalization

batch norm. normalizes each layer's activations according to the statistics of the <u>batch</u>

$$\mathbf{s}^{(\ell)} \leftarrow \gamma \frac{\mathbf{s}^{(\ell)} - \mu_{\mathcal{B}}}{\sigma_{\mathcal{B}}} + \beta$$

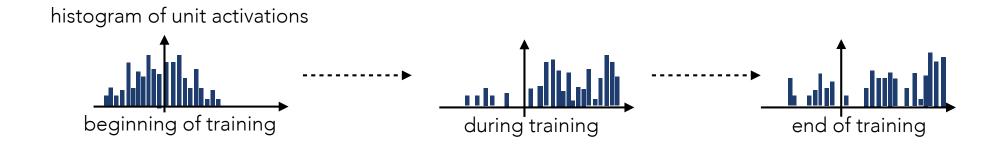
 $\mu_{\mathcal{B}}, \sigma_{\mathcal{B}}~~$  are the batch mean and std. deviation

 $\gamma,eta$  are additional parameters (affine transformation)

keeps internal activations in similar range, speeding up training adds stochasticity, improves generalization why does batch norm. work?

## original motivation: internal covariate shift

changing weights during training results in changing outputs; input to the next layer changes, making it difficult to learn

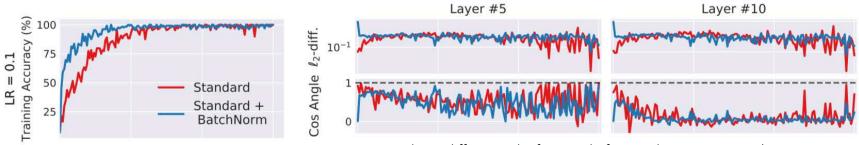


batch norm. should stabilize the activations during training

why does batch norm. work?

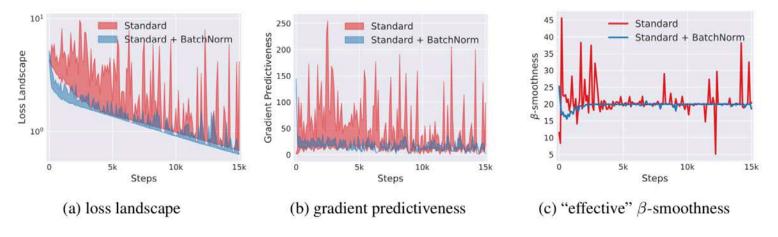
but actually...

batch norm. does *not* seem to significantly reduce internal covariate shift



gradient difference before and after updating previous layers

rather, it seems that batch norm. stabilizes and smooths the optimization surface



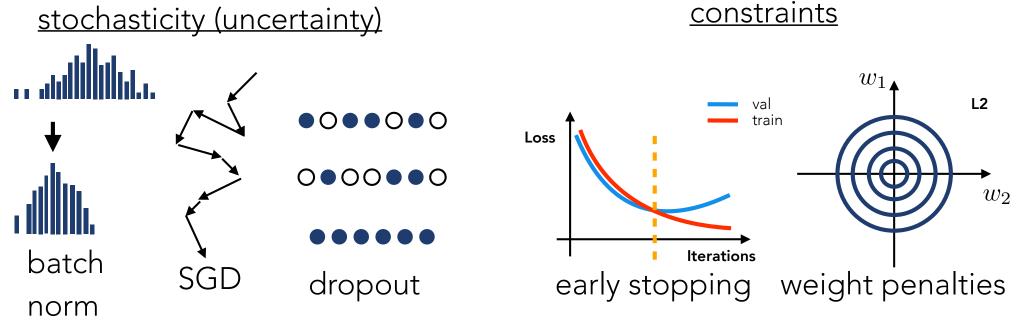
How Does Batch Normalization Help Optimization?, Santurkar et al., 2018

regularization

## neural networks are amazingly flexible...

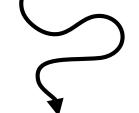
given enough parameters, they can perfectly fit random noise

regularization combats overfitting by formalizing <u>prior beliefs</u> on the model or data



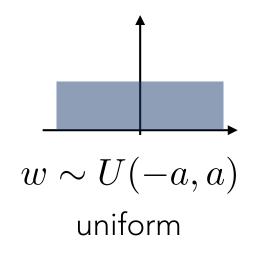
initialization

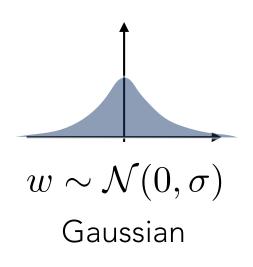
learning is formulated as an <u>optimization</u> problem, which can be sensitive to **initial conditions** 



"causes the network to blow up and/or not learn"

common strategies for weight initialization:





#### optimization

stochastic gradient descent (SGD):  $w = w - \alpha \tilde{\nabla}_w \mathcal{L}$ 

use stochastic gradient estimate to descend the surface of the loss function

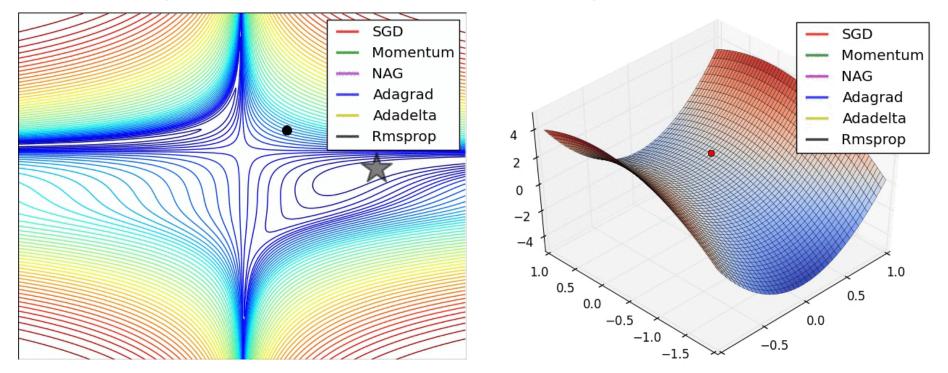
recent variants use additional terms to maintain"memory" of previous gradient information and scale gradients per parameter

## optimization

stochastic gradient descent (SGD):  $w = w - \alpha \tilde{\nabla}_w \mathcal{L}$ 

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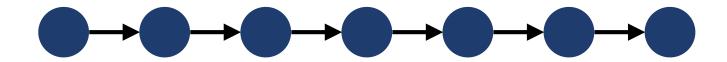
recent variants use additional terms to maintain"memory" of previous gradient information and scale gradients per parameter



local minima and saddle points are largely not an issue in many dimensions, can move in exponentially more directions

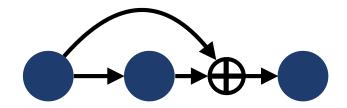
### connectivity

sequential connectivity: information must flow through the entire sequence to reach the output



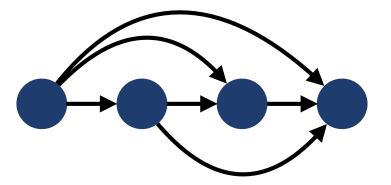
information may not be able to propagate easily *make shorter paths to output* 

residual & highway connections



Deep residual learning for image recognition, He et al., 2016 Highway networks, Srivastava et al., 2015 dense (concatenated)

connections

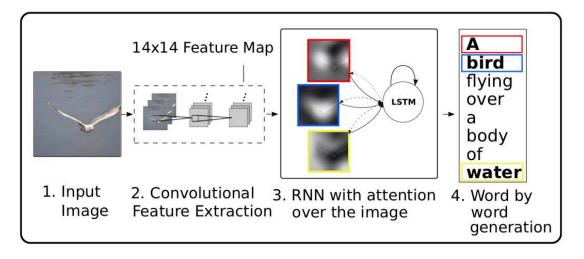


Densely connected convolutional networks, Huang et al., 2017

# A BUFFET OF IDEAS

#### attention

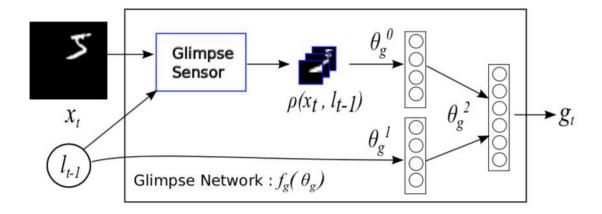
# soft attention $\mathbf{x}_{\mathrm{att.}} = \mathbf{a} \odot \mathbf{x}$ re-weighting



Show, Attend and Tell, Xu et al., 2015

hard attention

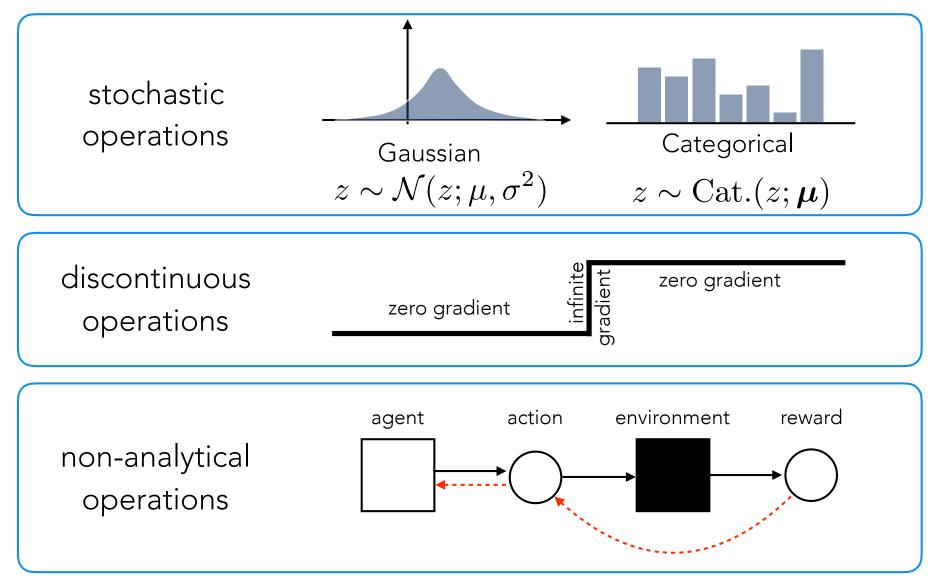
 $\mathbf{x}_{\mathrm{att.}} = \mathbf{x}[\mathbf{a}]$  extraction



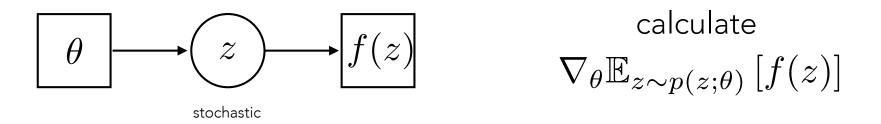
Recurrent Models of Visual Attention, Mnih et al., 2014

## gradients of non-differentiable operations

## examples of **non-differentiable** operations



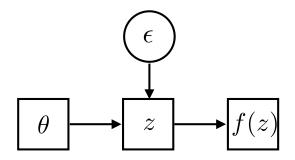
gradients of non-differentiable operations



Score Function Estimator (REINFORCE) Williams, 1992

$$\begin{array}{|c|c|} \hline \theta & & \hline f(z) \\ \hline \theta & & \hline f(z) \hline \theta & & \hline f(z) \\ \hline \theta & & \hline f(z) \hline \theta & & \hline f($$

Pathwise Derivative Estimator (Reparameterization) Kingma & Welling, 2014 Rezende et al., 2014



$$\nabla_{\theta} \mathbb{E}_{z \sim p(z;\theta)} \left[ f(z) \right] = \mathbb{E}_{\epsilon \sim p(\epsilon)} \left[ \nabla_{\theta} f(z(\epsilon;\theta)) \right]$$

e.g. 
$$z \sim \mathcal{N}(z; \mu, \sigma^2) \rightarrow z = \mu + \epsilon \cdot \sigma$$

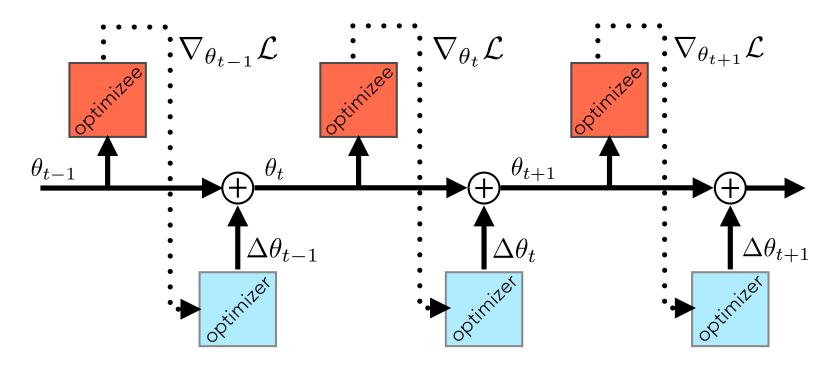
### learning to optimize

optimization is a **task**  $\Delta \theta = f(\theta, \nabla_{\theta} \mathcal{L})$ update estimate using current estimate and curvature

f is the <u>optimizer</u>

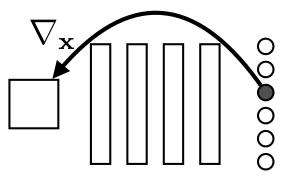
heta are the parameters of the <u>optimizee</u>

*learn* to perform optimization

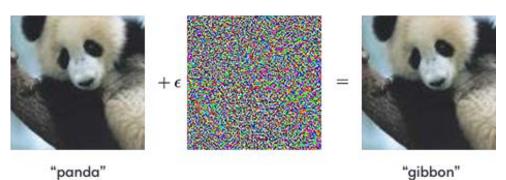


adversarial examples

current neural networks are susceptible to <u>adversarial</u> data examples: optimize the data *away* from correct output



data doesn't change qualitatively, yet is classified incorrectly



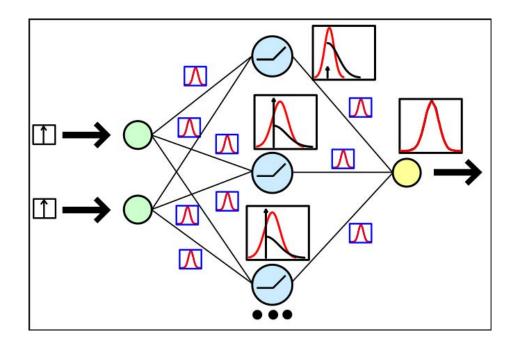
57.7% confidence

**"gibbon"** 99.3% confidence



Bayesian neural networks

maintain uncertainty in the network activations and/or weights



# place prior probabilities on these quantities

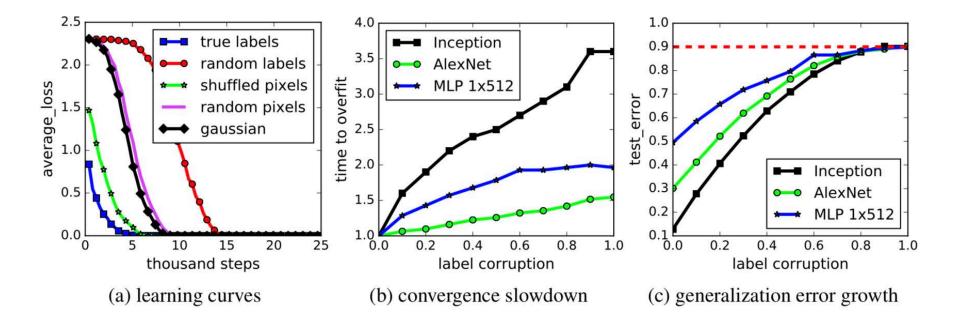
prevent overfitting in low-density data regions

### generalization

neural networks are incredibly flexible and can fit random noise

conventional wisdom of an abstract hierarchy of features may not hold

however, different learning behavior between fitting noise and data

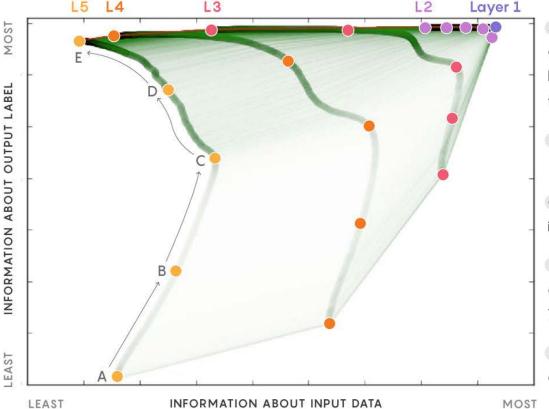


Understanding deep learning requires re-thinking generalization, Zhang et al., 2017

# information bottleneck

**information bottleneck theory**: maximize <u>mutual information</u> between the input and output while discarding all other input information

deep networks learn representations that compress the input while preserving the relevant information for predicting the output



A INITIAL STATE: Neurons in Layer 1 encode everything about the input data, including all information about its label. Neurons in the highest layers are in a nearly random state bearing little to no relationship to the data or its label.

**B** FITTING PHASE: As deep learning begins, neurons in higher layers gain information about the input and get better at fitting labels to it.

C PHASE CHANGE: The layers suddenly shift gears and start to "forget" information about the input.

**D COMPRESSION PHASE**: Higher layers compress their representation of the input data, keeping what is most relevant to the output label. They get better at predicting the label.

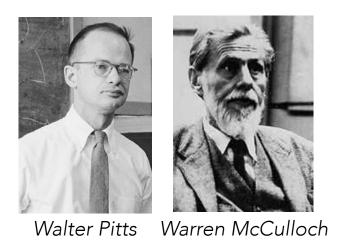
**E** FINAL STATE: The last layer achieves an optimal balance of accuracy and compression, retaining only what is needed to predict the label.

# PERSPECTIVE

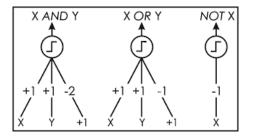
"Instead of trying to produce a program to simulate the adult mind, why not rather try to produce one which simulates the child's? If this were then subjected to an appropriate course of education one would obtain the adult brain."

-Alan Turing, 1950

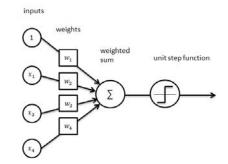




**1943** - McCulloch & Pitts introduce the Threshold Logic Unit to mimic a biological neuron



**1957** - Frank Rosenblatt introduces the Perceptron, with more flexible weights and a learning algorithm.





Frank Rosenblatt



**1969** - Minsky & Papert show that the perceptron is unable to learn the XOR function, essentially stopping all research on neural networks in the first *"Al winter."* 

Marvin Minksy Seymour Papert



**1982** - Hopfield introduces Hopfield networks, a type of recurrent network that is able to store auto-associative memory states.

**1985** - Sejnowski & Hinton provide a method of training restricted Boltzmann machines (RBMs), a type of unsupervised generative model.



Terry Sejnowski

Geoff Hinton



David Rumelhart



Hinton

Ronald Williams **1986** - Rumelhart, Hinton, and Williams introduce the backpropagation learning algorithm, which, in fact, had already been derived as early as 1960. Interest in neural networks increases as it is shown that non-linear functions can be learned.

**1989** - Yann LeCun introduces convolutional neural networks, which perform well on handwritten digit recognition.





1995 - Hochreiter & Schmidhuber introduce long short-term memory (LSTM), which uses gating mechanisms to read and write from a memory cell.

Sepp Jürgen Schmidhuber Hochreiter

**1995** - Hinton et al. introduce the Helmholtz machine, a generative model that uses a separate "inference model" to perform posterior inference, similar to modern autoencoders.





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Dayan

Radford Neal

Rich Zemel

**mid-1990s - mid-2000s** - Interest in neural networks fade, due to data and computational constraints as well as training difficulties (e.g. vanishing gradients). The field moves toward SVMs, kernel methods, etc. This is the second *"AI winter."* 



Geoff Hinton

Simon Yee Wh Osindero Teh

**2006** - Hinton et al. introduce a method for training deep belief networks through greedy layer-wise training. This work helps to ignite the move back to neural networks, which are rebranded as *"deep learning."* 

**mid-2000s - 2011** - Deep learning slowly begins to gain traction as methods, primarily for unsupervised pre-training of networks, are developed. Other techniques, such as non-saturating non-linearities, are introduced as well. Developments in hardware and software allow these models to be trained on GPUs, hugely speeding up the training process. However, *deep learning is not yet mainstream*.

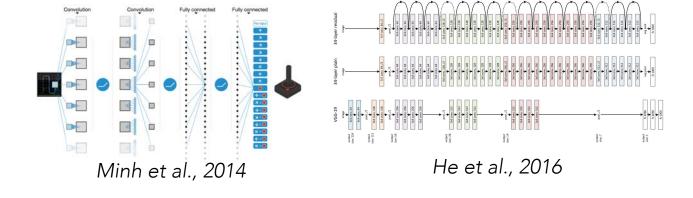


**2011, 2012** - Huge improvements on several machine learning benchmarks (speech recognition, computer vision) definitively show that deep learning outperforms other techniques for these tasks. The field grows enormously, dominating much of machine learning.

**2012 - ?** - Research in deep learning skyrockets as people join and new discoveries are made. New methods and discoveries make significant contributions to supervised learning, reinforcement learning, generative modeling, etc.



Goodfellow et al., 2014 Rezende et al., 2014 Kingma & Welling, 2014

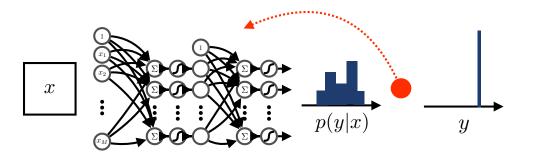


### we are in a golden era for research on neural networks

# big picture

# deep networks are **function approximators**

 parameterize conditional probability distributions

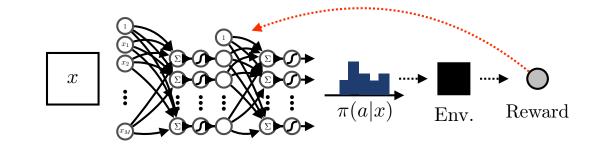


 $x \xrightarrow{y} \\ x_{2} \\ x_{3} \\ x_{4} \\ x_{5} \\ x_{$ 

most success has been in supervised learning

(fit the posterior of a latent variable using <u>labels</u>)

in deep (model-free) RL, can approximate an agent's <u>value function</u> or <u>policy</u>



### deep networks are a tool,

real progress depends on developing better learning algorithms



deep learning has allowed us to extend our learning algorithms to many new and relevant domains





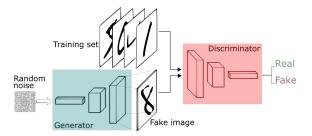


can learn more complex conditional probabilities

"hello"

### deep learning has also enabled the development of new learning algorithms

Generative Adversarial Networks (GANs)



big picture

### but many (human-relevant) tasks are unsolved

### progress depends on...



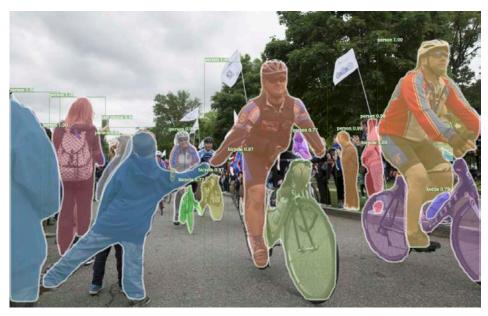
# looking forward

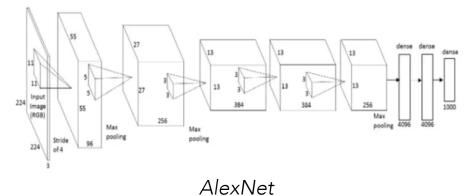
### deep learning in its current form may get replaced

$$x \longrightarrow p(y|x)$$

but only by something that allows us to more easily approximate more complex probability distributions

# NEXT TIME





Mask R-CNN

# convolutional neural networks

&

### recurrent neural networks

