Lecture 3: Basic Neural Networks: multi-layer neural networks

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Announcement

- Tutorial and TA office hour
  - Location & Tutorial & Office hour
  - Please vote on Piazza

- Quiz 1 results are out
  - Check with TAs if you have any question

- A1 will be out soon
  - Check with TAs
- Reference reading is listed at the end of lecture slides.

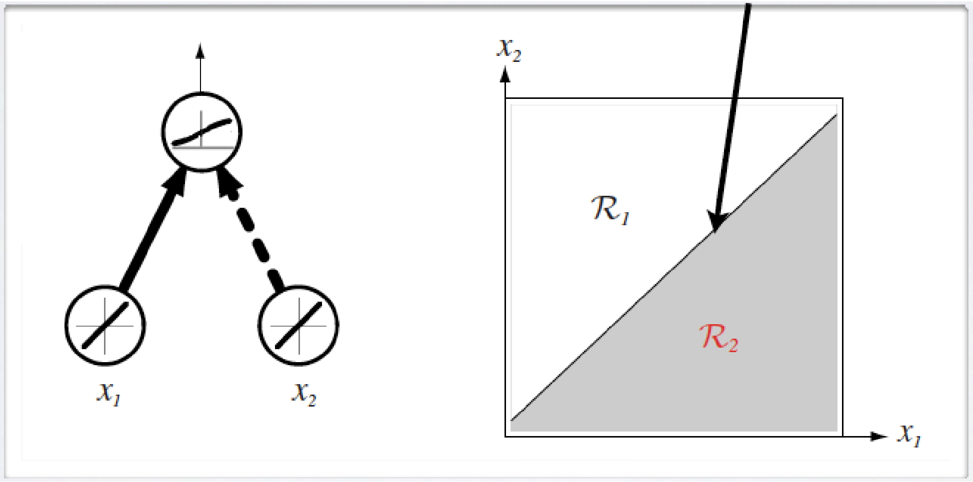
Outline

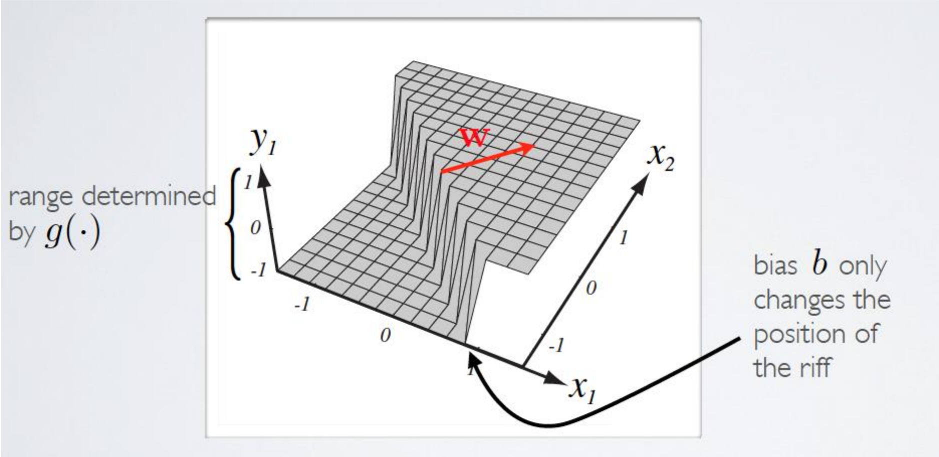
- Multi-layer neural networks
  - Limitations of single layer networks
  - Networks with single hidden layer
  - Sequential network architecture and variants
- Inference and learning
  - Forward and Backpropagation
  - Examples: one-layer network
  - General BP algorithm

Acknowledgement: Hugo Larochelle's, Mehryar Mohri@NYU's & Yingyu Liang@Princeton's course notes

Capacity of single neuron

- Binary classification
  - A neuron estimates $P(y = 1|\mathbf{x}) = \sigma(\mathbf{w}^\intercal \mathbf{x})$
  - Its decision boundary is linear, determined by its weights





Capacity of single neuron

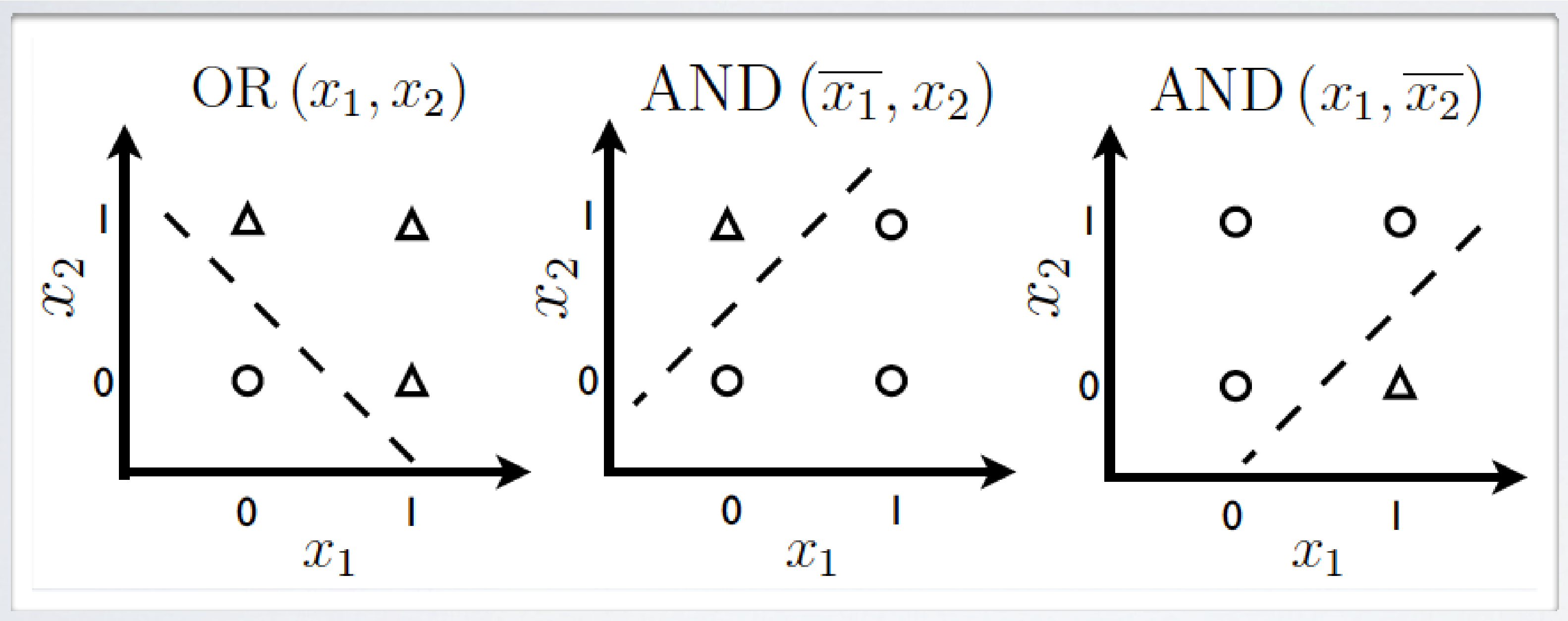
- Can solve linearly separable problems

$$\mathcal{D} = \mathcal{D}^+ \cup \mathcal{D}^-$$

$$\exists\ \mathbf{w}^*, \mathbf{w}^{*\mathsf{T}}\mathbf{x} > 0,\ \ \forall \mathbf{x} \in \mathcal{D}^+$$

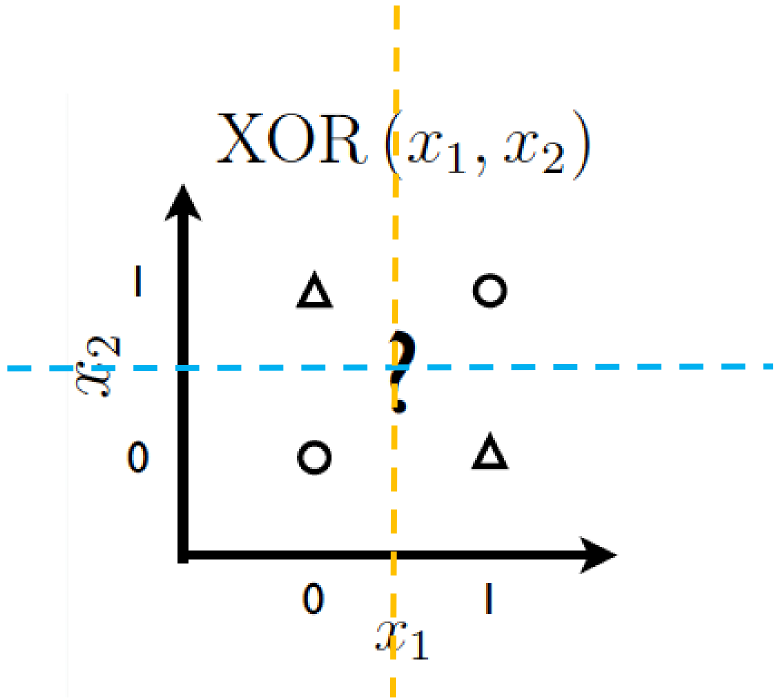
$$\mathbf{w}^{*\mathsf{T}}\mathbf{x} < 0,\ \ \forall \mathbf{x} \in \mathcal{D}^-$$

  - Examples



Capacity of single neuron

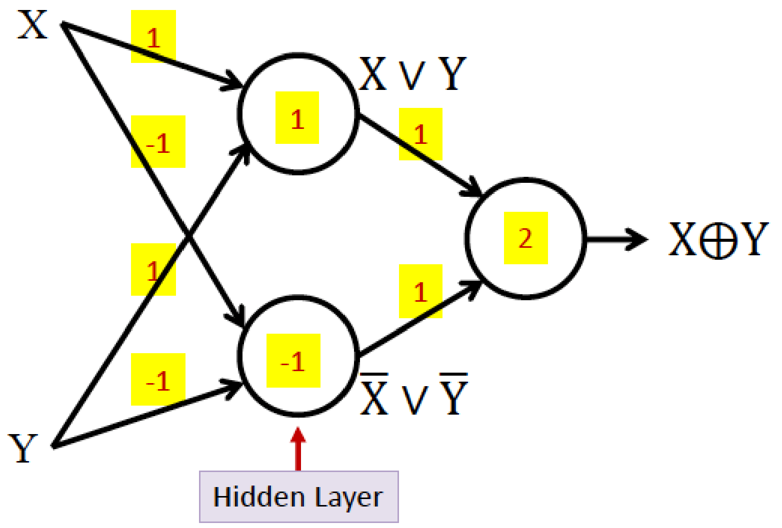
- Can't solve non linearly separable problems



- Can we use multiple neurons to achieve this?

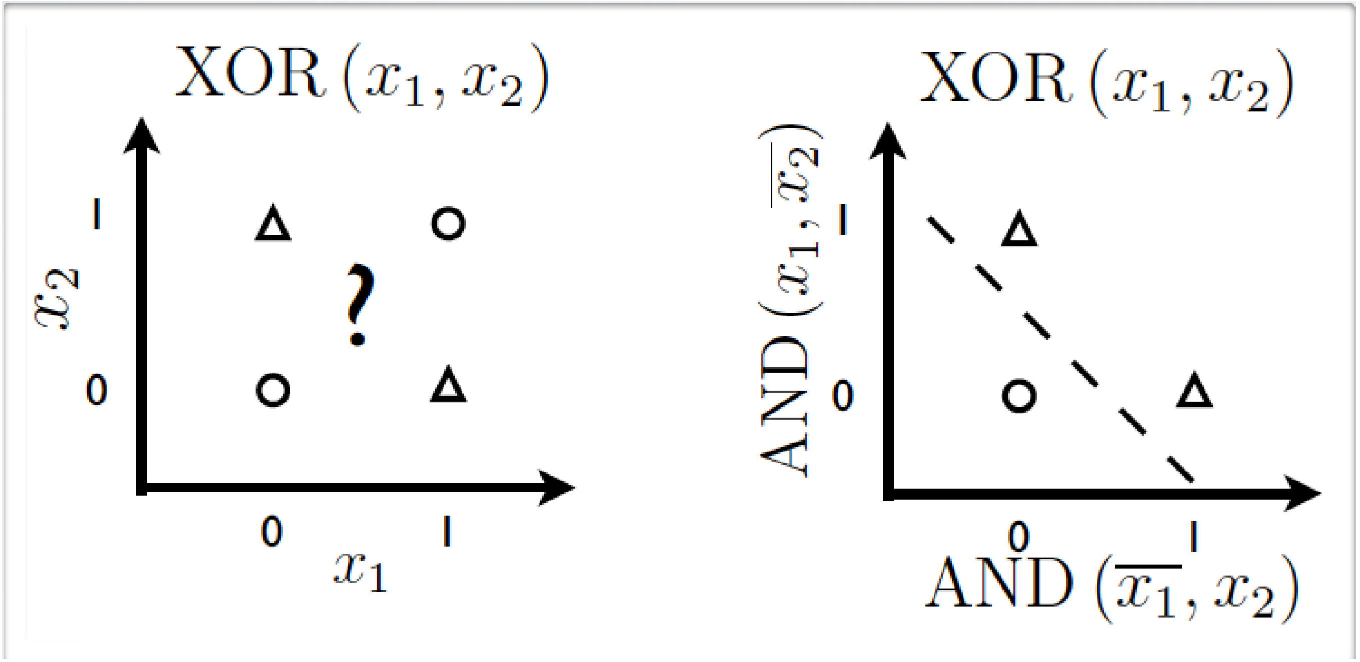
Capacity of single neuron

- Can't solve non linearly separable problems
- Unless the input is transformed in a better representation



Capacity of single neuron

- Can't solve non linearly separable problems



- Unless the input is transformed in a better representation

Adding one more layer

- Single hidden layer neural network
  - 2-layer neural network: ignoring input units

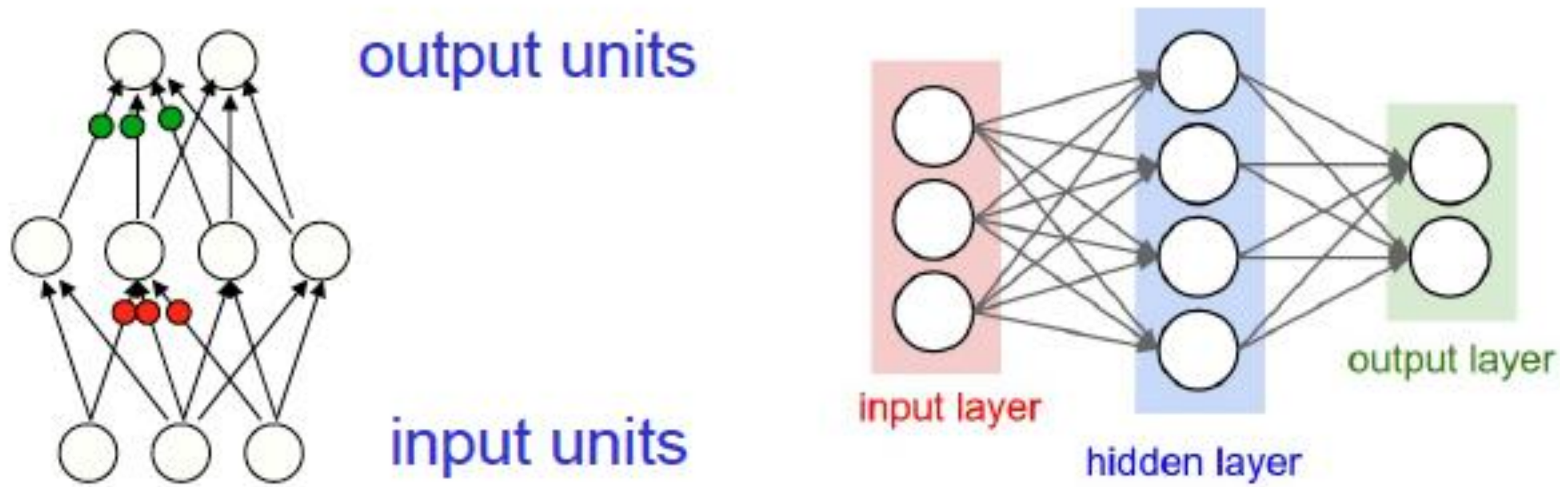
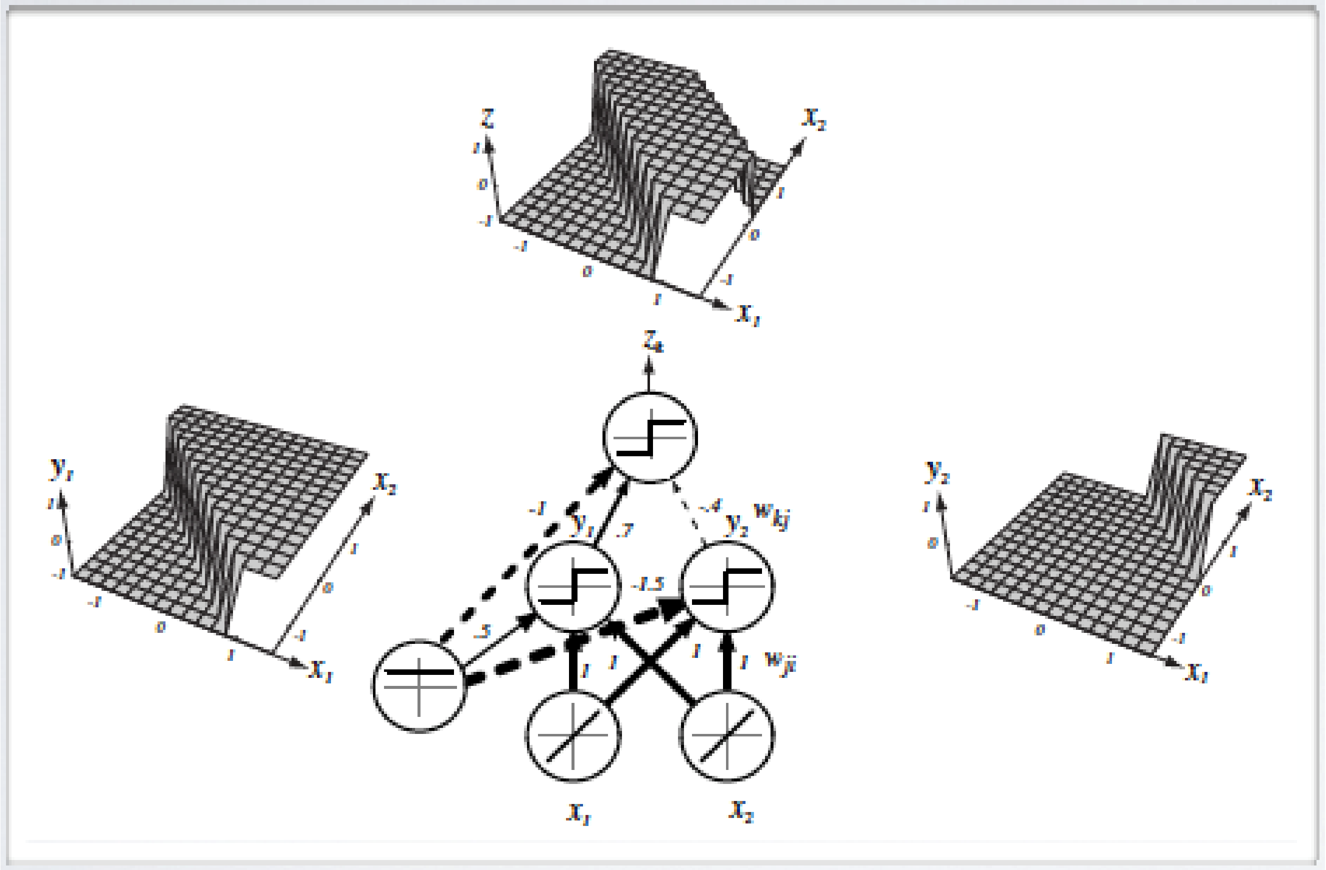


Figure : Two different visualizations of a 2-layer neural network. In this example: 3 input units, 4 hidden units and 2 output units

- Q: What if using linear activation in hidden layer?

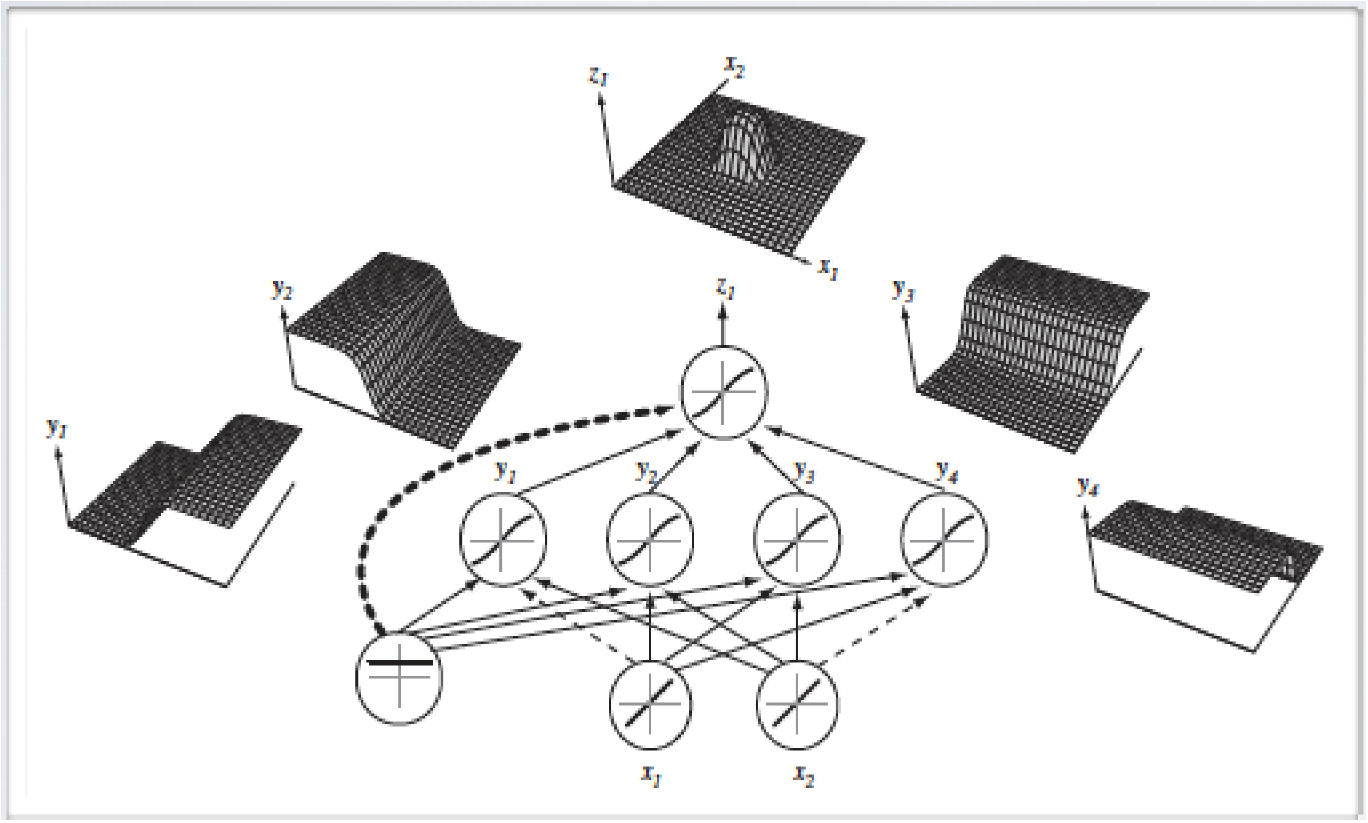
Capacity of neural network

- Single hidden layer neural network
  - Partition the input space into regions



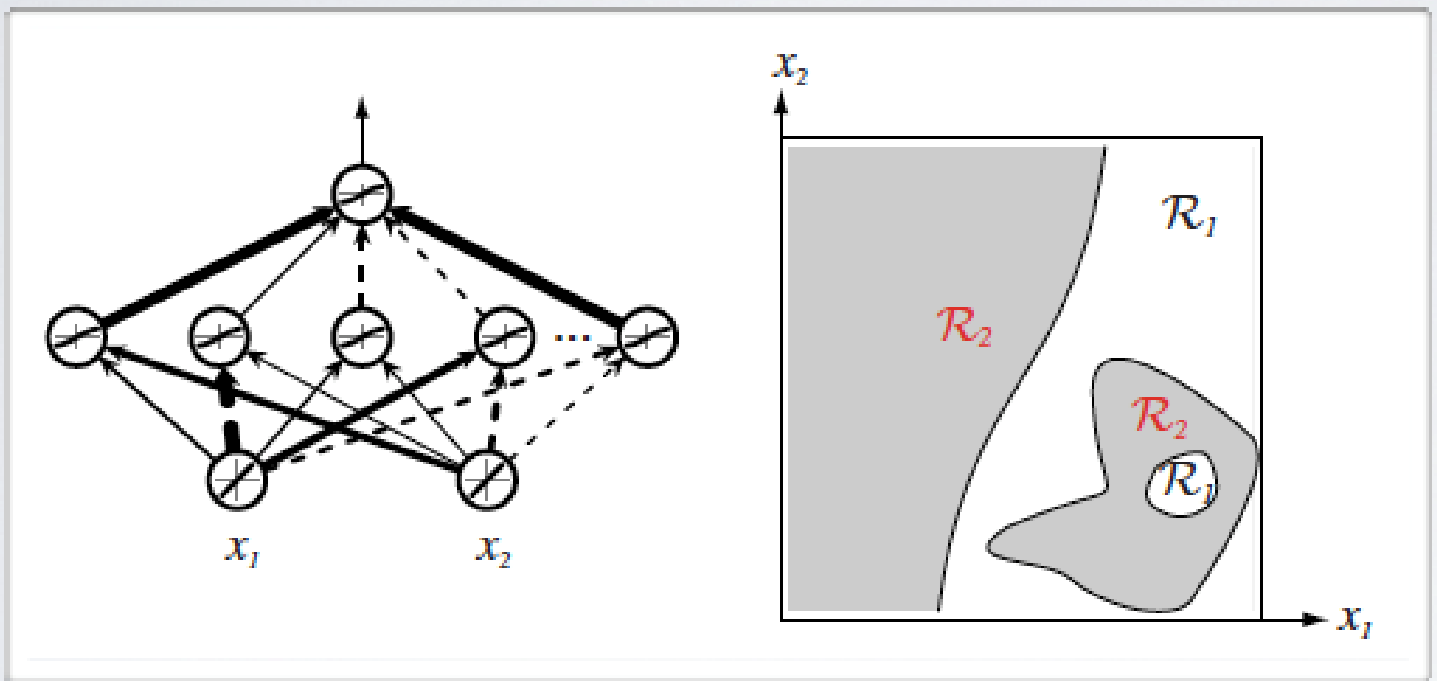
Capacity of neural network

- Single hidden layer neural network
  - Form a stump/delta function



Capacity of neural network

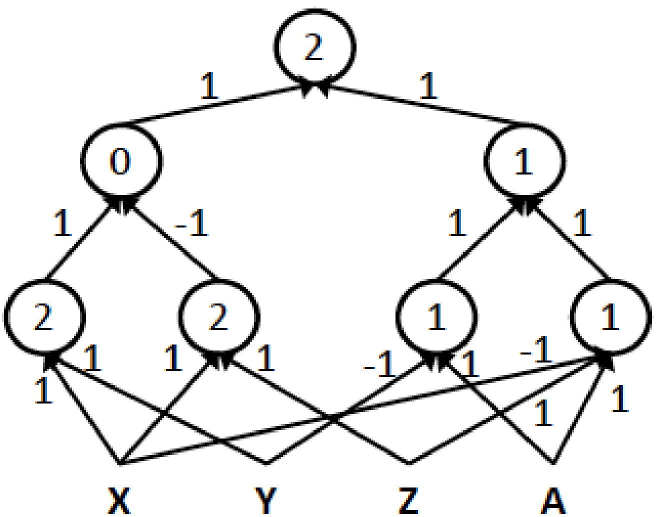
- Single hidden layer neural network



Multi-layer perceptron

- Boolean case
  - Multilayer perceptrons (MLPs) can compute more complex Boolean functions
  - MLPs can compute ***any*** Boolean function
    - Since they can emulate individual gates
  - MLPs are *universal Boolean functions*

$$((A\&\bar{X}\&Z)|(A\&\bar{Y}))\&((X\ \&\ Y)|\overline{(X\&Z)})$$



Capacity of neural network

- Universal approximation
  - Theorem (Hornik, 1991)

    A single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units.
  - The result applies for sigmoid, tanh and many other hidden layer activation functions

- Caveat: good result but not useful in practice
  - How many hidden units?
  - How to find the parameters by a learning algorithm?

General neural network

- Multi-layer neural network

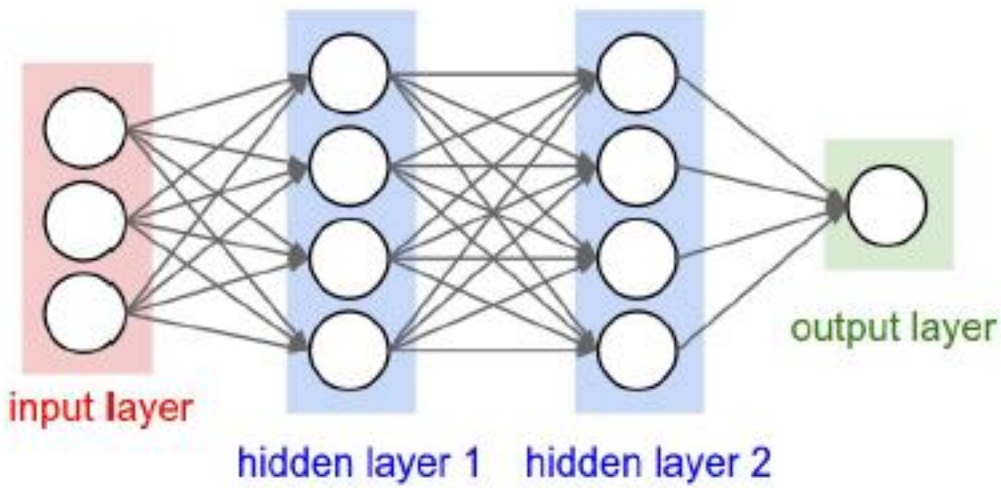
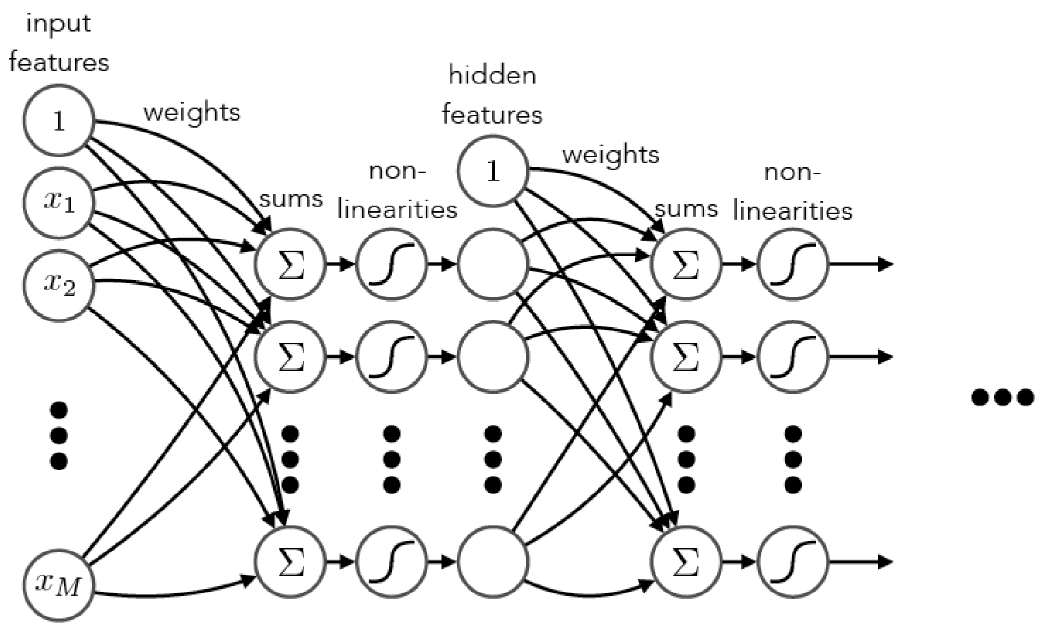


Figure : A 3-layer neural net with 3 input units, 4 hidden units in the first and second hidden layer and 1 output unit

- Naming conventions; a N-layer neural network:
  - $N-1$ layers of hidden units
  - One output layer

Multilayer networks



network: *sequence of parallelized weighted sums and non-linearities*

DEFINE $\mathbf{x}^{(0)} \equiv \mathbf{x}$, $\mathbf{x}^{(1)} \equiv \mathbf{h}$, ETC.

1st layer

$$\mathbf{s}^{(1)} = \mathbf{W}^{(1)\intercal}\mathbf{x}^{(0)}$$

$$\mathbf{x}^{(1)} = \sigma(\mathbf{s}^{(1)})$$

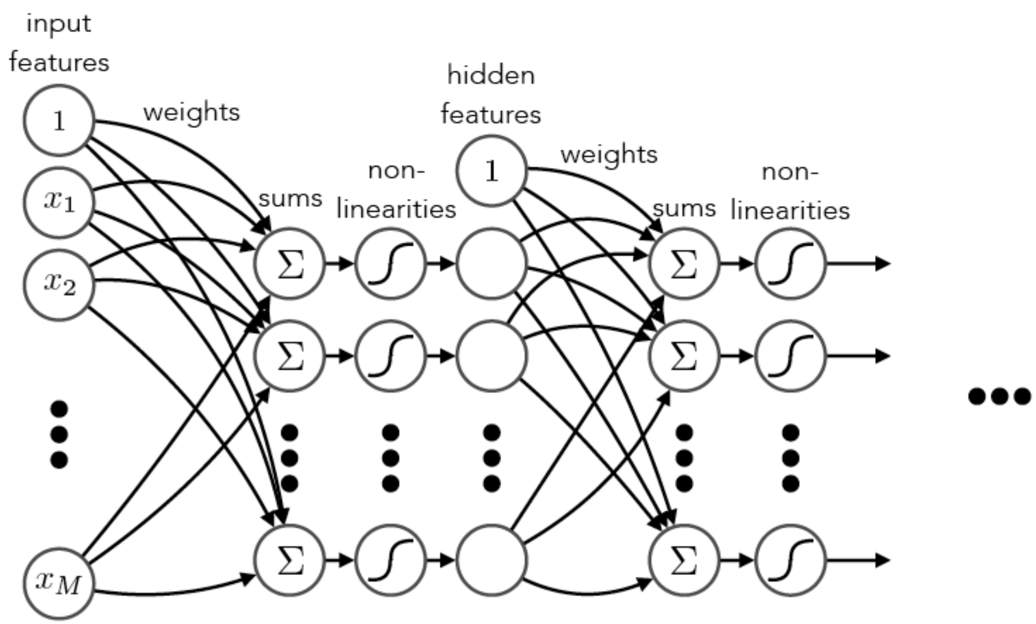
2nd layer

$$\mathbf{s}^{(2)} = \mathbf{W}^{(2)\intercal}\mathbf{x}^{(1)}$$

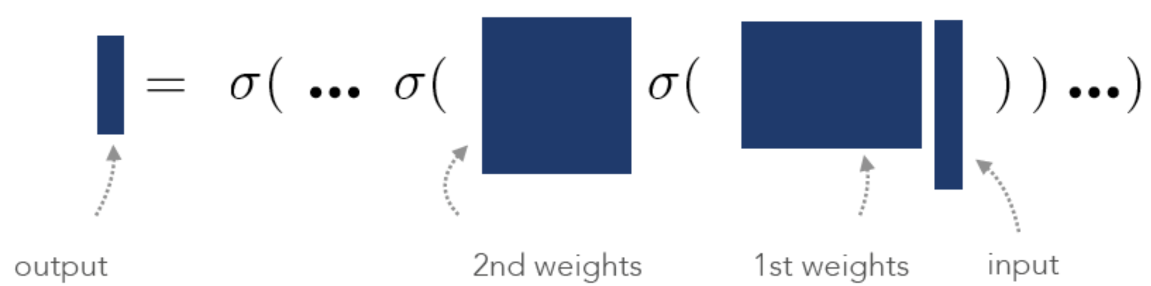
$$\mathbf{x}^{(2)} = \sigma(\mathbf{s}^{(2)})$$

•••

Multilayer networks

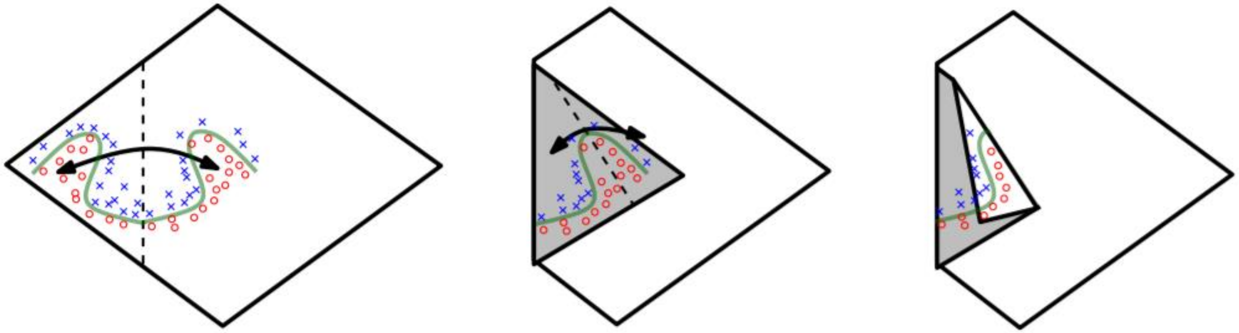


network: *sequence of parallelized weighted sums and non-linearities*



Why more layers (deeper)?

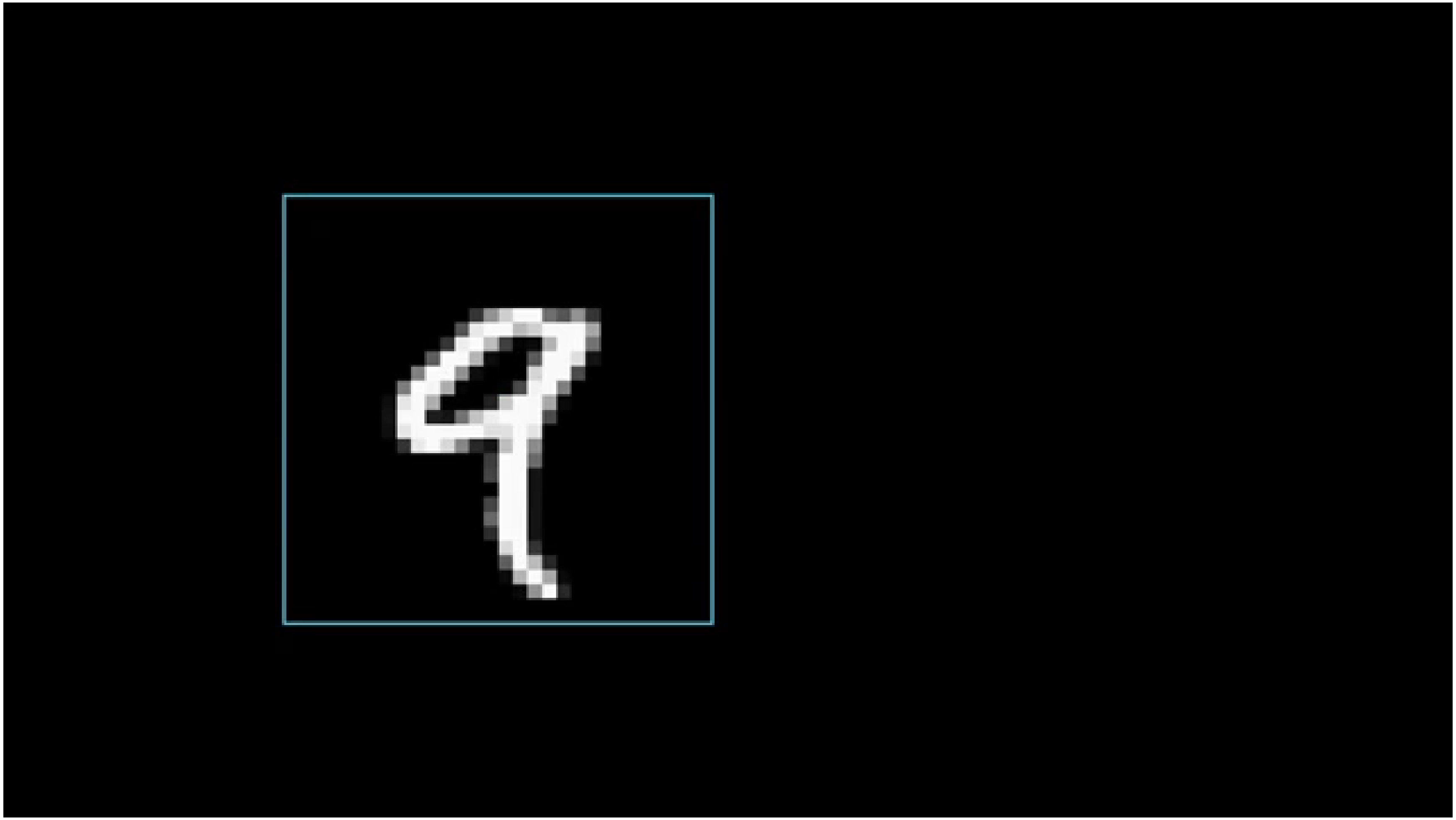
- A deep architecture can represent certain functions more compactly
  - (Montufar et al., NIPS'14)
    - Functions representable with a deep rectifier net can require an exponential number of hidden units with a shallow one.



Why more layers (deeper)?

- A deep architecture can represent certain functions more compactly
  - Example: Boolean functions
    - There are Boolean functions which require an exponential number of hidden units in the single layer case
    - require a polynomial number of hidden units if we can adapt the number of layers
  - Example: multivariate polynomials (Rolnick & Tegmark, ICLR'18)
    - Total number of neurons m required to approximate natural classes of multivariate polynomials of n variables
    - grows only linearly with n for deep neural networks, but grows exponentially when merely a single hidden layer is allowed.

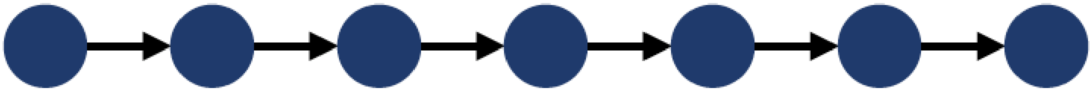
Why more layers (deeper)?



https://youtu.be/aircAruvnKk?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi

Other network connectivity

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

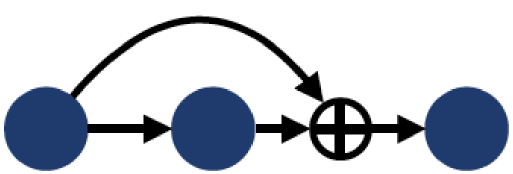


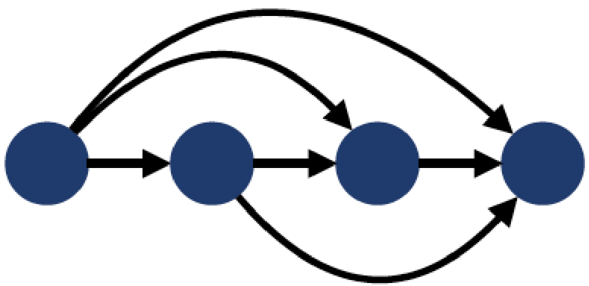
information may not be able to propagate easily

→ *make shorter paths to output*

residual & highway connections

dense (concatenated) connections

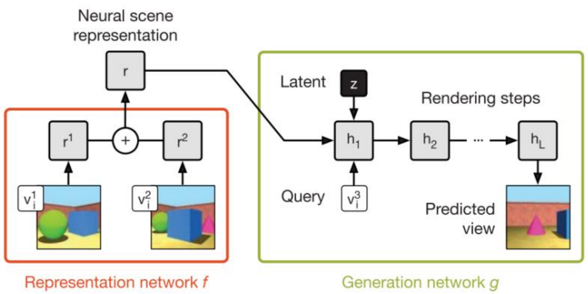




Deep residual learning for image recognition, He et al., 2016
Highway networks, Srivastava et al., 2015

Densely connected convolutional networks, Huang et al., 2017

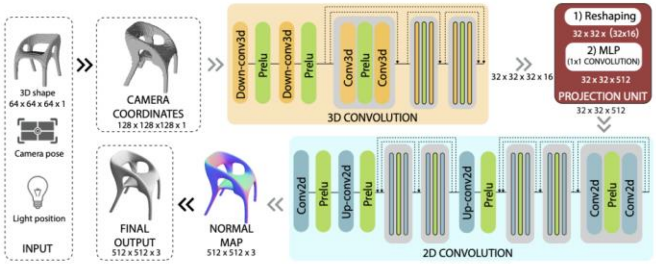
Modern MLP as Implicit Representation



Generative Query Networks
[Eslami et al. 2018]

[Flynn et al., 2016; Zhou et al., 2018b;
Mildenhall et al. 2019]

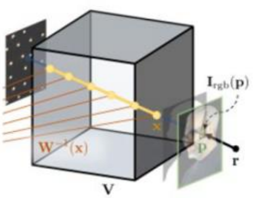
Multiplane Images (MPIs)



RenderNet [Nguyen-Phuoc et al. 2018]

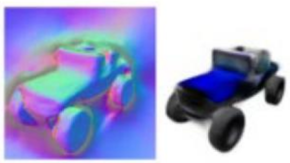
Voxel Grids + CNN decoder

DeepVoxels
[Sitzmann et al. 2019]

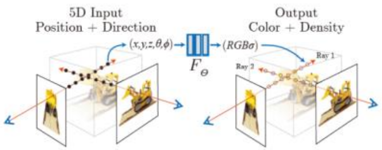


Neural Volumes
[Lombardi et al. 2019]

Voxel Grids + Ray Marching



SRN
[Sitzmann et al. 2019b]



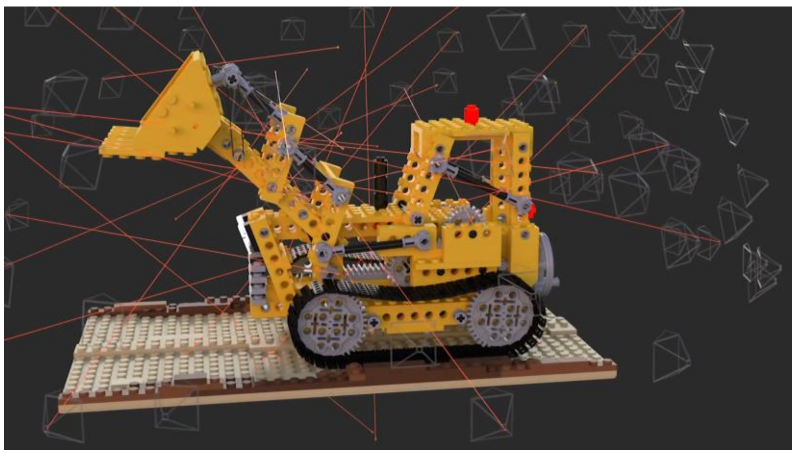
NeRF
[Mildenhall et al. 2020]

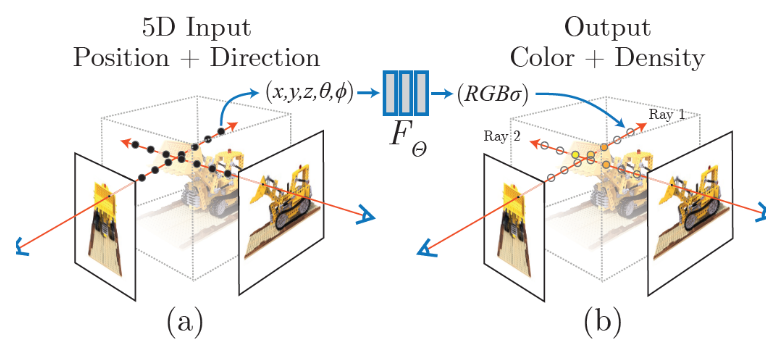
IDR
[Yariv et al. 2020]

Implicit Fields

Modern MLP in NeRF

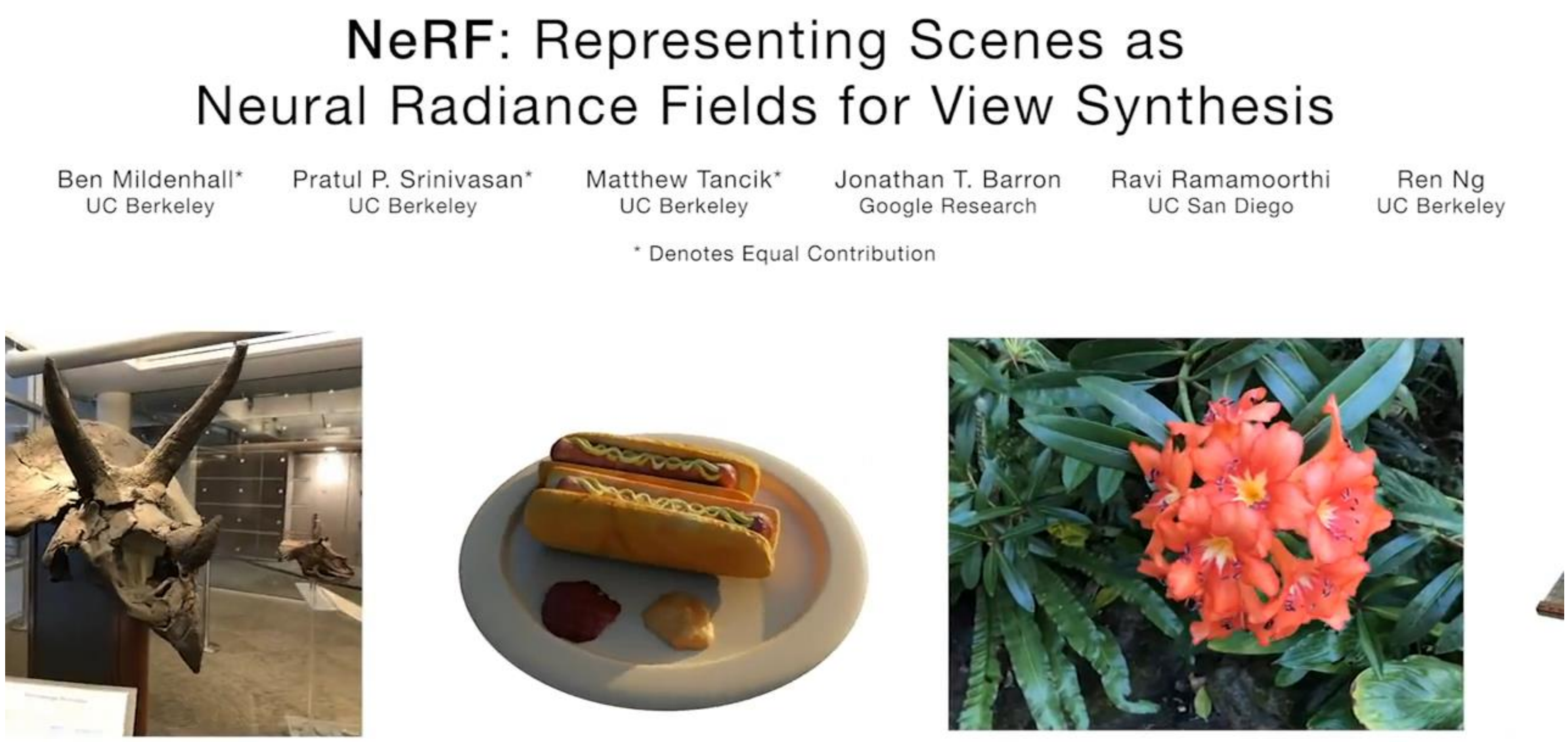
- - Color + Density
- Positional Encoding
- Volume Rendering





Representing Scenes as Neural Radiance Fields for View Synthesis, Mildenhall et al., *ECCV 2020 Oral - Best Paper Honorable Mention*

Modern MLP in NeRF



https://youtu.be/JuH79E8rdKc

Outline

- Multi-layer neural networks
  - Limitations of single layer networks
  - Neural networks with single hidden layer
  - Sequential network architecture and variants
- Inference and learning
  - Forward and Backpropagation
  - Examples: one-layer network
  - General BP algorithm

Computation in neural network

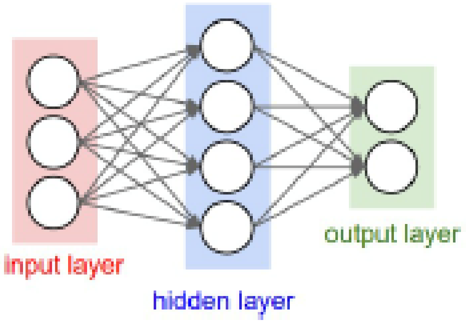
- We only need to know two algorithms
  - Inference/prediction: simply forward pass
  - Parameter learning: needs backward pass
- Basic fact:
  - A neural network is a function of composed operations

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

  - All the f functions are linear + (simple) nonlinear (differentiable a.e.) operators

Inference example: Forward Pass

- What does the network compute?



- Output of the network can be written as:

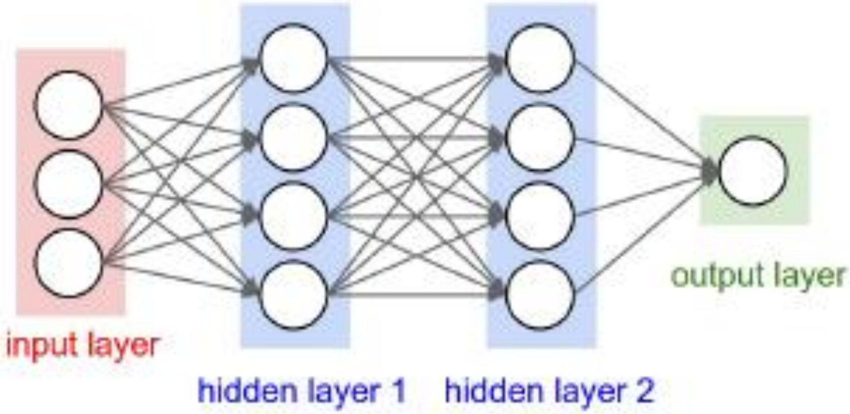
$$h_j(\mathbf{x}) = f(v_{j0} + \sum_{i=1}^{D} x_i v_{ji})$$

$$o_k(\mathbf{x}) = g(w_{k0} + \sum_{j=1}^{J} h_j(\mathbf{x}) w_{kj})$$

(j indexing hidden units, k indexing the output units, D number of inputs)

Forward Pass in Python

- Example code for a forward pass for a 3-layer network in Python:




```
# 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)
```

- Can be implemented efficiently using matrix operations

Parameter learning: Backward Pass

- Supervised learning framework
  - Find weights:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{n=1}^{N} \operatorname{loss}(\mathbf{o}^{(n)}, \mathbf{t}^{(n)})$$

    where $\mathbf{o} = f(\mathbf{x}; \mathbf{w})$ is the output of a neural network

  - Define a loss function, eg:
    - Squared loss: $\sum_k \frac{1}{2}(o_k^{(n)} - t_k^{(n)})^2$
    - Cross-entropy loss: $-\sum_k t_k^{(n)} \log o_k^{(n)}$
  - Gradient descent:

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{\partial E}{\partial \mathbf{w}^t}$$

    where η is the learning rate (and E is error/loss)

Backward pass

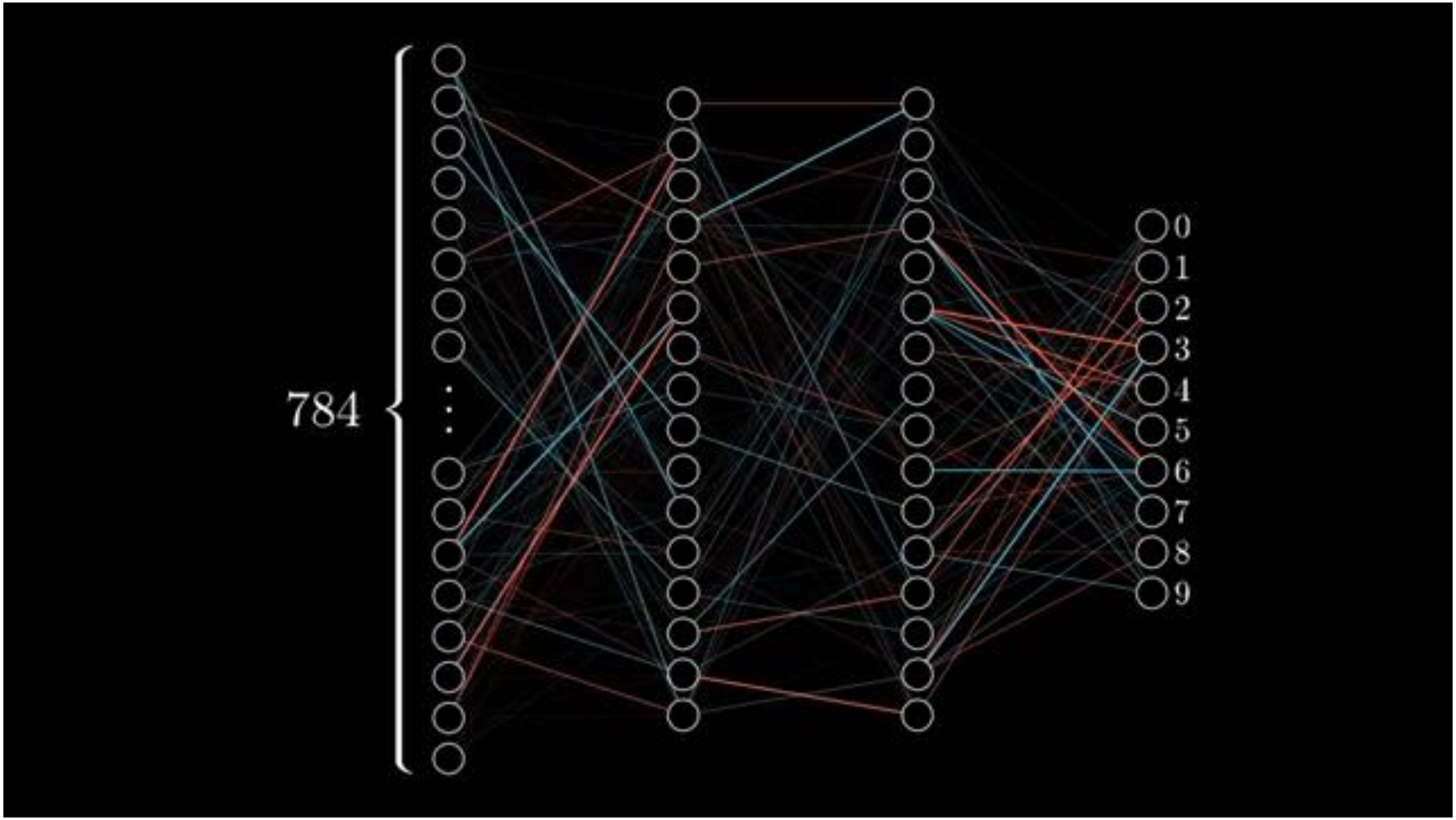
- Backpropagation
  - An efficient method for computing gradients in NNs
  - A neural network as a function of composed operations

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

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

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

Backward pass



https://www.youtube.com/watch?v=Ilg3gGewQ5U

Gradient descent iteration

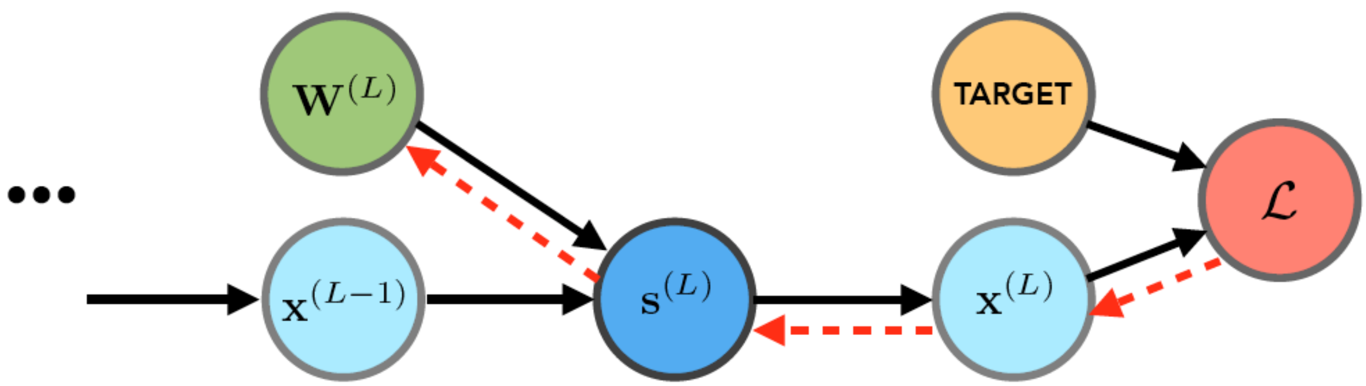
- Forward pass

1st layer	2nd layer		Loss
$\mathbf{s}^{(1)} = \mathbf{W}^{(1)\intercal}\mathbf{x}^{(0)}$	$\mathbf{s}^{(2)} = \mathbf{W}^{(2)\intercal}\mathbf{x}^{(1)}$	•••	$\mathcal{L}$
$\mathbf{x}^{(1)} = \sigma(\mathbf{s}^{(1)})$	$\mathbf{x}^{(2)} = \sigma(\mathbf{s}^{(2)})$		

- Backward pass

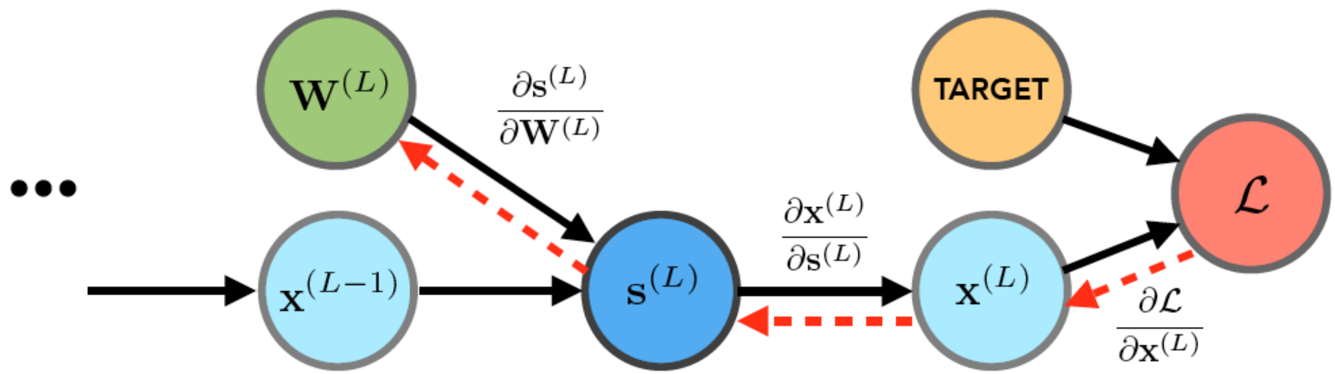
calculate $\nabla_{W^{(1)}}\mathcal{L}, \nabla_{W^{(2)}}\mathcal{L}, \ldots$ let's start with the final layer: $\nabla_{W^{(L)}}\mathcal{L}$

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



Gradient descent iteration

- Backward pass



$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{W}^{(L)}}$$

depends on the form of the loss

derivative of the non-linearity

$$\frac{\partial}{\partial \mathbf{W}^{(L)}} (\mathbf{W}^{(L)\intercal} \mathbf{x}^{(L-1)}) = \mathbf{x}^{(L-1)\intercal}$$

The order needs to be reversed for Jacobians! See LN04 for details

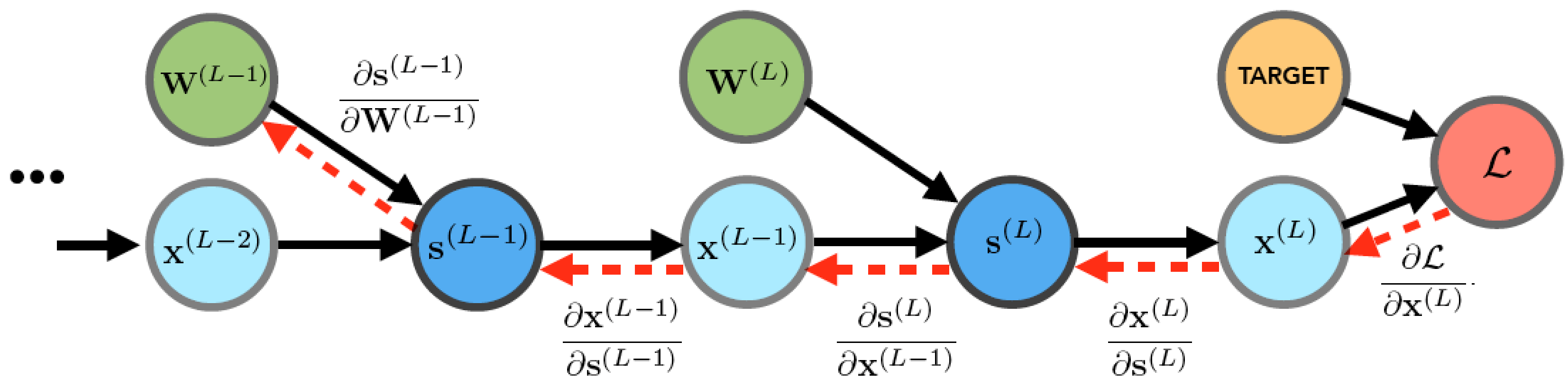
note $\nabla_{\mathbf{W}^{(L)}} \mathcal{L} \equiv \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$ is notational convention

Gradient descent iteration

- Backward pass

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

again we'll draw the dependency graph:

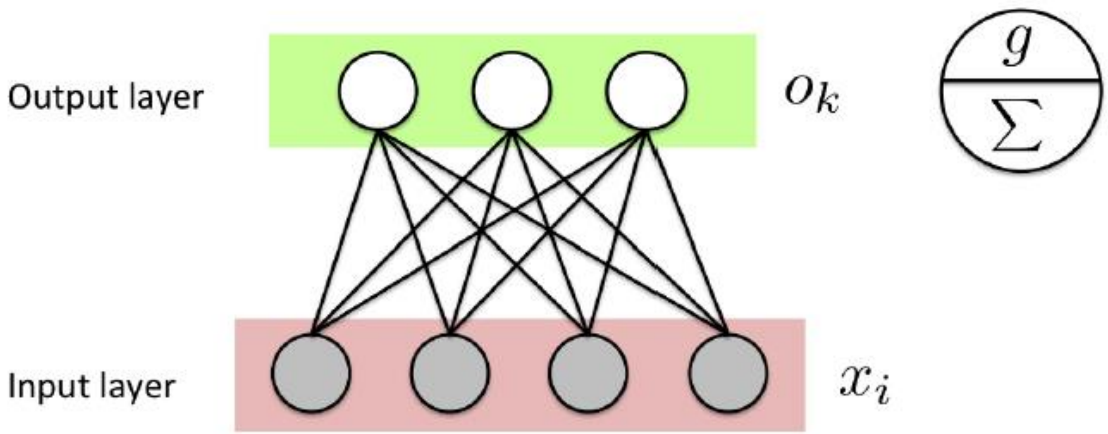


$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{x}^{(L-1)}} \frac{\partial \mathbf{x}^{(L-1)}}{\partial \mathbf{s}^{(L-1)}} \frac{\partial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

The order needs to be reversed for Jacobians! See LN04 for details

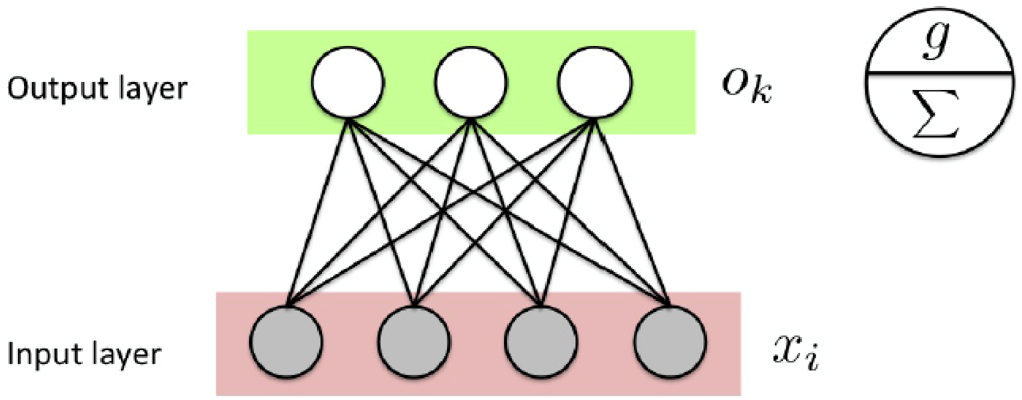
Example: Single Layer Network

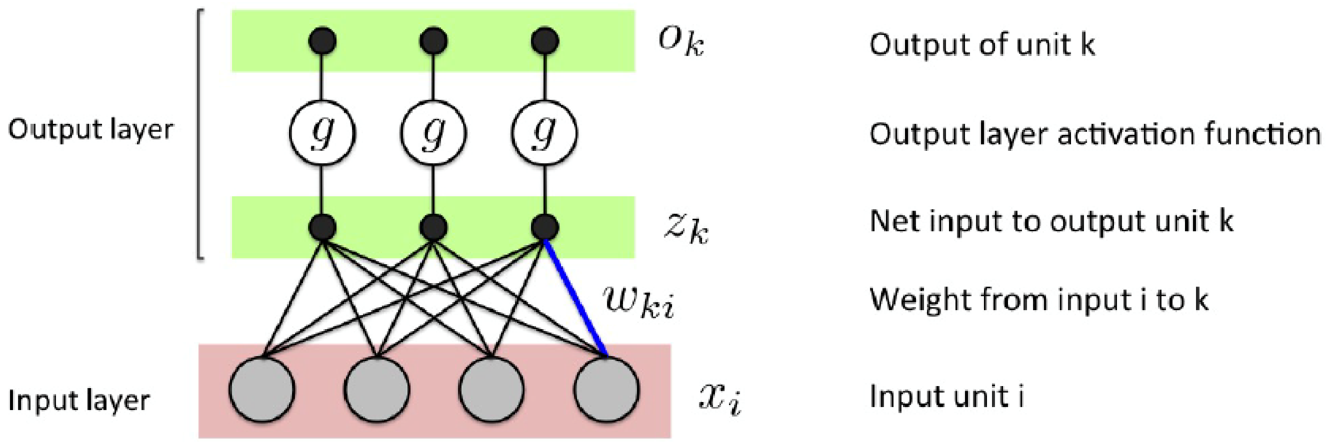
- Let's take a single layer network



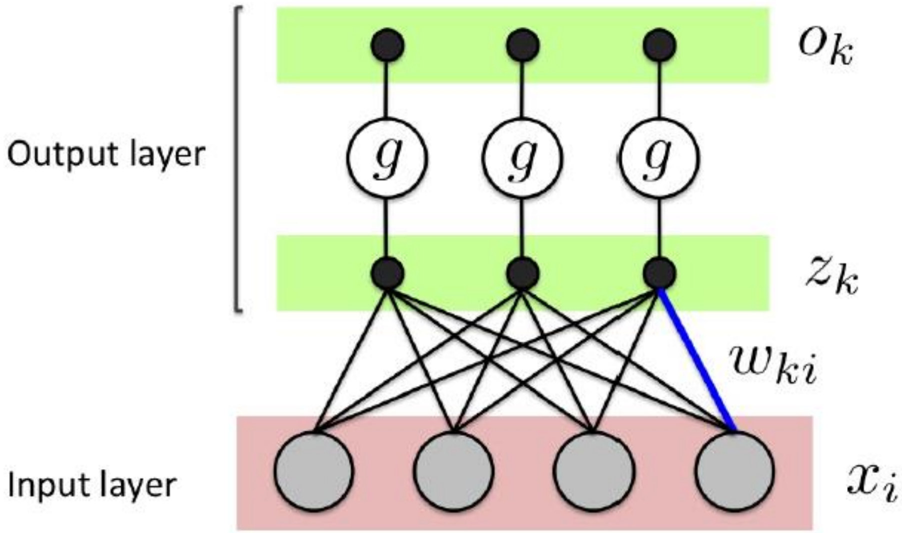
Example: Single Layer Network

- Let's take a single layer network and draw it a bit differently





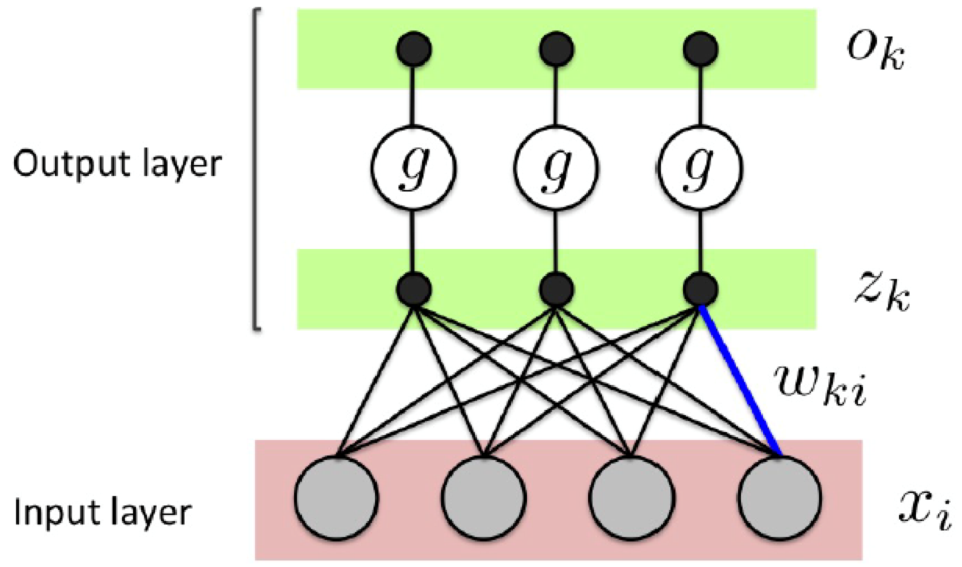
Example: Single Layer Network



- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} =$$

Example: Single Layer Network

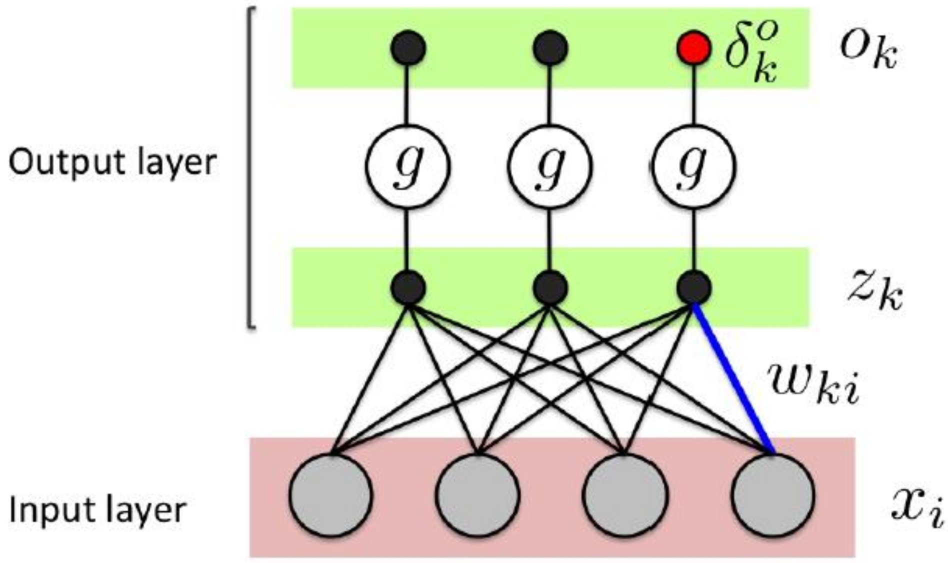


- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k} \frac{\partial o_k}{\partial z_k} \frac{\partial z_k}{\partial w_{ki}}$$

- Error gradient is computable for any continuous activation function $g()$, and any continuous error function

Example: Single Layer Network

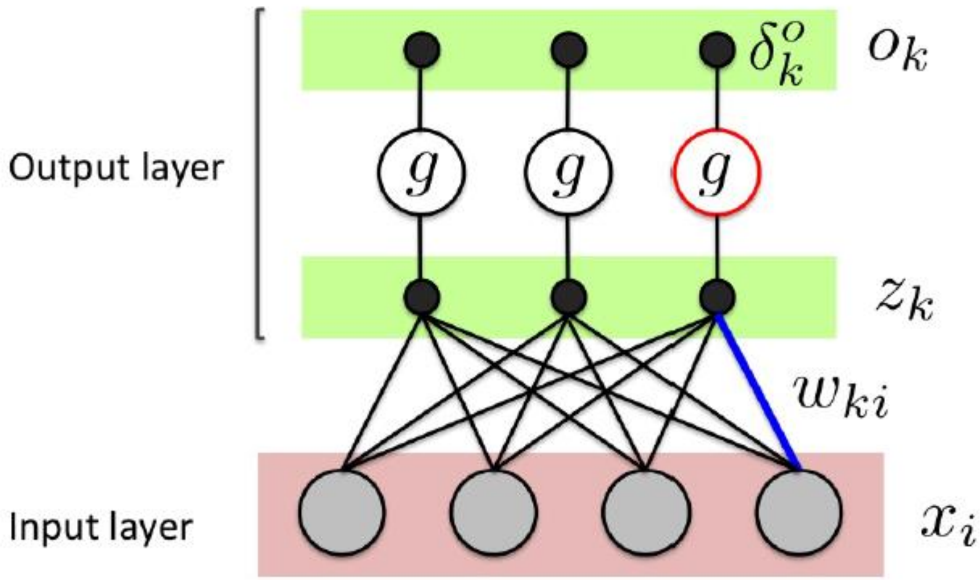


$$\delta_k^o = \frac{\partial E}{\partial o_k}$$

- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \underbrace{\frac{\partial E}{\partial o_k}}_{\delta_k^o} \frac{\partial o_k}{\partial z_k} \frac{\partial z_k}{\partial w_{ki}}$$

Example: Single Layer Network

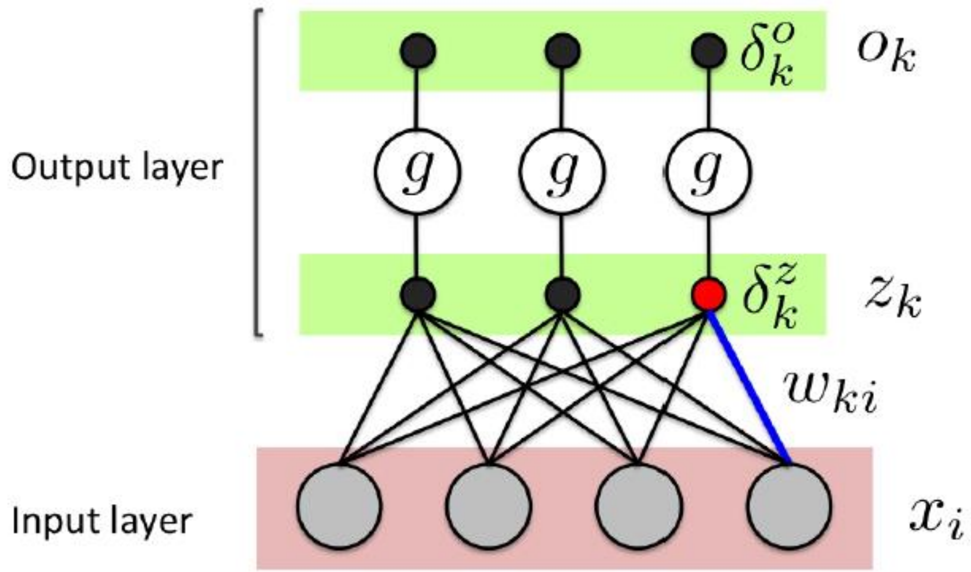


$$\frac{\partial o_k}{\partial z_k}$$

- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial z_k}\frac{\partial z_k}{\partial w_{ki}} = \delta_k^o \frac{\partial o_k}{\partial z_k}\frac{\partial z_k}{\partial w_{ki}}$$

Example: Single Layer Network

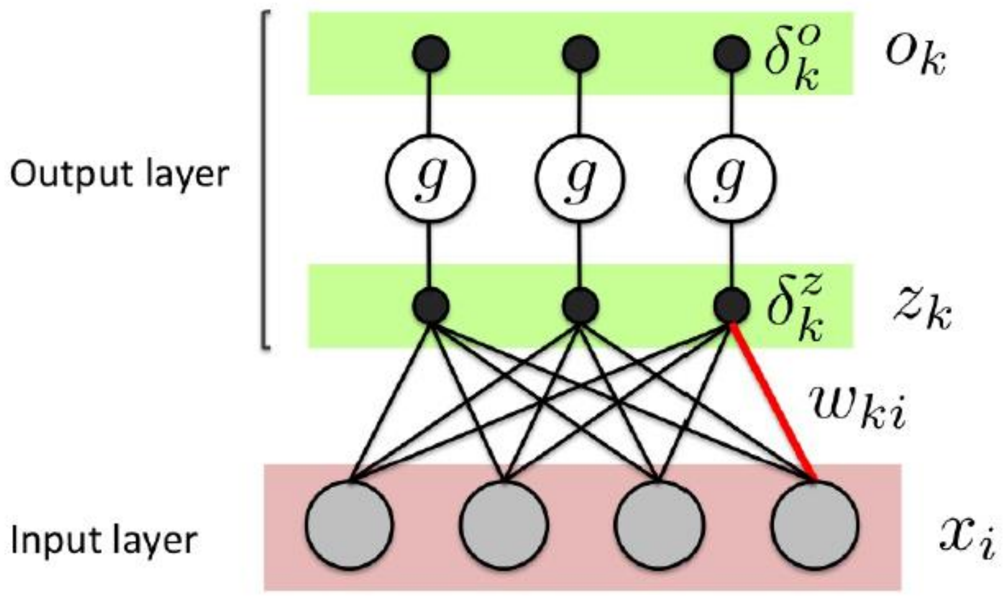


$$\delta_k^z = \delta_k^o \cdot \frac{\partial o_k}{\partial z_k}$$

- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial z_k}\frac{\partial z_k}{\partial w_{ki}} = \underbrace{\delta_k^o \cdot \frac{\partial o_k}{\partial z_k}}_{\delta_k^z}\frac{\partial z_k}{\partial w_{ki}}$$

Example: Single Layer Network



$$\frac{\partial z_k}{\partial w_{ki}}$$

- Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k}\frac{\partial o_k}{\partial z_k}\frac{\partial z_k}{\partial w_{ki}} = \delta_k^z \frac{\partial z_k}{\partial w_{ki}} = \delta_k^z \cdot x_i$$

Outline

- Multi-layer neural networks
  - Limitations of single layer networks
  - Neural networks with single hidden layer
  - Sequential network architecture and variants
- Inference and learning
  - Forward and Backpropagation
  - Examples: one-layer network
  - General BP algorithm

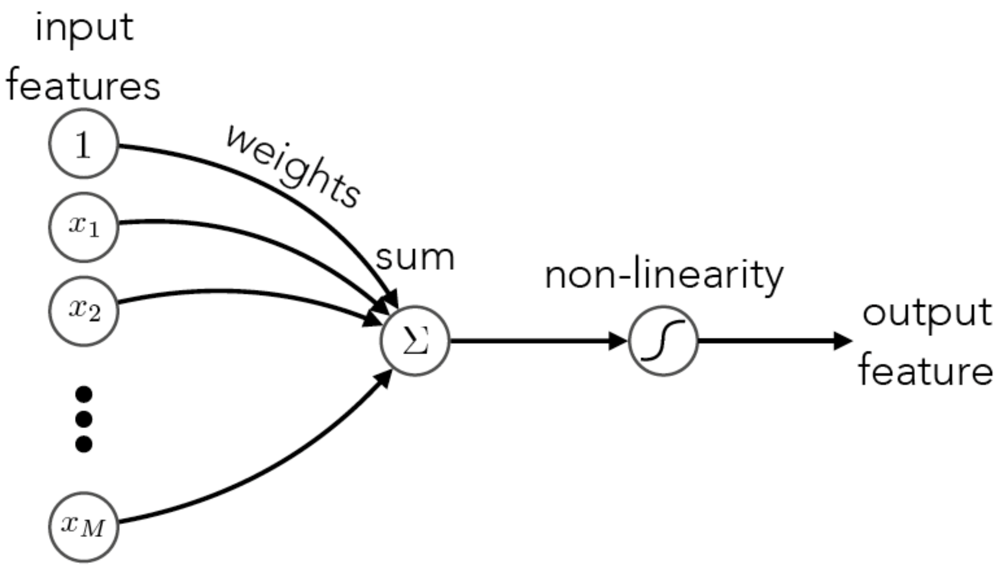
An implementation perspective

- Example: Univariate logistic least square model

$$s = wx + b$$

$$y = \sigma(s)$$

$$\mathcal{L} = \frac{1}{2}(y - t)^2$$



Univariate chain rule

- A structured way to implement it
  - The goal is to write a program that efficiently computes the derivatives

Computing the loss:

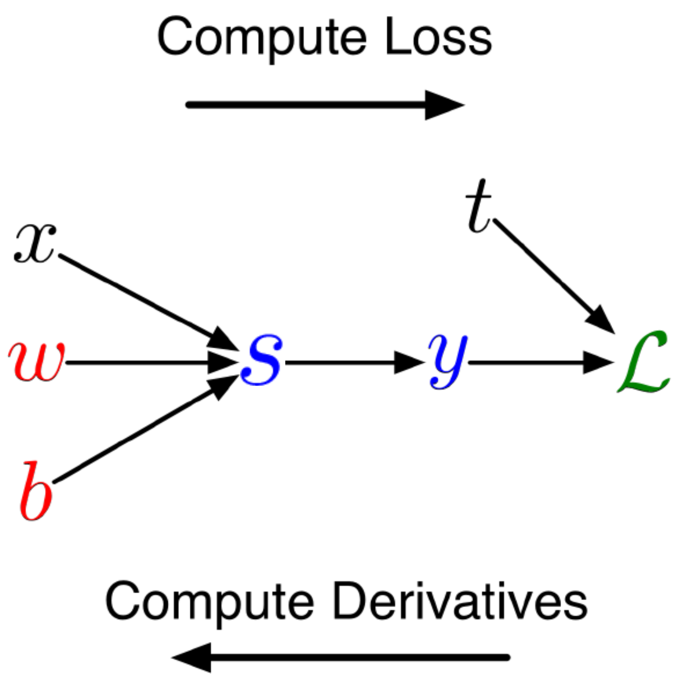
$$s = wx + b$$
$$y = \sigma(s)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Computing the derivatives:

$$\frac{d\mathcal{L}}{dy} = y - t$$
$$\frac{d\mathcal{L}}{ds} = \frac{d\mathcal{L}}{dy}\sigma'(s)$$
$$\frac{d\mathcal{L}}{dw} = \frac{d\mathcal{L}}{ds}x$$
$$\frac{d\mathcal{L}}{db} = \frac{d\mathcal{L}}{ds}$$

Computation graph

- Represent the computations using a computation graph
  - Nodes: inputs & computed quantities
  - Edges: which nodes are computed directly as function of which other nodes



Univariate chain rule

- A shorthand notation
  - Use $\delta_y := d\mathcal{L}/dy$, called the error signal
  - Note that the error signals are values computed by the program

Computing the loss:

$$s = wx + b$$

$$y = \sigma(s)$$

$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

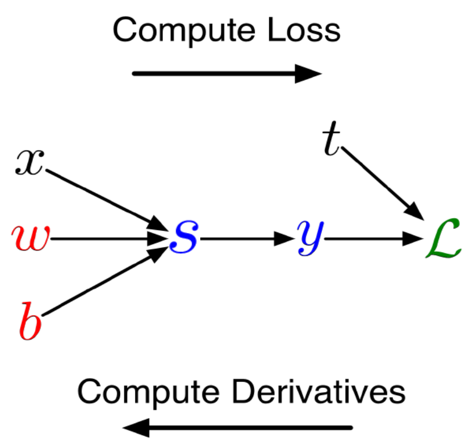
Computing the derivatives:

$$\delta_y = y - t$$

$$\delta_s = \delta_y \sigma'(s)$$

$$\delta_w = \delta_s x$$

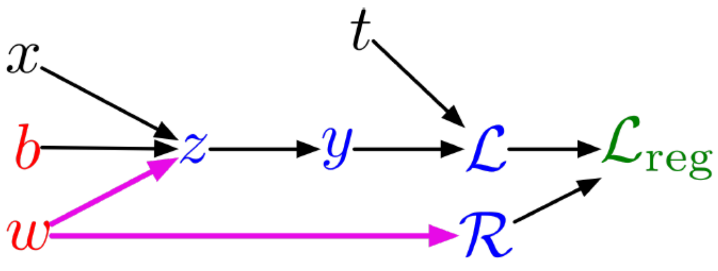
$$\delta_b = \delta_s$$



Multivariate chain rule

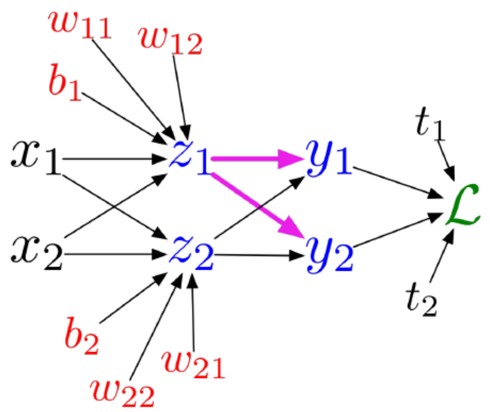
- The computation graph has fan-out > 1

L_2-Regularized regression



$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$
$$\mathcal{R} = \frac{1}{2}w^2$$
$$\mathcal{L}_{\mathrm{reg}} = \mathcal{L} + \lambda\mathcal{R}$$

Multiclass logistic regression



$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$
$$\mathcal{L} = -\sum t_k \log y_k$$

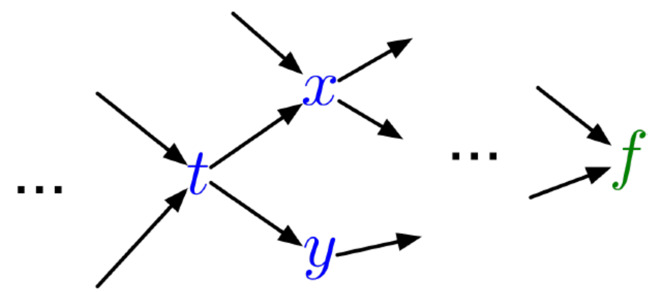
Multivariable chain rule

- Recall the distributed chain rule

Mathematical expressions
to be evaluated

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Values already computed
by our program



- The shorthand notation:

$$\delta_t = \delta_x \frac{dx}{dt} + \delta_y \frac{dy}{dt}$$

General Backpropagation

- Given a computation graph

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss)

forward pass

For $i = 1, \ldots, N$

Compute v_i as a function of $\mathrm{Pa}(v_i)$

backward pass

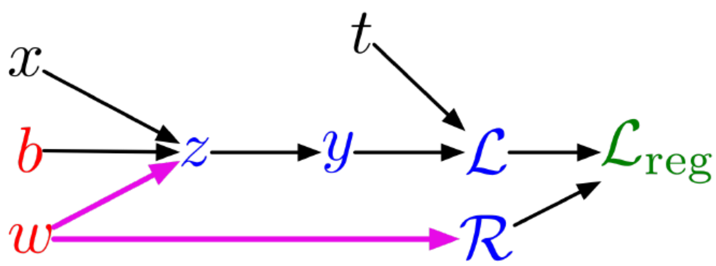
$\delta_{v_N} = 1$

For $i = N-1, \ldots, 1$

$\delta_{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \delta_{v_j} \frac{\partial v_j}{\partial v_i}$

General Backpropagation

- Example: univariate logistic least square regression



Forward pass:

$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$
$$\mathcal{R} = \frac{1}{2}w^2$$
$$\mathcal{L}_{\text{reg}} = \mathcal{L} + \lambda \mathcal{R}$$

Backward pass:

$\delta_{\mathcal{L}_{\text{reg}}} =$

$\delta_{\mathcal{R}} =$

$=$

$\delta_{\mathcal{L}} =$

$=$

$\delta_y =$

$=$

$\delta_z =$

$=$

$\delta_w =$

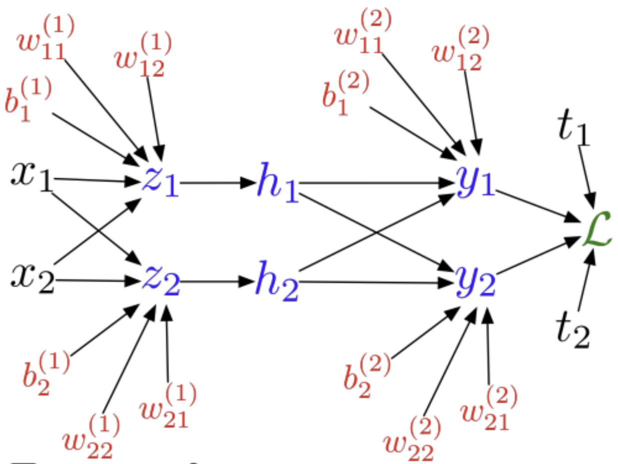
$=$

$\delta_b =$

$=$

General Backpropagation

- Example: Multilayer Perceptron (multiple outputs)



Forward pass:

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

$$h_i = \sigma(z_i)$$

$$y_k = \sum_i w_{ki}^{(2)} h_i + b_k^{(2)}$$

$$\mathcal{L} = \frac{1}{2} \sum_k (y_k - t_k)^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$

$$\overline{y_k} = \overline{\mathcal{L}}\,(y_k - t_k)$$

$$\overline{w_{ki}^{(2)}} = \overline{y_k}\, h_i$$

$$\overline{b_k^{(2)}} = \overline{y_k}$$

$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

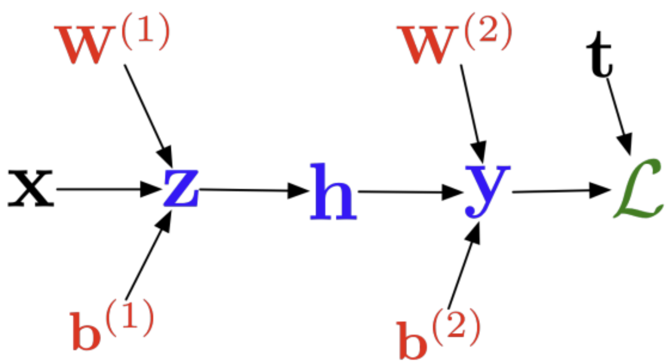
$$\overline{z_i} = \overline{h_i}\, \sigma'(z_i)$$

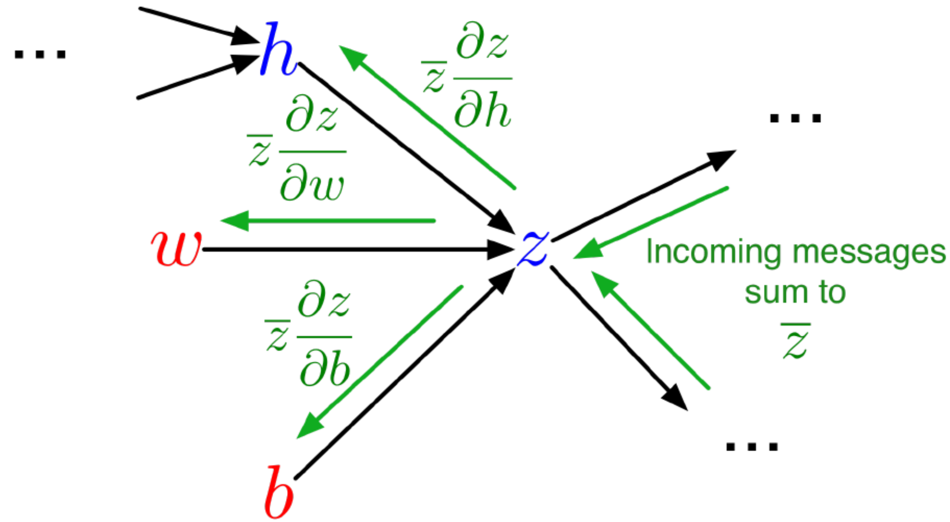
$$\overline{w_{ij}^{(1)}} = \overline{z_i}\, x_j$$

$$\overline{b_i^{(1)}} = \overline{z_i}$$

General Backpropagation

- Backprop as message passing:

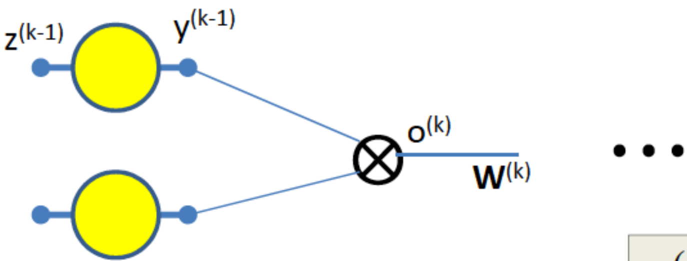




  - Each node receives a set of messages from its children, which are aggregated into its error signal, then it passes messages to its parents
  - Modularity: each node only has to know how to compute derivatives w.r.t. its arguments – local computation in the graph

Patterns in backward flow

- Multiplicative node

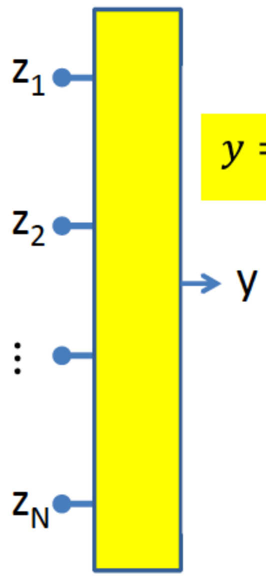


Forward: $o_i^{(k)} = y_j^{(k-1)} y_l^{(k-1)}$

$$\frac{\partial L}{\partial y_j^{(k-1)}} = \frac{\partial L}{\partial o_i^{(k)}} \frac{\partial o_i^{(k)}}{\partial y_j^{(k-1)}} = y_l^{(k-1)} \frac{\partial L}{\partial o_i^{(k)}}$$

Patterns in backward flow

- Max node



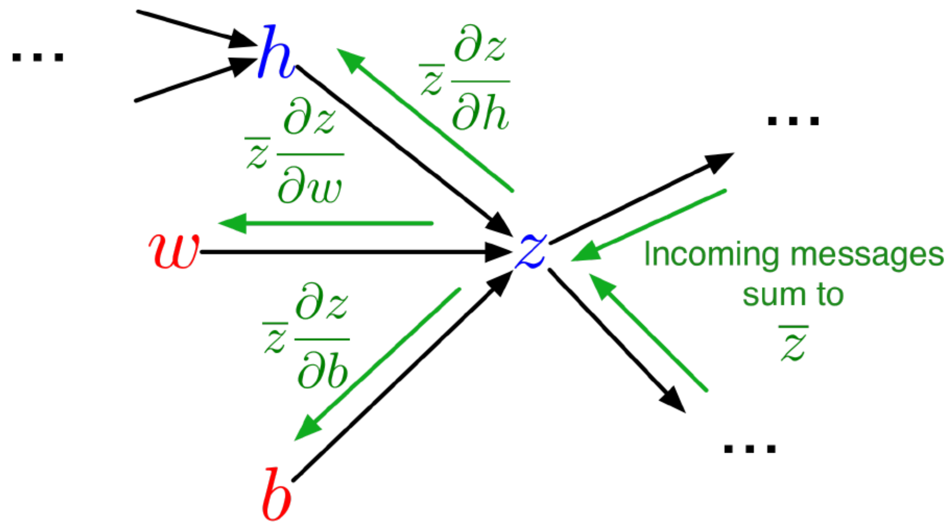
$$y = \max_j z_j$$

$$\frac{\partial y}{\partial z_i} = \begin{cases} 1, & i = \operatorname{argmax}_j z_j \\ 0, & otherwise \end{cases}$$

- Vector equivalent of subgradient
  - 1 w.r.t. the largest incoming input
    - Incremental changes in this input will change the output
  - 0 for the rest
    - Incremental changes to these inputs will not change the output

Computation cost

- Forward pass: one add-multiply operation per weight
- Backward pass: two add-multiply operations per weight



$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

$$\overline{w_{ki}^{(2)}} = \overline{y_k}\, h_i$$

$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

- For a multilayer network, the cost is linear in the number of layers, quadratic in the number of units per layer

Backpropagation

- Backprop is used to train the majority of neural nets
  - Even generative network learning, or advanced optimization algorithms (second-order) use backprop to compute the update of weights
- However, backprop seems biologically implausible
  - No evidence for biological signals analogous to error derivatives
  - All the existing biologically plausible alternatives learn much more slowly on computers.
  - So how on earth does the brain learn???

Coding examples

- Getting familiar with Pytorch
  - Python Tutorial: https://cs231n.github.io/python-numpy-tutorial/
  - PyTorch in 60 mins: https://pytorch.org/tutorials/beginner/deep_learning_60min_blitz.html

- Predicting house prices
  - https://d2l.ai/chapter_multilayer-perceptrons/kaggle-house-price.html

Summary

- Multi-layer neural networks
- Inference and learning
  - Forward and Backpropagation
- Next time …
  - Modern topics about MLP, CNN
  - Quiz 2: Open book, but no electronic device is allowed.
- **Reference:**
  - d2l.ai: 4.1-4.3, 4.7
  - DLBook: Chapter 6