Multi-Layer Networks

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Deep Learning

Sharif University of Technology

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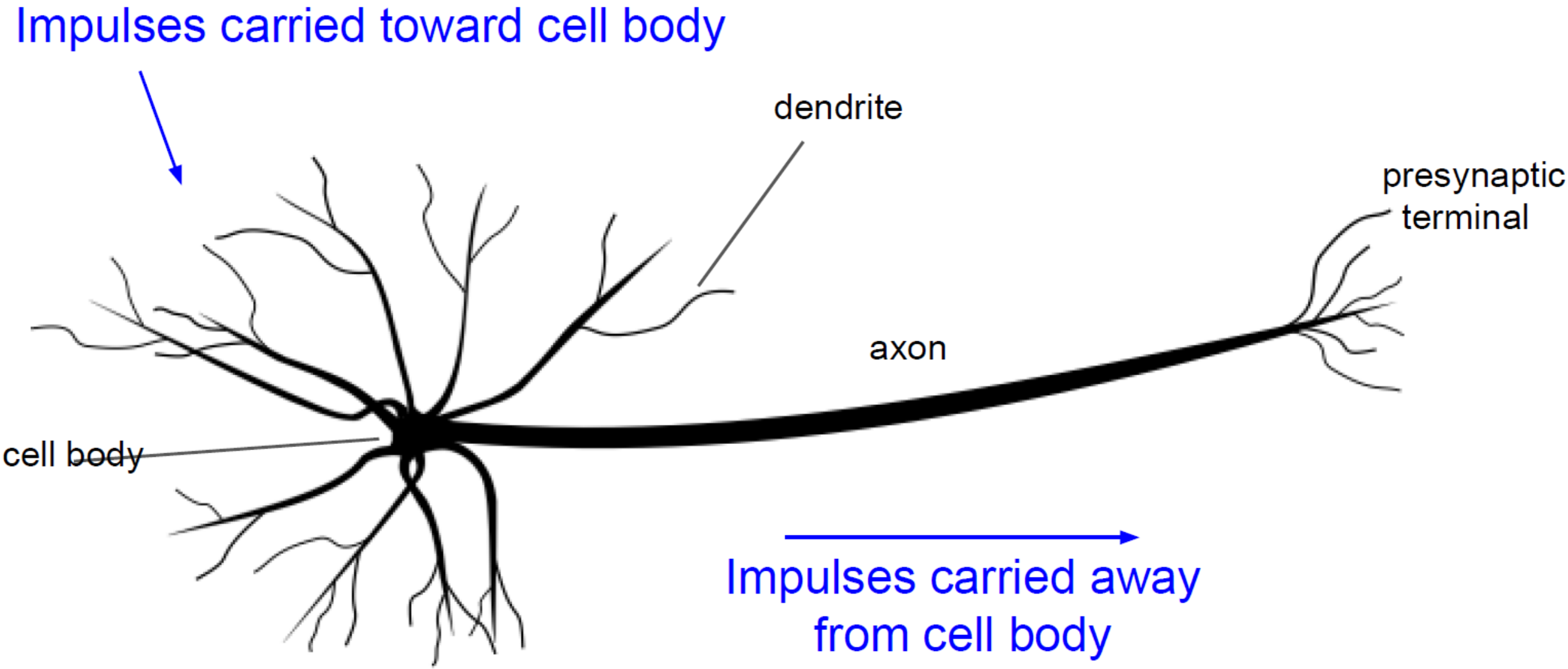
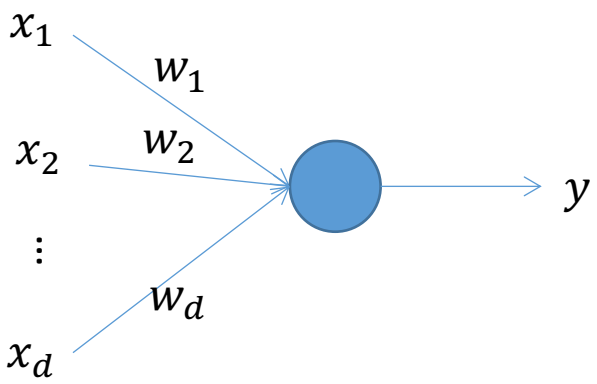
Most slides have been adapted from:

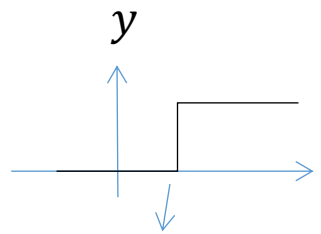
Bhiksha Raj, 11-785, CMU



McCulloch-Pitts neuron: binary threshold

binary McCulloch-Pitts neuron

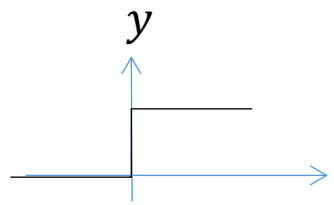


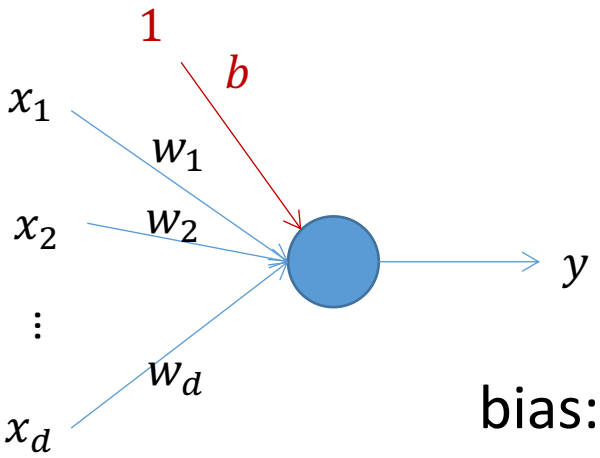


θ: activation threshold

$$y = \begin{cases} 1, & z \geq \theta \\ 0, & z < \theta \end{cases}$$

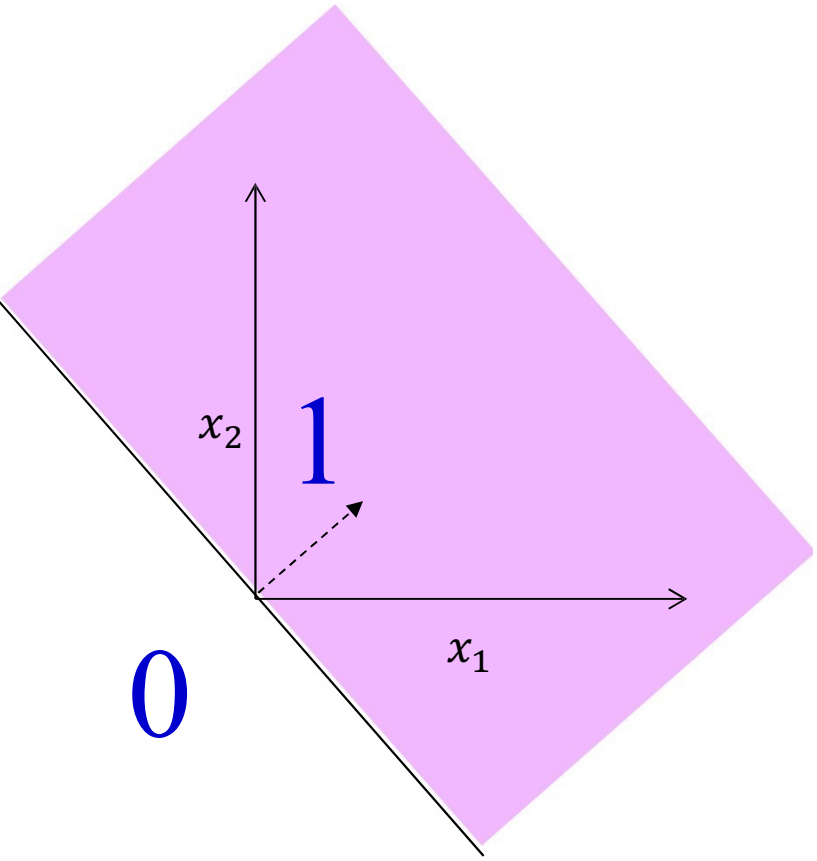
Equivalent to

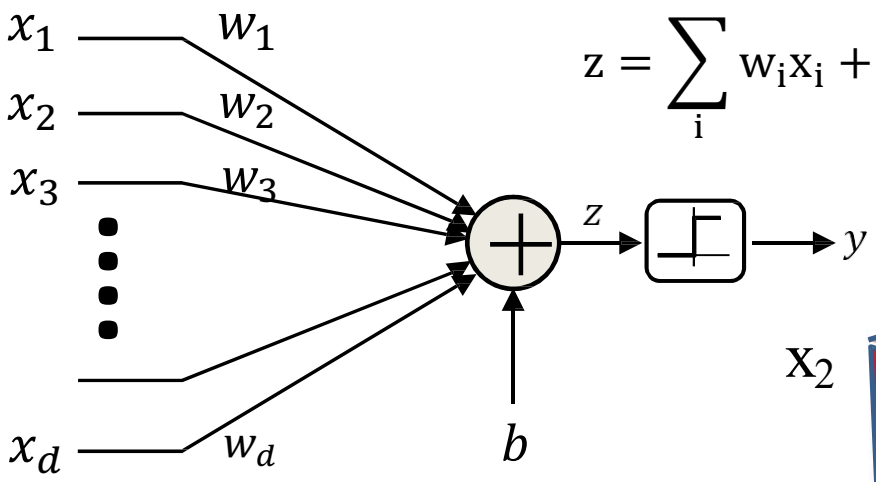


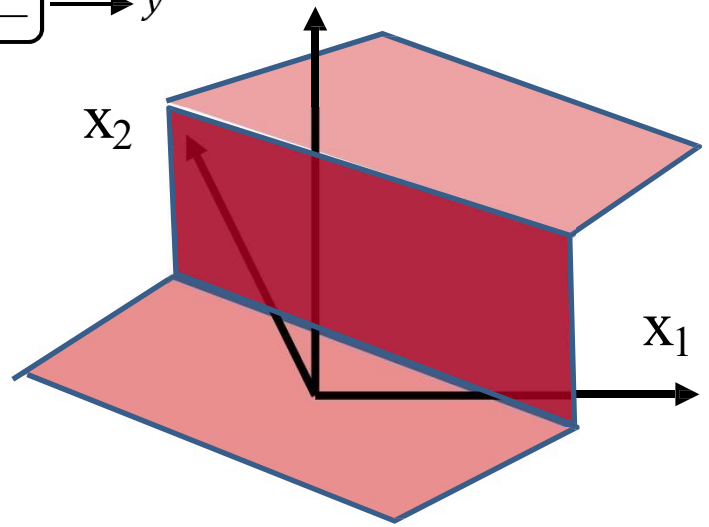


bias: $b = -\theta$

Perceptron

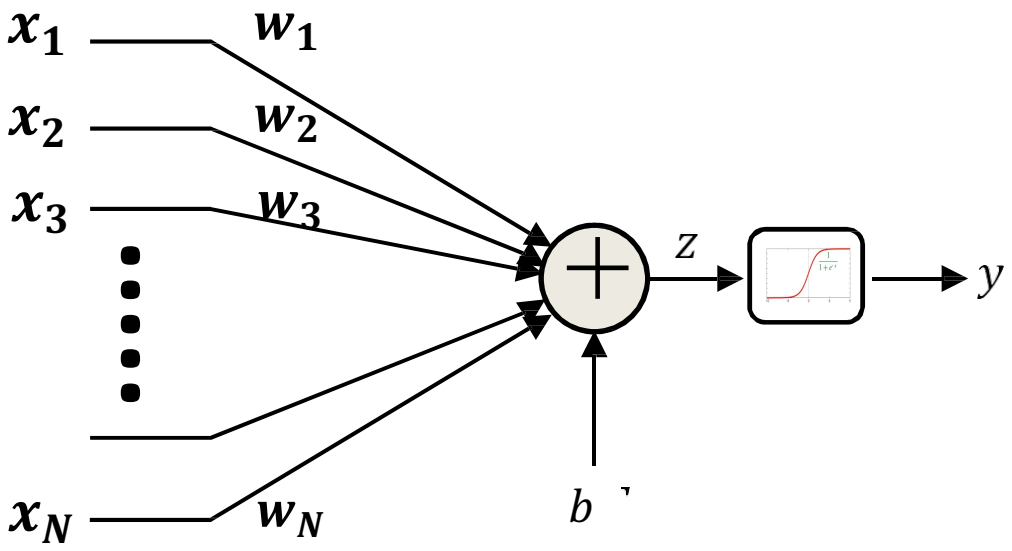






- Learn this function
  - A step function across a hyperplane

The “soft” perceptron (logistic)

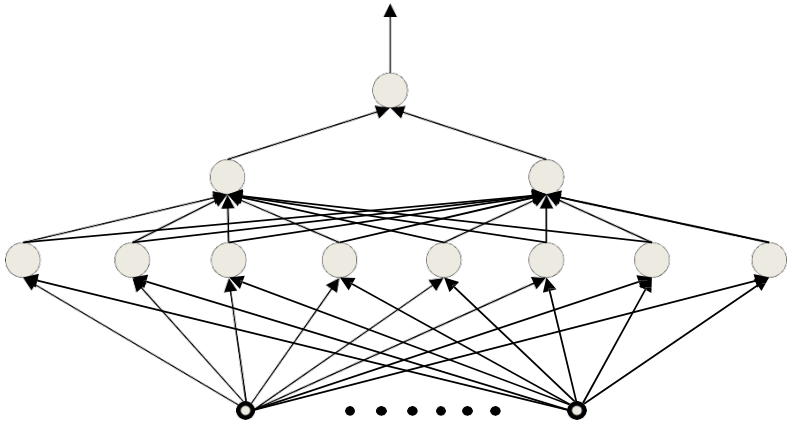


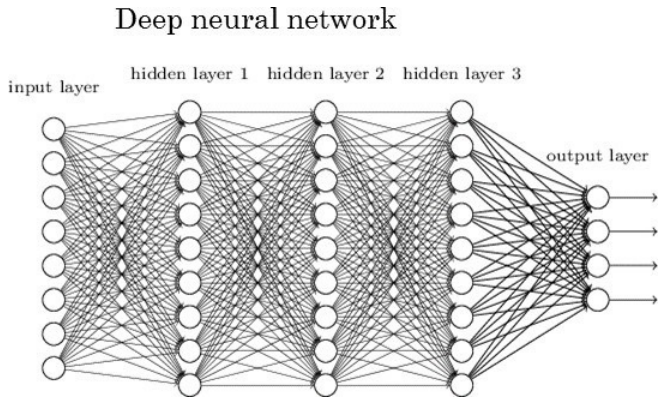
$$z = \sum_i w_i x_i + b$$

$$y = \frac{1}{1 + \exp(-z)}$$

- A “squashing” function instead of a threshold at the output
  - The sigmoid “activation” replaces the threshold
    - Activation: The function that acts on the weighted combination of inputs (and threshold)

The multi-layer perceptron

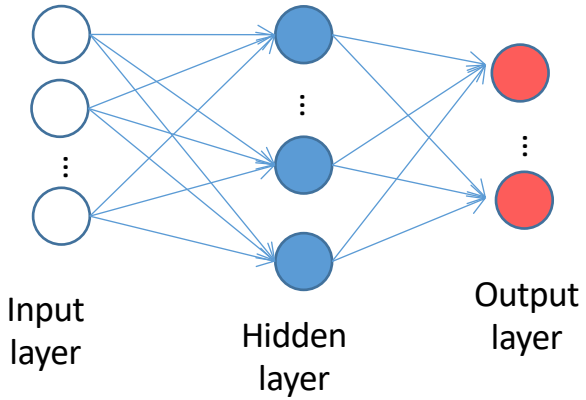




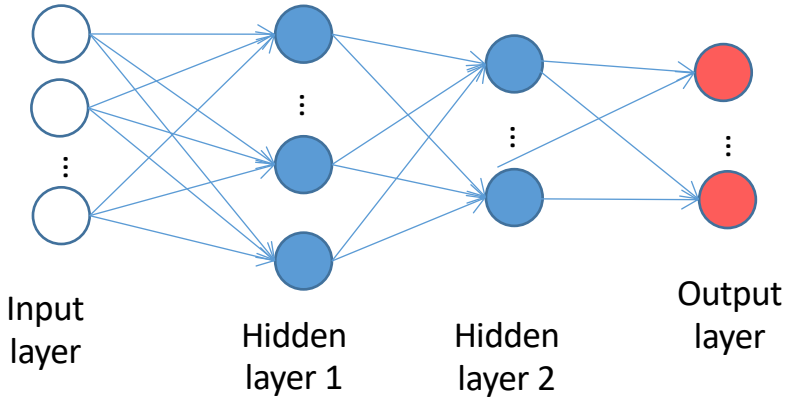
- A network of perceptrons
  - Generally “layered”

Feed-forward neural networks

- Also called **Multi-Layer Perceptron (MLP)**



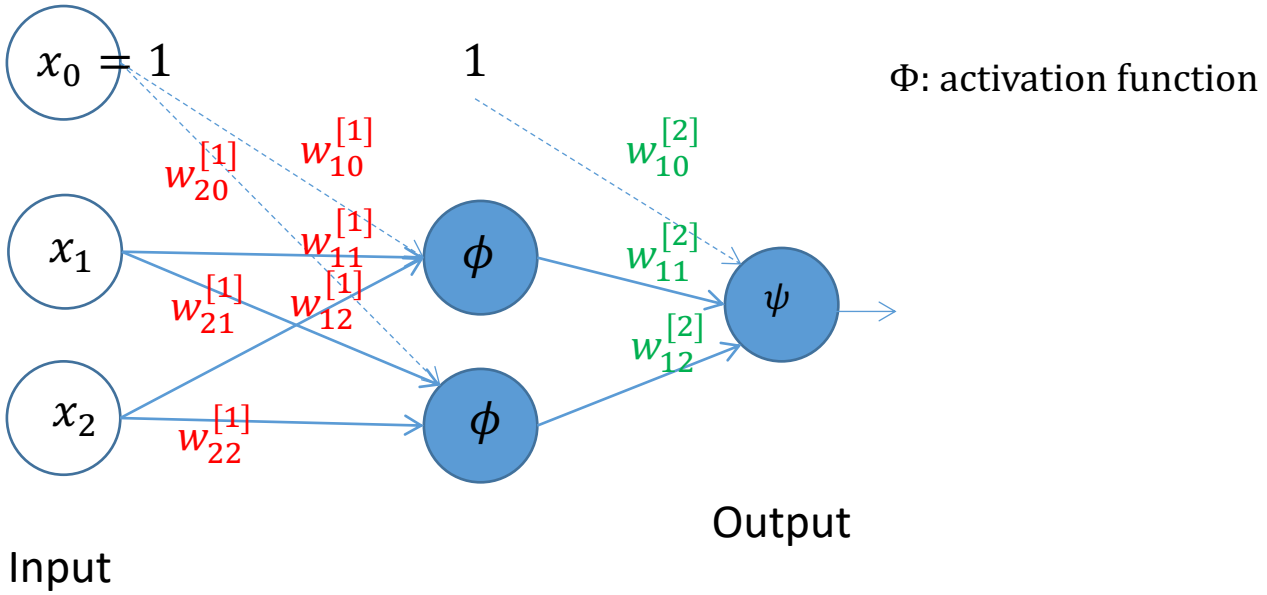
1-Hidden Layer
or 2-layer network



2-Hidden Layers
or 3-layer network

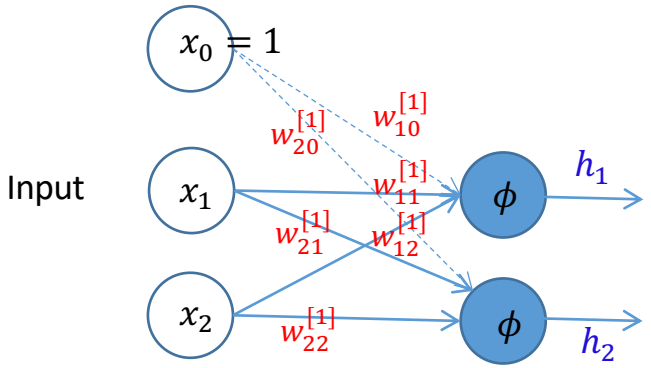
Multi-layer Neural Network

- MLP with single hidden layer
  - Called two-layer MLP (Number of layers of adaptive weights is counted)



Multi-layer Neural Network

$$\boldsymbol{W}^{[1]} = \begin{bmatrix} w_{10}^{[1]} & w_{11}^{[1]} & w_{12}^{[1]} \\ w_{20}^{[1]} & w_{21}^{[1]} & w_{22}^{[1]} \end{bmatrix}$$



$$h_j = \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)$$

Matrix form: $$\boldsymbol{h} = \phi\left(W^{[1]}\boldsymbol{x}\right)$$

ϕ: fixed activation function

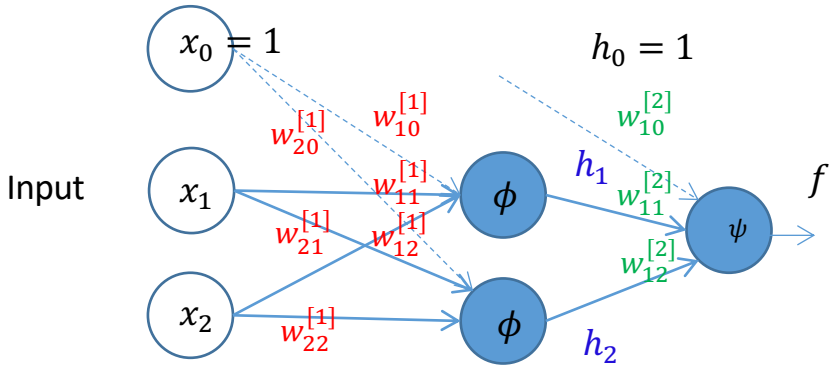
Examples:

$$\phi(z) = \max(0, z)$$

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

Multi-layer Neural Network

$$\boldsymbol{W}^{[1]} = \begin{bmatrix} w_{10}^{[1]} & w_{11}^{[1]} & w_{12}^{[1]} \\ w_{20}^{[1]} & w_{21}^{[1]} & w_{22}^{[1]} \end{bmatrix}$$



ϕ: fixed activation function

Examples:

$$\phi(z) = \max(0, z)$$

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

$$h_j = \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right) \qquad f = \psi\left(\sum_{j=0}^{2} w_{kj}^{[2]} h_j\right)$$

Matrix form:

$$\boldsymbol{h} = \phi\left(W^{[1]}\boldsymbol{x}\right)$$

$$\begin{aligned} & f(\boldsymbol{x}) \\ & = \psi\left(\boldsymbol{W}^{[2]}\boldsymbol{h}\right) \\ & = \psi\left(\boldsymbol{W}^{[2]}\phi\left(\boldsymbol{W}^{[1]}\boldsymbol{x}\right)\right) \end{aligned}$$

Beyond linear models

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

(**Now**) 2-layer Neural Network $f = W_2\phi(W_1x)$
or 3-layer Neural Network

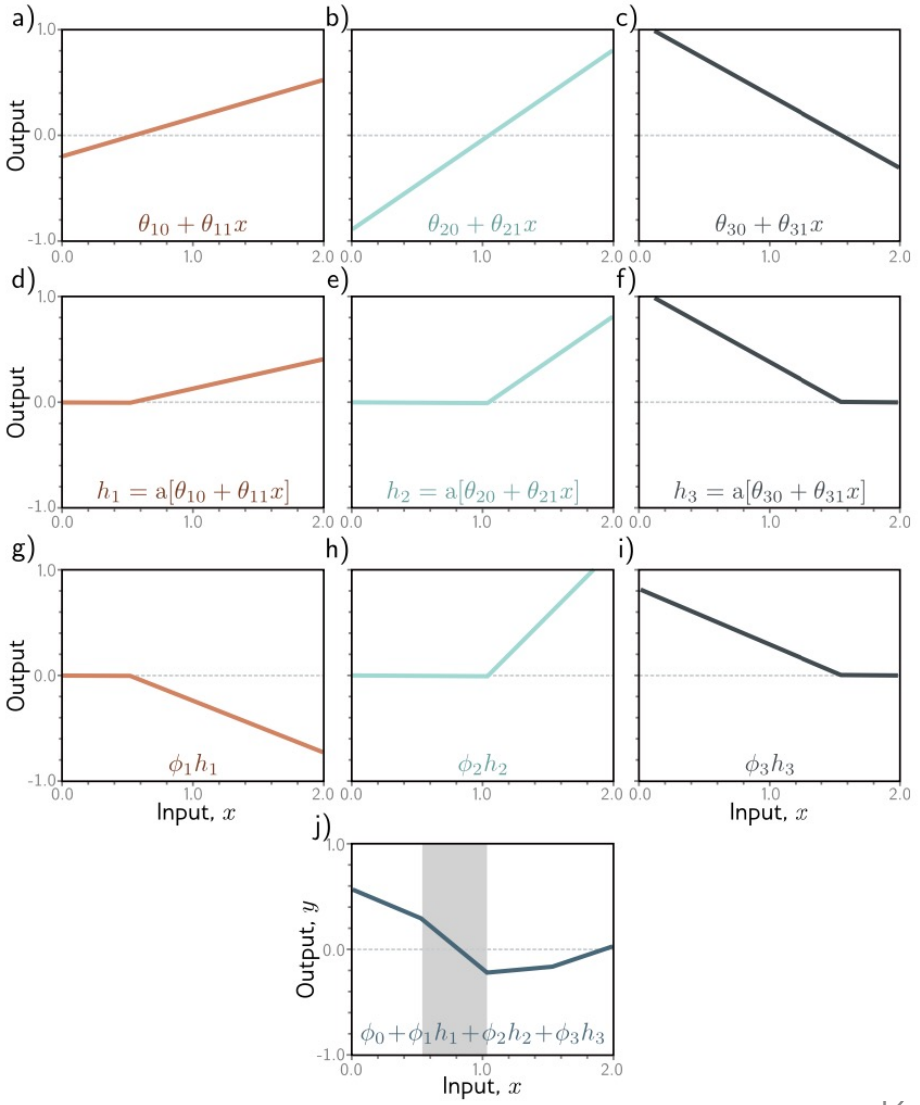
$$f = W_3\phi\big(W_2\phi(W_1x)\big)$$

Question 1

Pre-activation of the hidden layer

Post-activation of the hidden layer

Weighted hidden values



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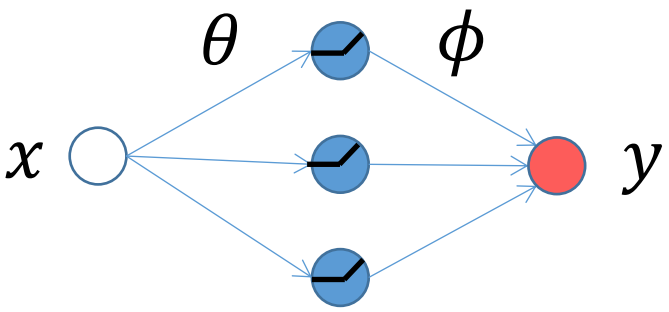
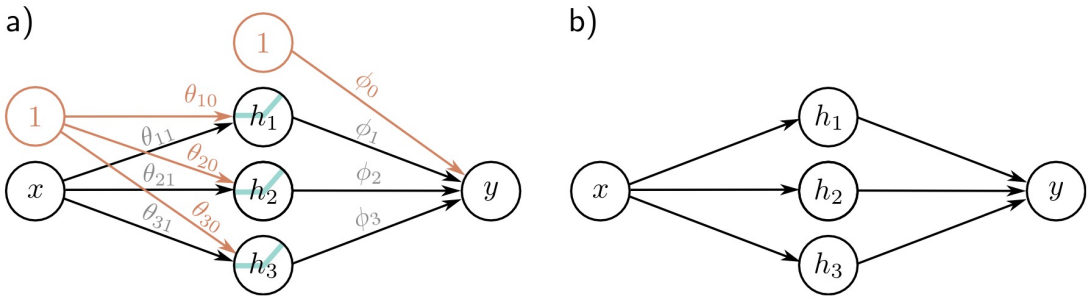
Question 1

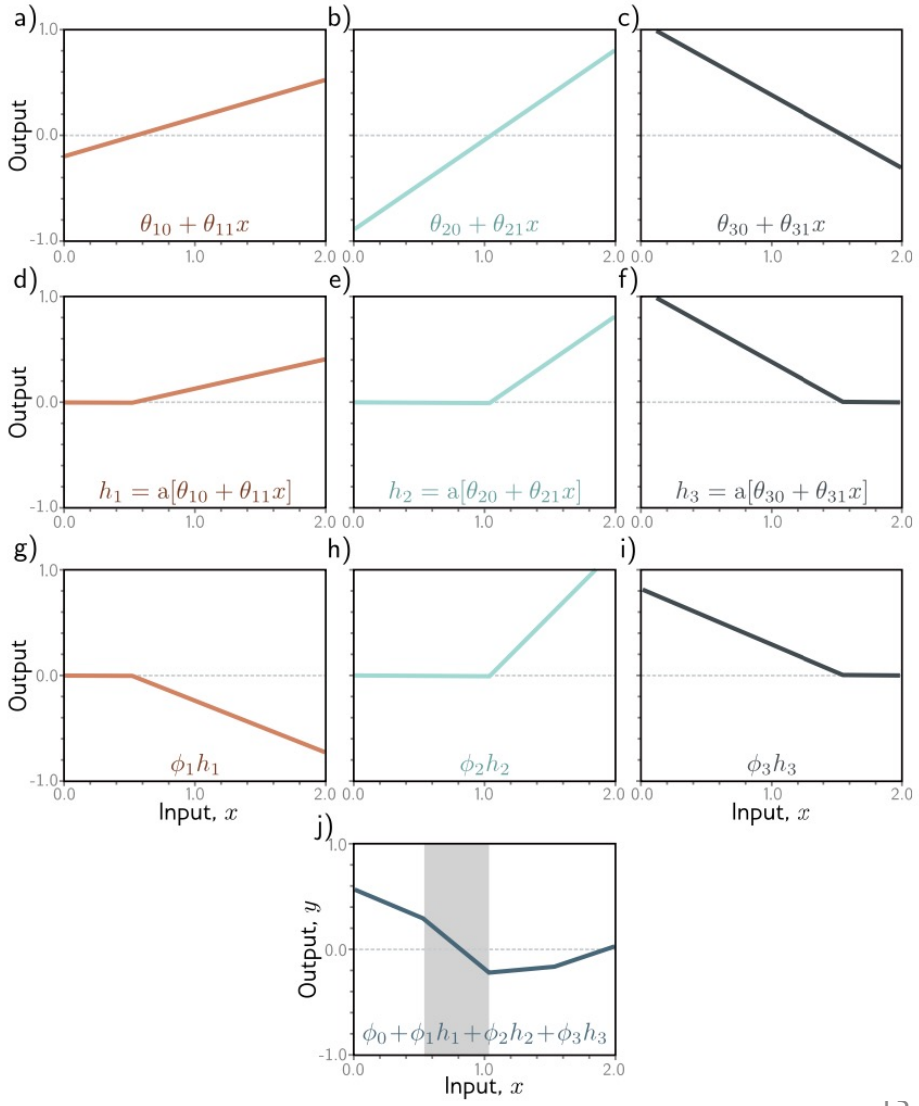


Pre-activation of the hidden layer

Post-activation of the hidden layer

Weighted hidden values





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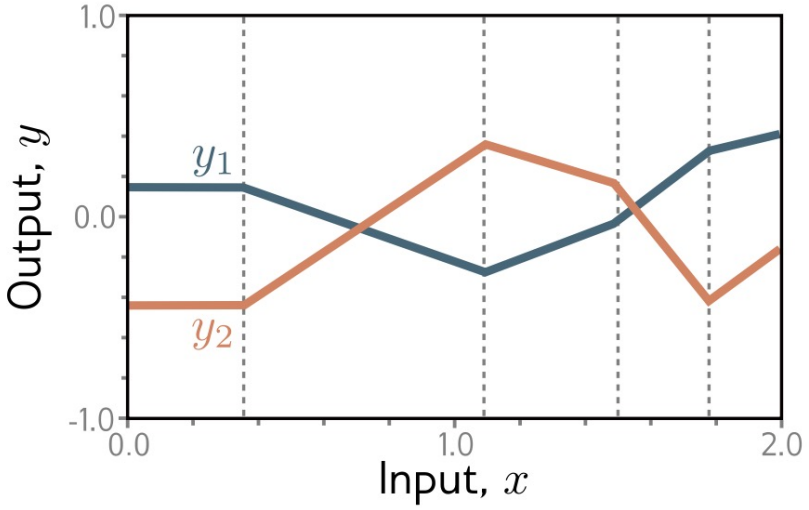
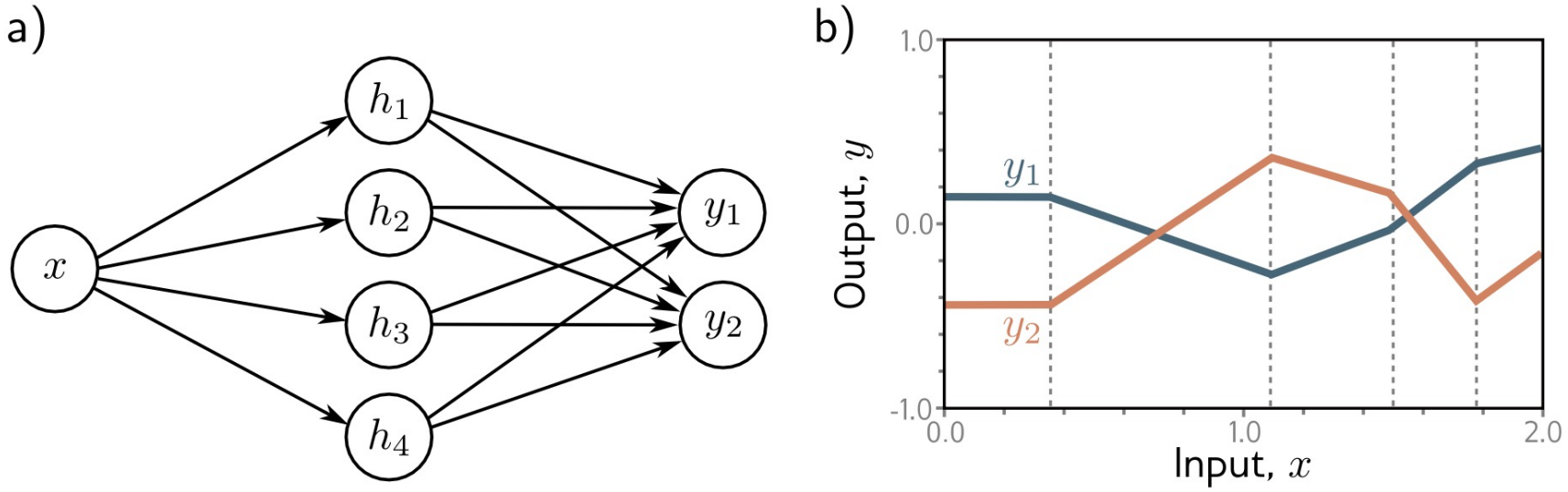
Question 2



Question 2



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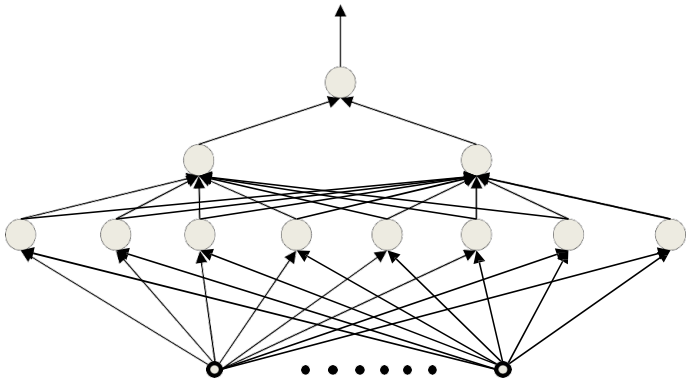
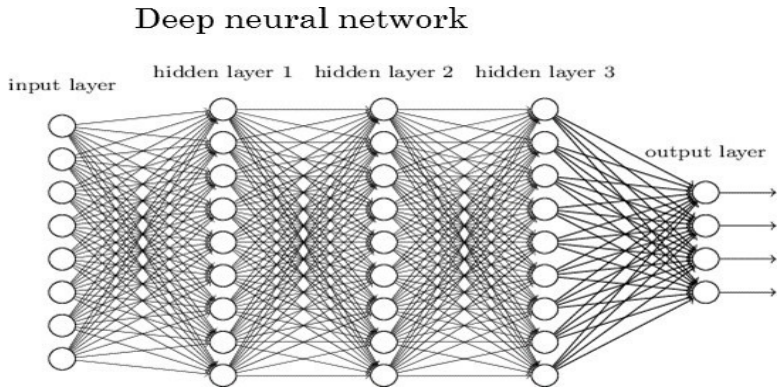
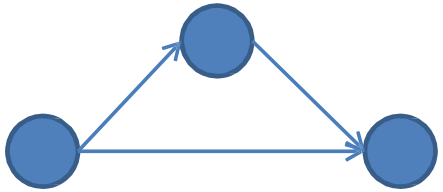
Deep Structures

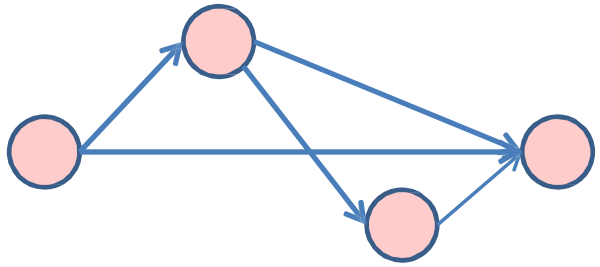




- "depth" is the length of the longest path from an input source to an output sink



Left: Depth =2



Right: Depth =3

- "Deep" ⇨ Depth > 2

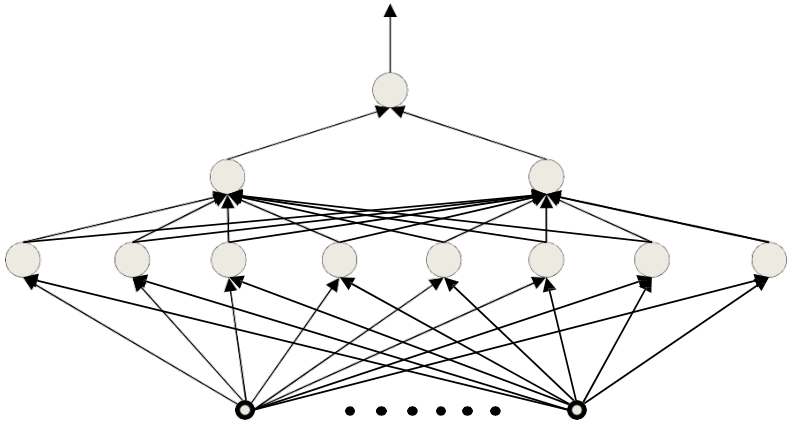
MLP Universal Approximator

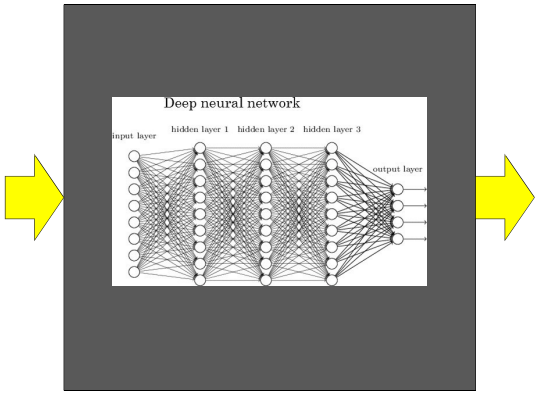
- A feed-forward net with a single hidden layer and linear outputs can approximate any continuous function on a compact subset of $\mathbb{R}^D$ to an arbitrary accuracy
  - under mild assumptions on the activation function
    - e.g., sigmoid activation functions (Cybenko,1989)
  - when sufficiently large (but finite) number of hidden units is used

$$F_k(x) = \sum_{j=1}^{M} w_{kj}^{[2]} \phi\left(\sum_{i=0}^{d} w_{ji}^{[1]} x_i\right)$$

- It is of greater theoretical interest than practical
  - the construction of such a network requires weight values which are unknown

The multi-layer perceptron

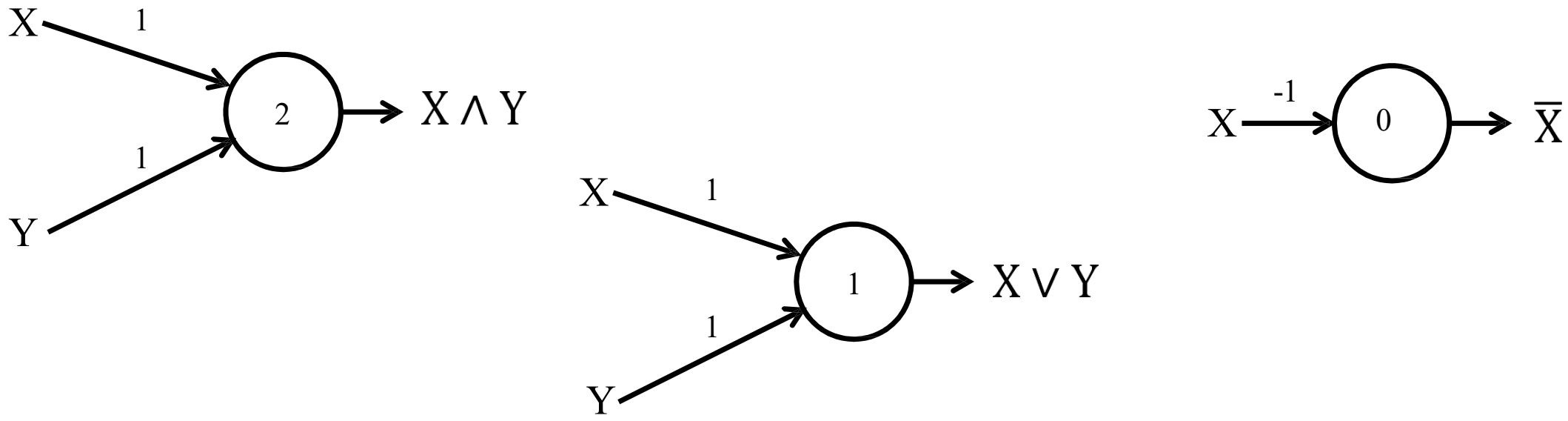




- Inputs are real or Boolean stimuli
- Outputs are real or Boolean values
  - Can have multiple outputs for a single input
- What can this network compute?
  - What kinds of input/output relationships can it model?

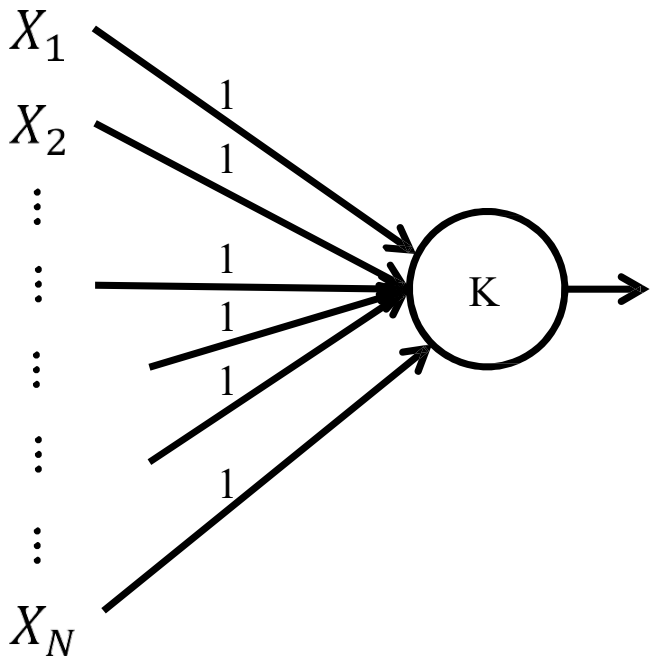
Multi-layer Perceptrons as universal Boolean functions

The perceptron as a Boolean gate



- A perceptron can model any simple binary Boolean gate

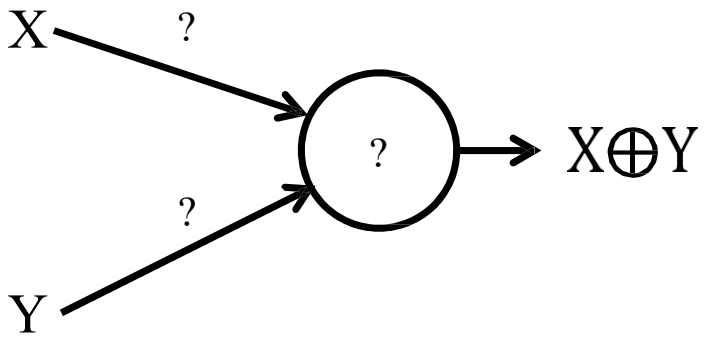
Perceptron as a majority gate



Will fire only if at least K inputs are 1

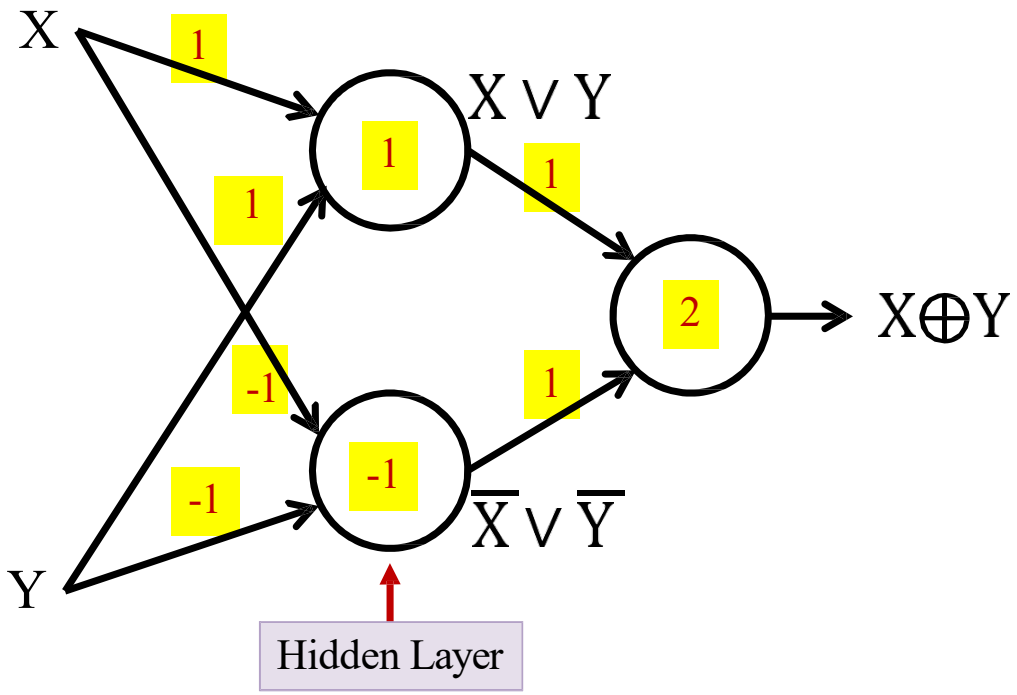
- Generalized majority gate
  - Fire if at least K inputs are of the desired polarity

The perceptron is not enough



- Cannot compute an XOR

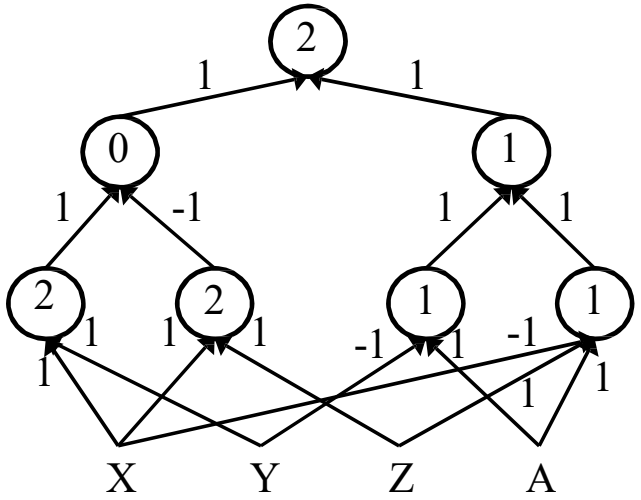
Multi-layer perceptron XOR



- An XOR takes three perceptrons

Multi-layer perceptron

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



- MLPs can compute more complex Boolean functions
- MLPs can compute any Boolean function
  - Since they can emulate individual gates
- MLPs are universal Boolean functions

How many layers for a Boolean MLP?

Truth Table

X_1	X_2	X_3	X_4	X_5	Y
0	0	1	1	0	1
0	1	0	1	1	1
0	1	1	0	0	1
1	0	0	0	1	1
1	0	1	1	1	1
1	1	0	0	1	1

Truth table shows all input combinations for which output is 1

- A Boolean function is just a truth table

How many layers for a Boolean MLP?

Truth Table

X_1	X_2	X_3	X_4	X_5	Y
0	0	1	1	0	1
0	1	0	1	1	1
0	1	1	0	0	1
1	0	0	0	1	1
1	0	1	1	1	1
1	1	0	0	1	1

Truth table shows all input combinations for which output is 1

$$y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3X_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$$

- Expressed in disjunctive normal form

How many layers for a Boolean MLP?

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X_1	X_2	X_3	X_4	X_5	Y
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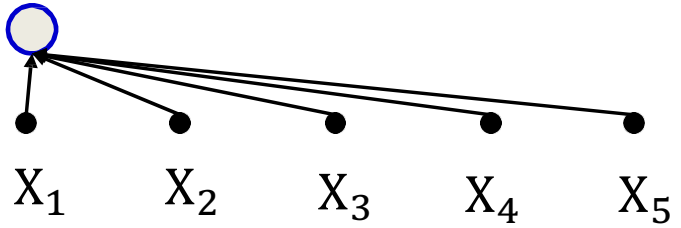

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Truth table shows all input combinations for which output is 1

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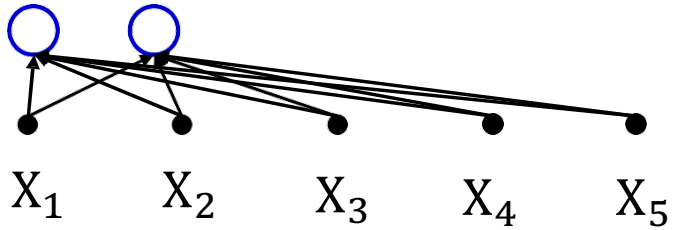

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How many layers for a Boolean MLP?

Truth Table

X_1	X_2	X_3	X_4	X_5	Y
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0	1	0	1	1	1
0	1	1	0	0	1
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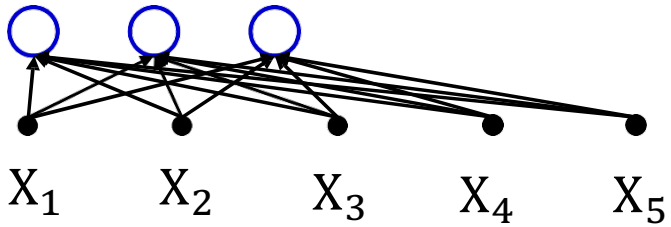
Truth table shows all input combinations for which output is 1

$$y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3X_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$$



- Expressed in disjunctive normal form

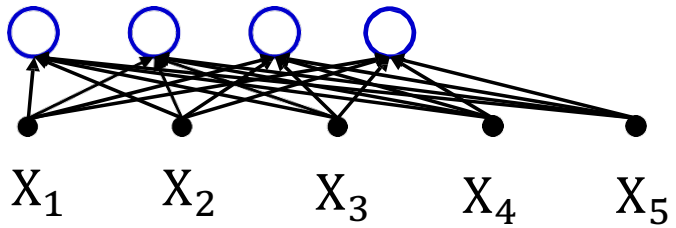
How many layers for a Boolean MLP?

Truth Table

X_1	X_2	X_3	X_4	X_5	Y
0	0	1	1	0	1
0	1	0	1	1	1
0	1	1	0	0	1
1	0	0	0	1	1
1	0	1	1	1	1
1	1	0	0	1	1

Truth table shows all input combinations for which output is 1

$$y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3X_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$$



- Expressed in disjunctive normal form

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0	1	0	1	1	1
0	1	1	0	0	1
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1	0	1	1	1	1
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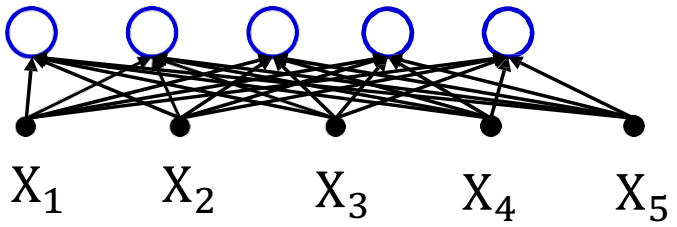

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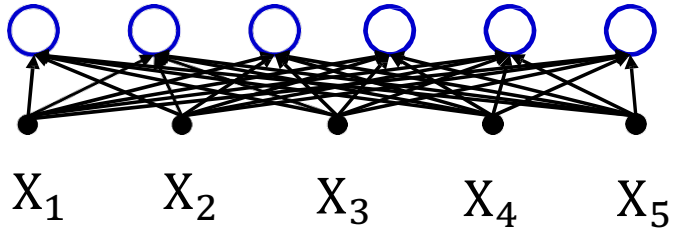

- Expressed in disjunctive normal form

How many layers for a Boolean MLP?

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X_1	X_2	X_3	X_4	X_5	Y
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Truth table shows all input combinations for which output is 1

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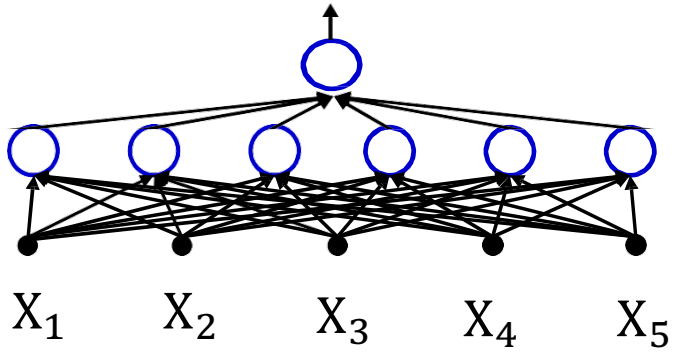


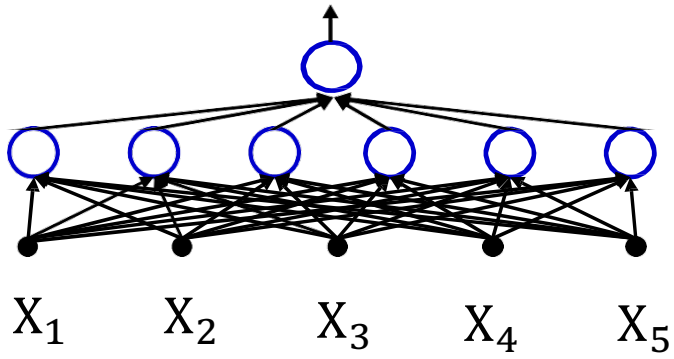
- Expressed in disjunctive normal form

How many layers for a Boolean MLP?

Truth Table

X_1	X_2	X_3	X_4	X_5	Y
0	0	1	1	0	1
0	1	0	1	1	1
0	1	1	0	0	1
1	0	0	0	1	1
1	0	1	1	1	1
1	1	0	0	1	1

$$y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3X_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$$



- Any truth table can be expressed in this manner!
- A one-hidden-layer MLP is a Universal Boolean Function
- But what is the largest number of perceptrons required in the single hidden layer for an N-input-variable function?

Worst case

- Which truth tables cannot be reduced further simply?

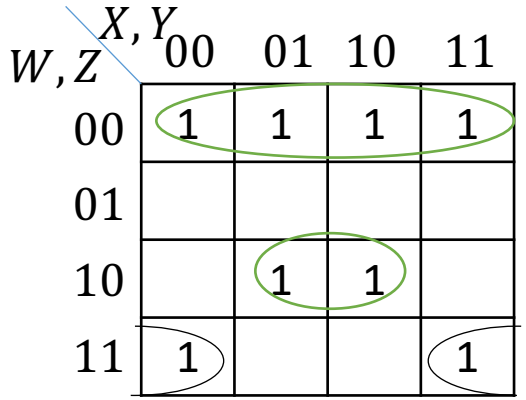
- Largest width needed for a single-layer Boolean network on N inputs
  - Worst case: 2^{N-1}
    - Example: Parity function

W, Z \ X, Y	00	01	11	10
00	1	0	1	0
01	0	1	0	1
11	1	0	1	0
10	0	1	0	1

$X \oplus Y \oplus Z \oplus W$

Boolean functions

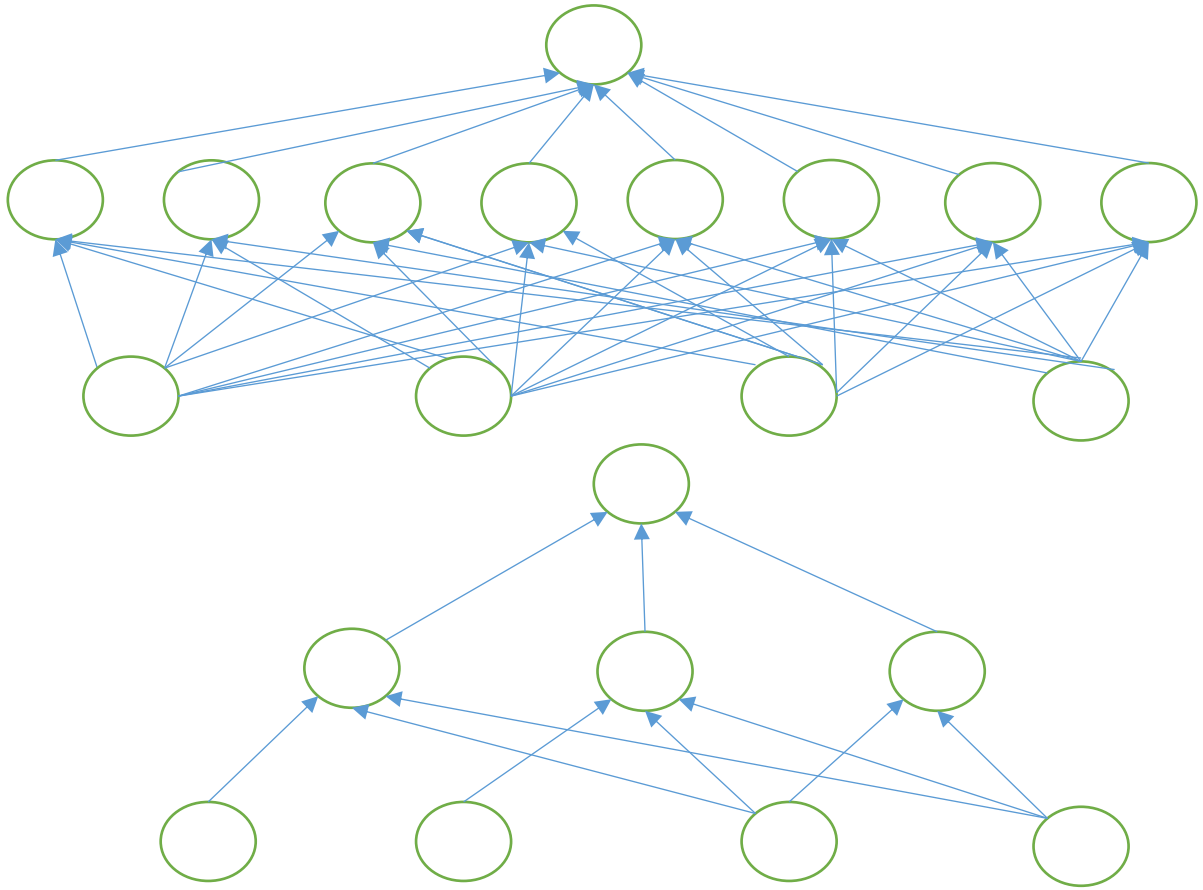
- Input: N Boolean variable
- How many neurons in a one hidden layer MLP is required?
- More compact representation of a Boolean function
  - "Karnaugh Map"
    - representing the truth table as a grid
    - Grouping adjacent boxes to reduce the complexity of the Disjunctive Normal Form (DNF) formula



How many neurons in the hidden layer?

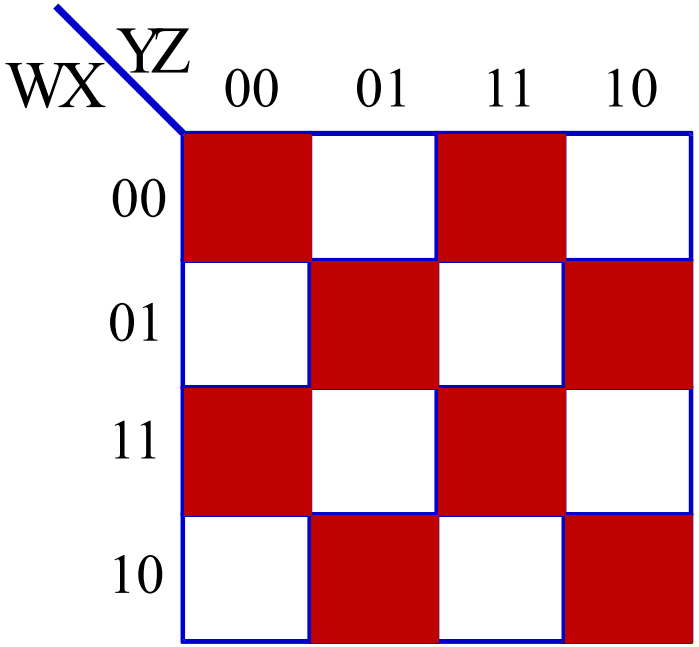
- $\bar{X}\bar{Y}\bar{W}\bar{Z} \vee \bar{X}Y\bar{W}\bar{Z} \vee X\bar{Y}\bar{W}\bar{Z} \vee XY\bar{W}\bar{Z} \vee \bar{X}\bar{Y}WZ \vee X\bar{Y}W\bar{Z} \vee XYW\bar{Z} \vee X\bar{Y}WZ$

W,Z \ X,Y	00	01	11	10
00	1	1	1	1
01				
11	1			1
10			1	1



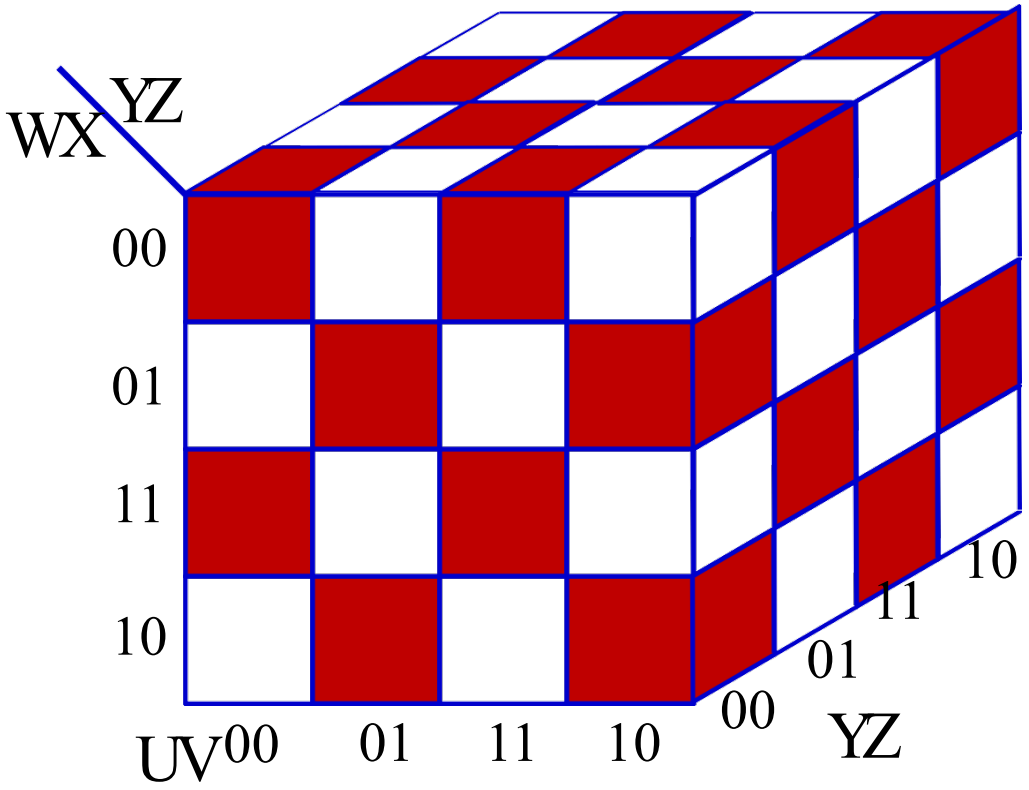
- $\bar{W}\bar{Z} \vee \bar{Y}WZ \vee XW\bar{Z}$

Largest irreducible DNF?



- What arrangement of ones and zeros simply cannot be reduced further?
- How many neurons in a DNF (one hidden-layer) MLP for this Boolean function?

Width of a single-layer Boolean MLP



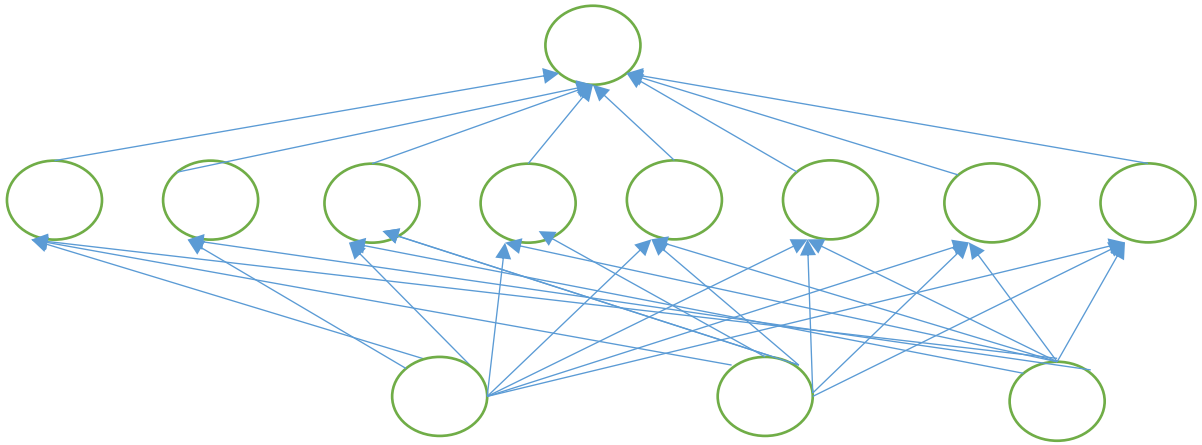
- How many neurons in a DNF (one hidden-layer) MLP for this Boolean function of 6 variables?
- Can be generalized: Will require 2^{D-1} perceptrons in hidden layer Exponential in D
- How many units if we use multiple layers?

Using deep network: Parity function on N inputs

- Simple MLP with one hidden layer:

2^{D-1} Hidden units

$(D+2)2^{D-1}+1$ Weights and biases



Using deep network: Parity function on N inputs

- Simple MLP with one hidden layer:

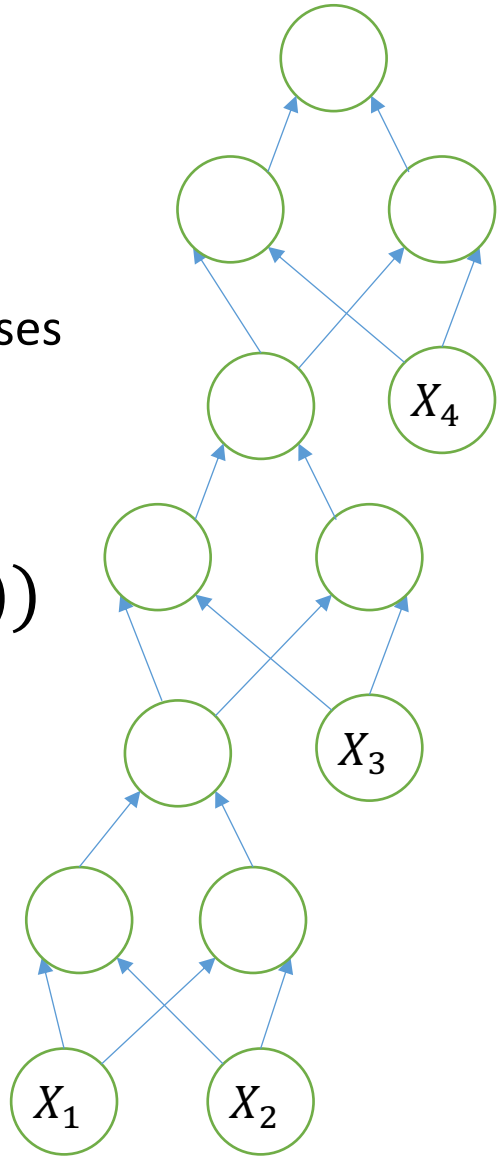
2^{D-1} Hidden units

$(D+2)2^{D-1}+1$ Weights and biases

- $f = ((X_1 \oplus X_2) \oplus X_2) \ldots \oplus X_D))))$

$3(D-1)$ Nodes

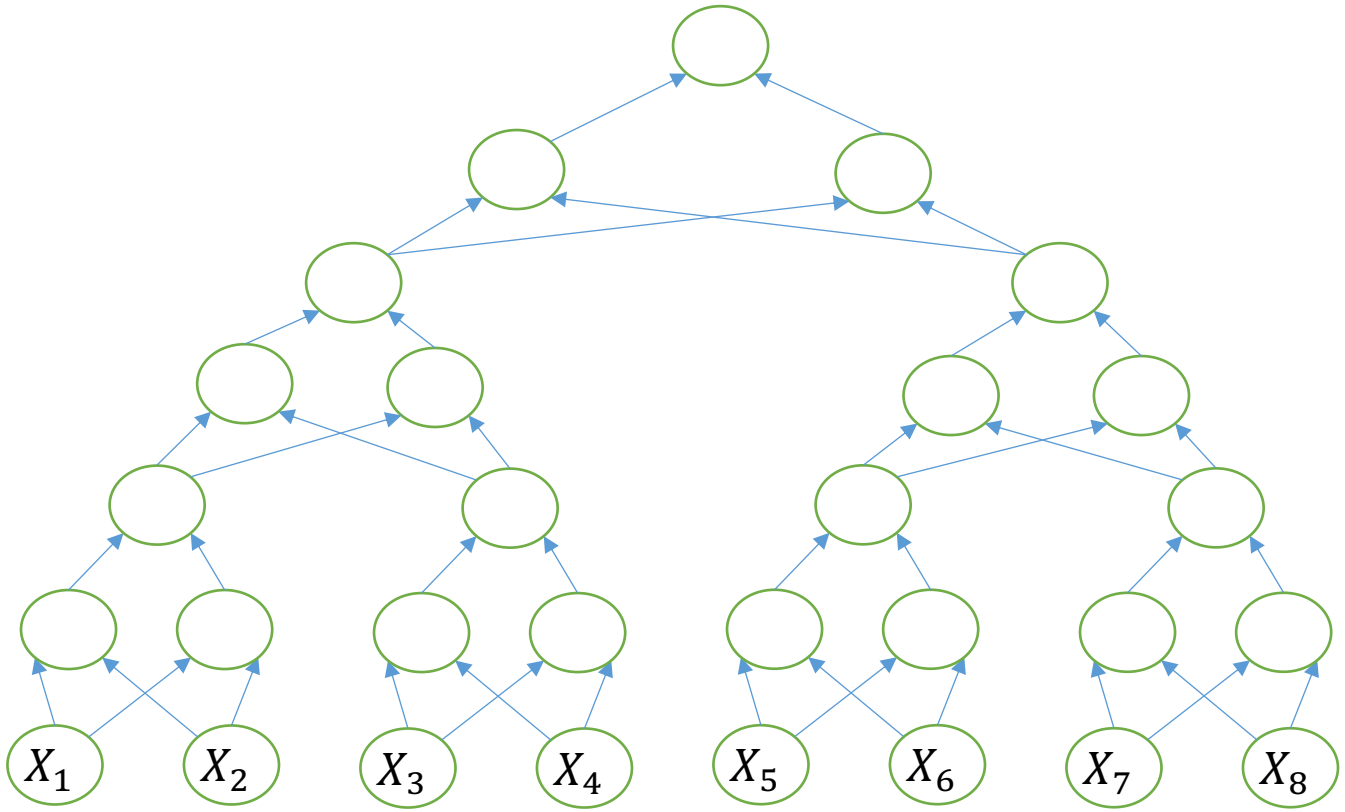
$9(D-1)$ Weights and biases



The actual number of parameters in a network is the number that really matters in software or hardware implementations

A better architecture

- Only requires $2\log N$ layers
- $f = \big((X_1 \oplus X_2) \oplus (X_3 \oplus X_4)\big) \oplus \big((X_4 \oplus X_5) \oplus (X_6 \oplus X_7)\big)$

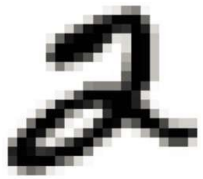


Summary: Wide vs. deep network

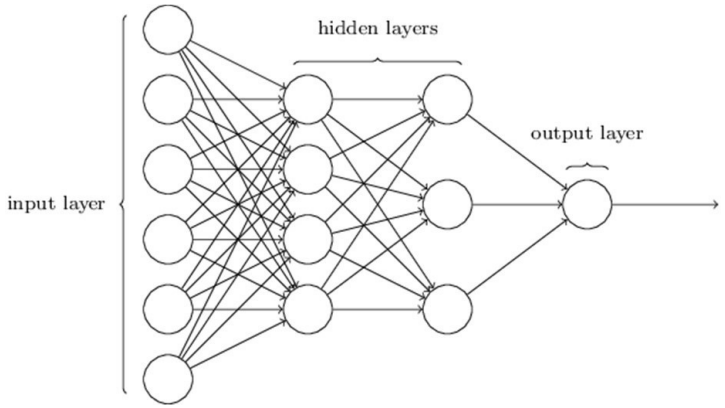
- MLP with a single hidden layer is a universal Boolean function
- However, a single-layer network might need an exponential number of hidden units w.r.t. the number of inputs
- Depth efficiency: Deeper networks may require far fewer neurons than shallower networks to express the same function
  - Could be exponentially smaller
- Optimal width and depth depend on the number of variables and the complexity of the Boolean function
  - Complexity: minimal number of terms in DNF formula to represent it

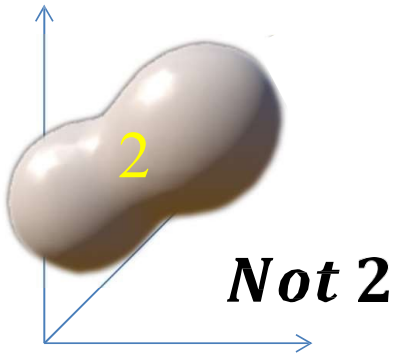
MLPs as universal classifiers

The MLP as a classifier



784 dimensions
(MNIST)

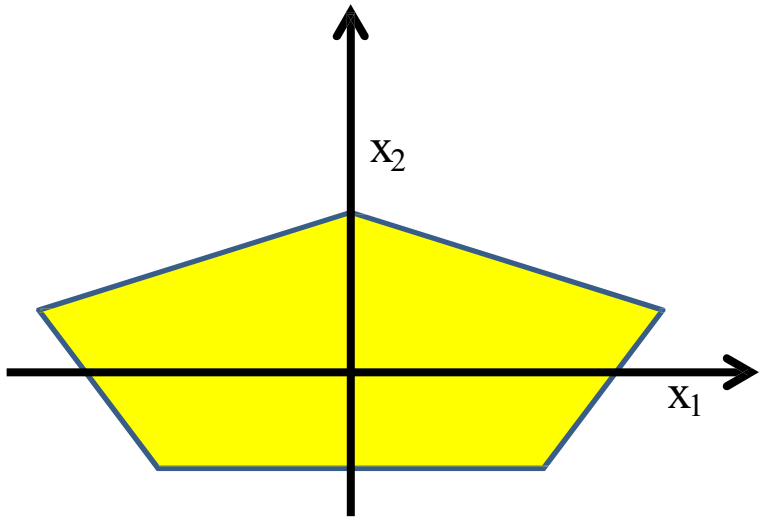




784 dimensions

- MLP as a function over real inputs
- MLP as a function that finds a complex “decision boundary” over a space of reals

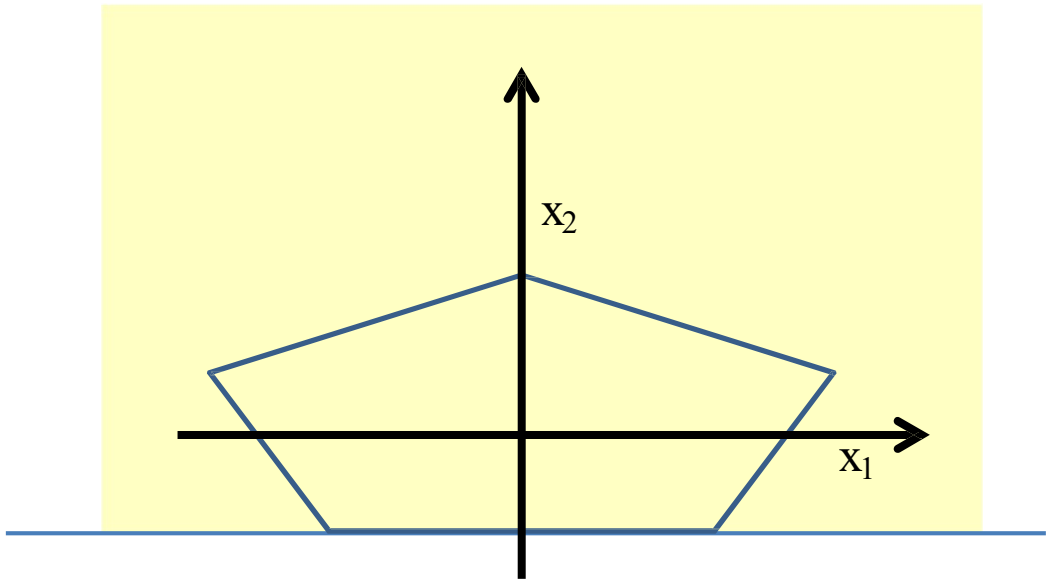
Composing complicated “decision” boundaries

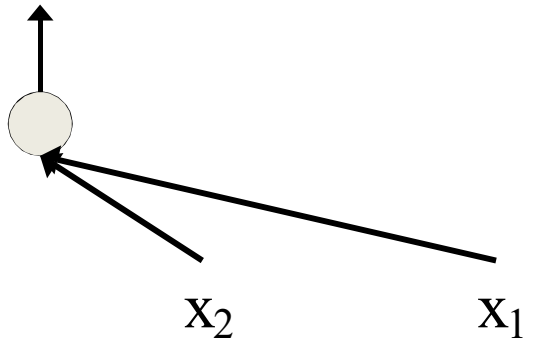


Can now be composed into “networks” to compute arbitrary classification “boundaries”

- Build a network of units with a single output that fires if the input is in the coloured area

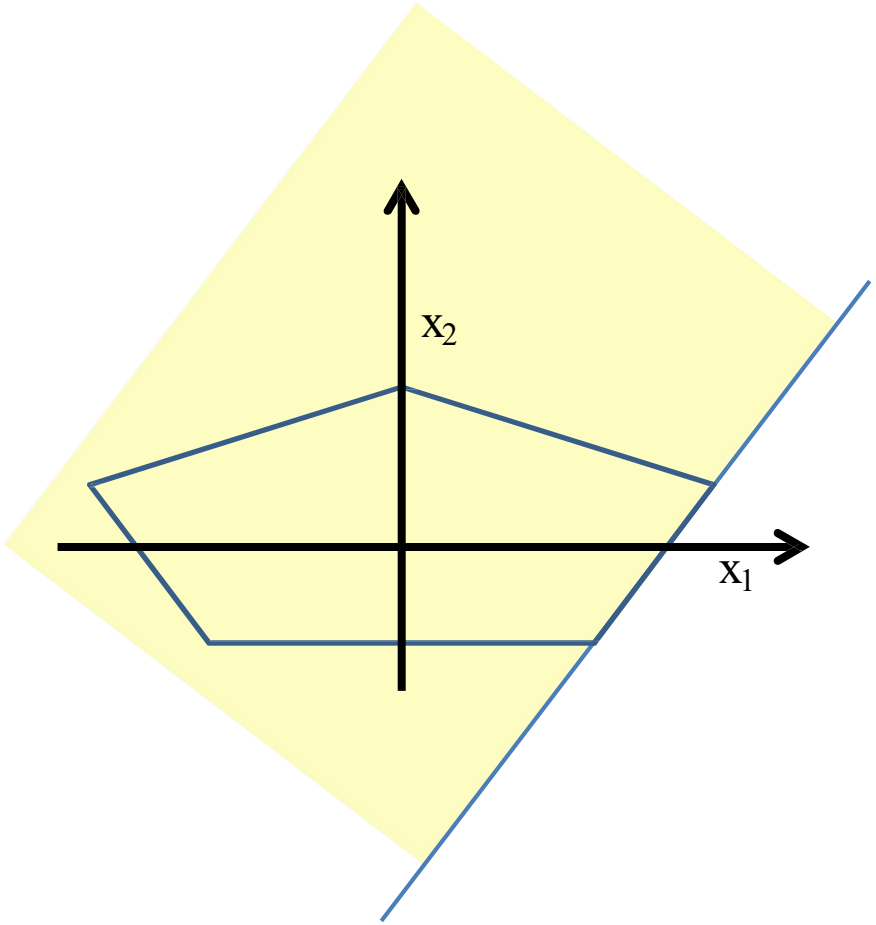
Booleans over the reals

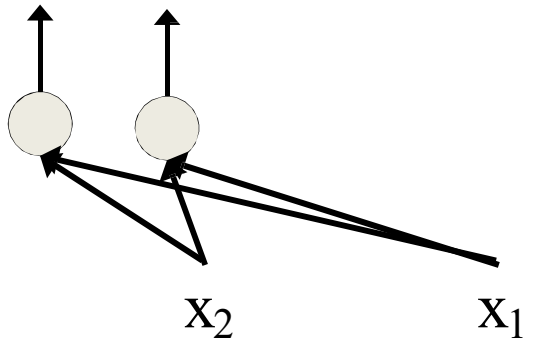




- The network must fire if the input is in the coloured area

Booleans over the reals





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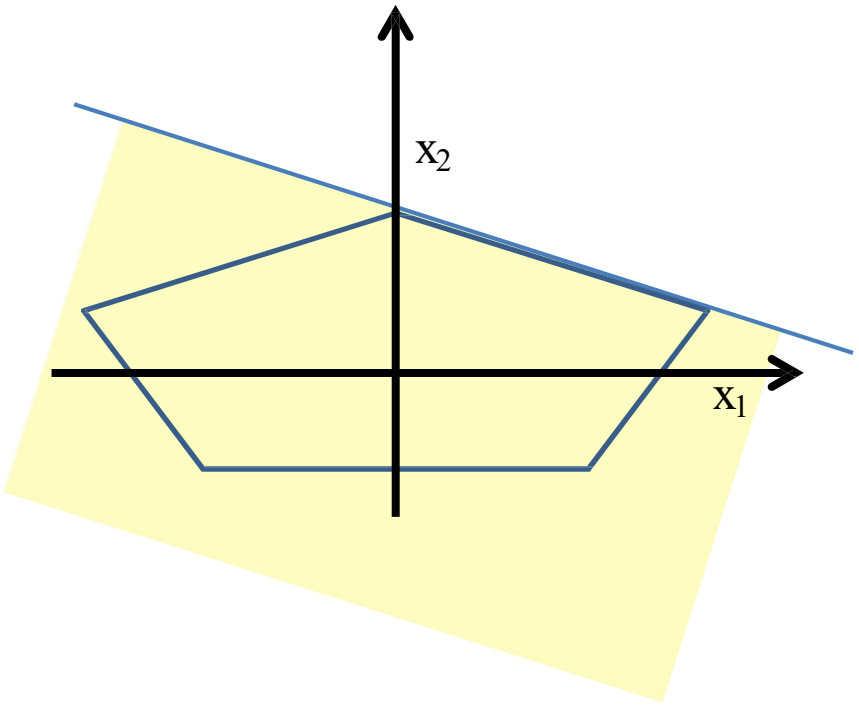
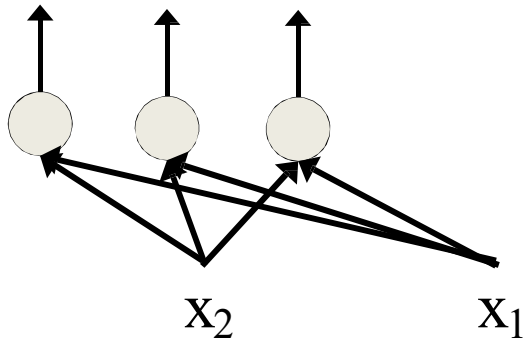
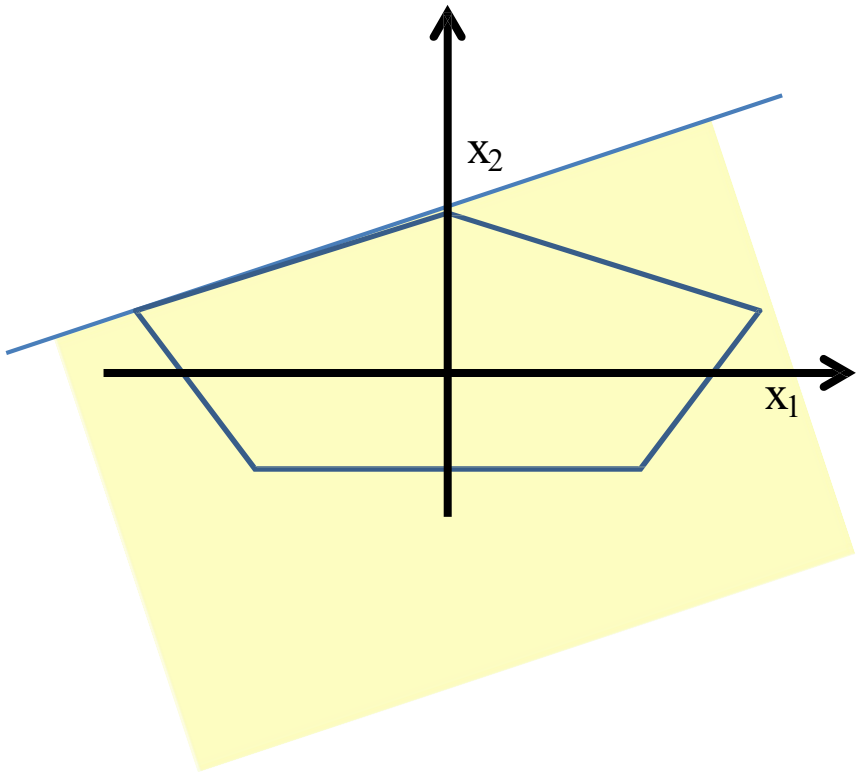
Booleans over the reals

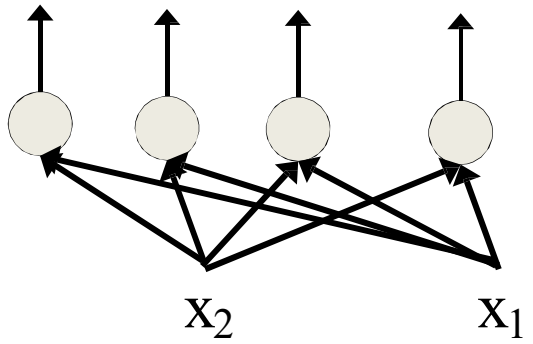




- The network must fire if the input is in the coloured area

Booleans over the reals





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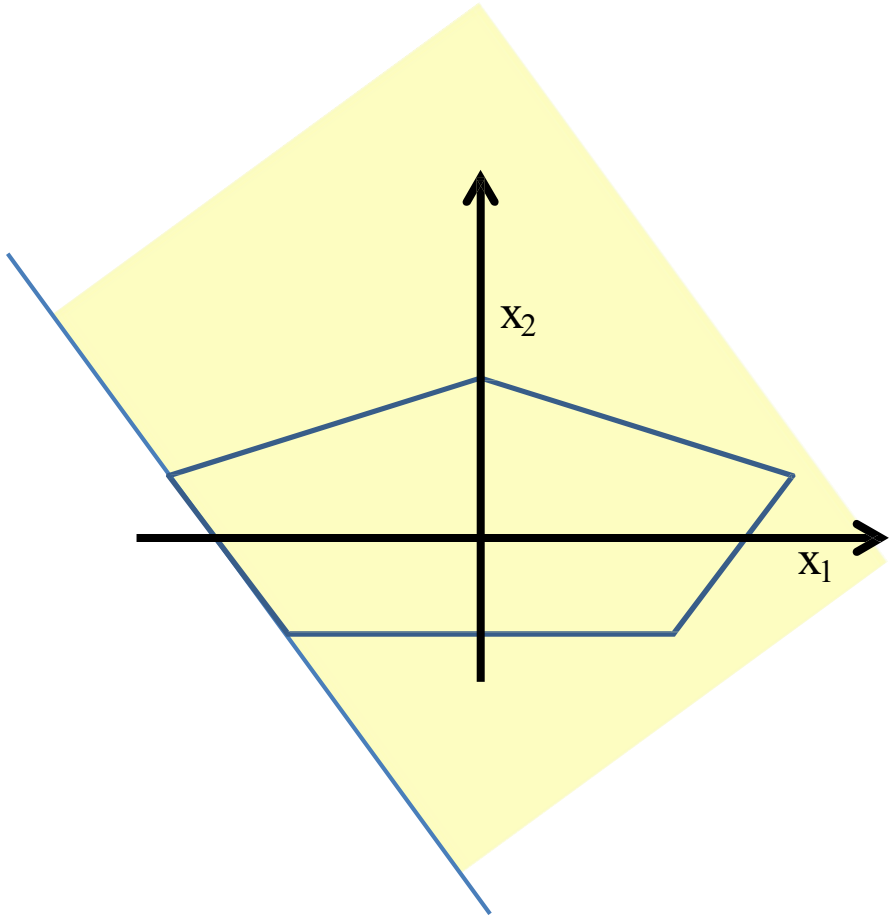
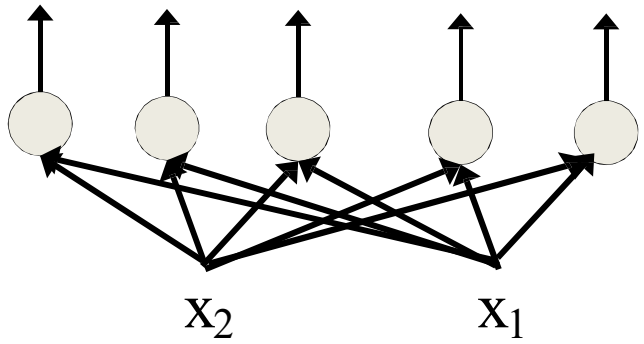
Booleans over the reals





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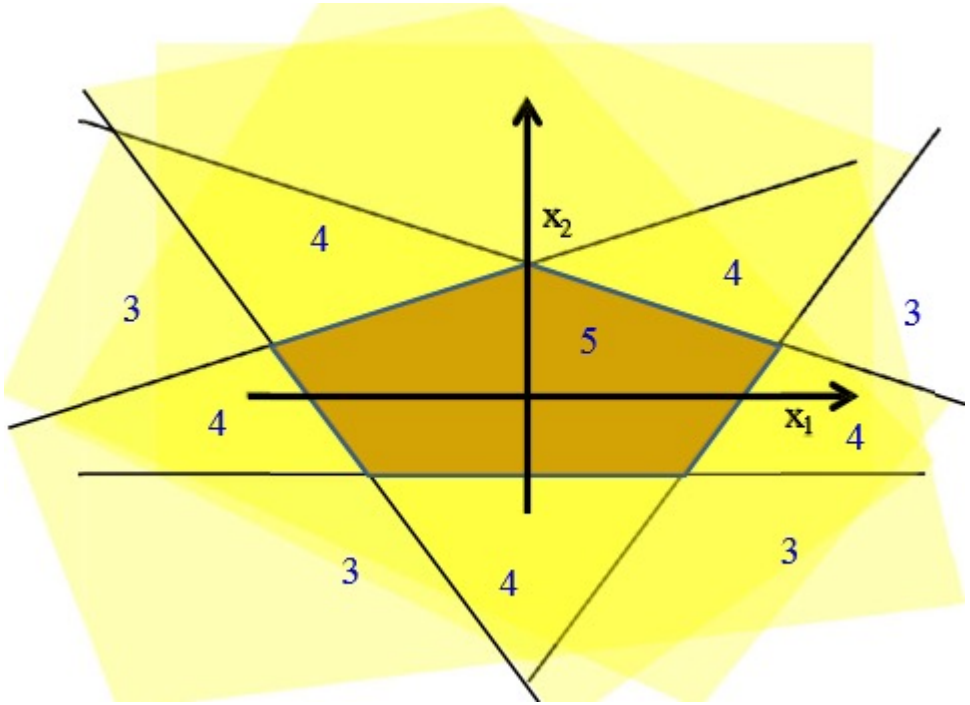
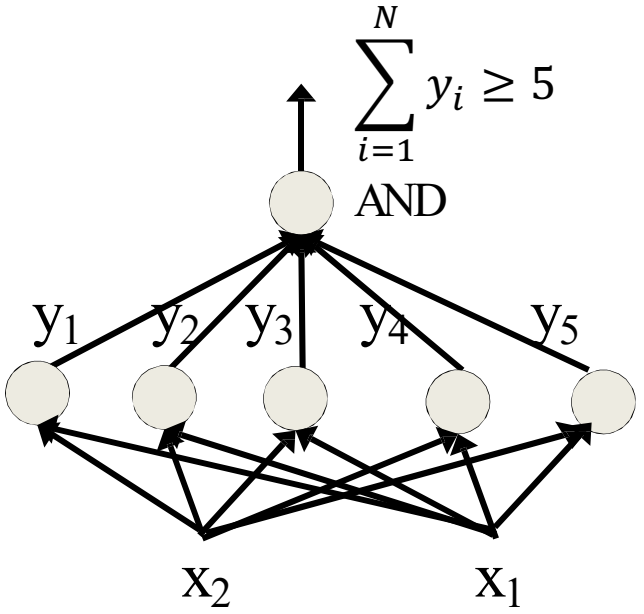
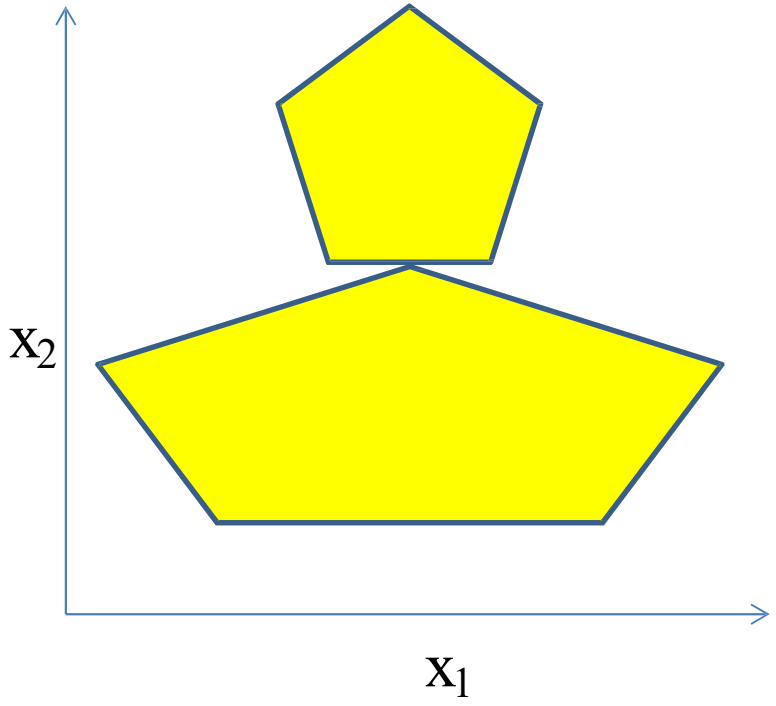
Booleans over the reals

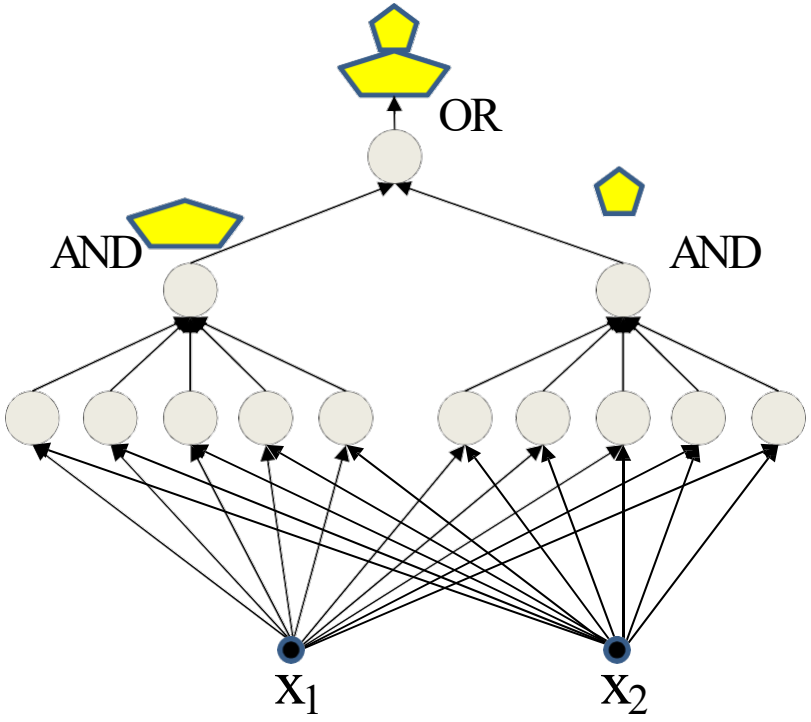




- The network must fire if the input is in the coloured area

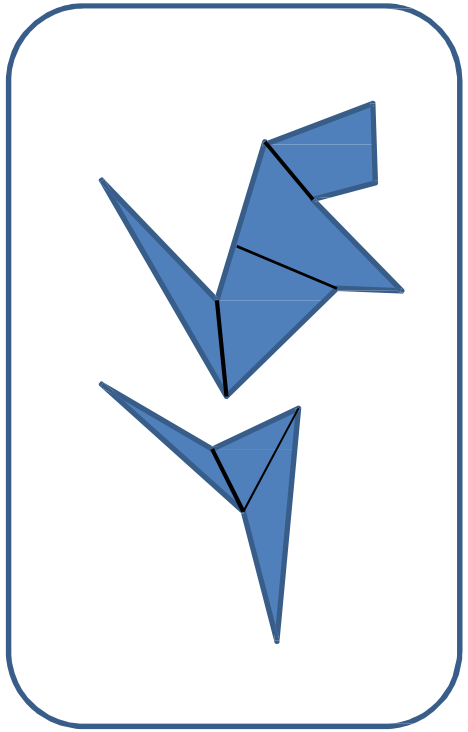
More complex decision boundaries

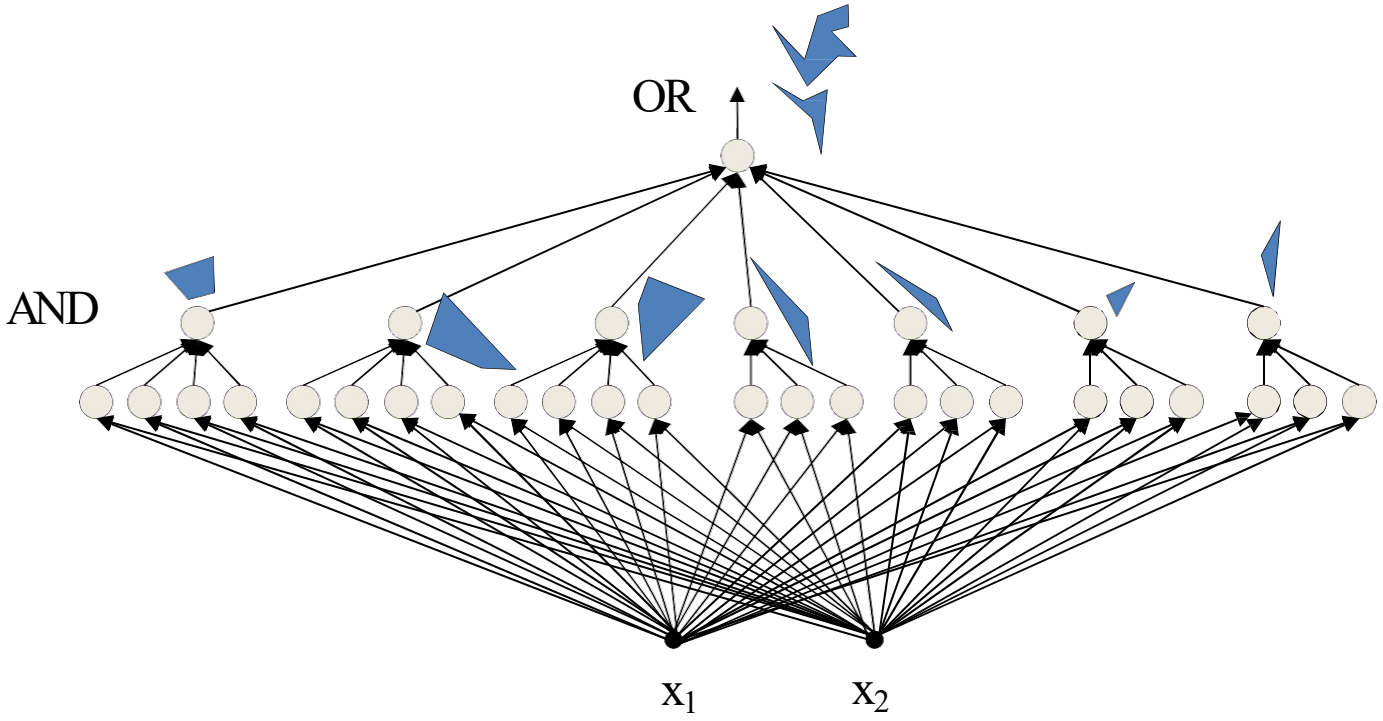




- Network to fire if the input is in the yellow area
  - "OR" two polygons
  - A third layer is required

Complex decision boundaries



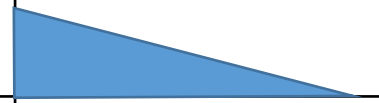
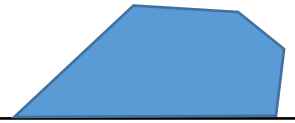
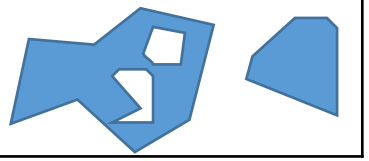


- Can compose arbitrarily complex decision boundaries
  - With only one hidden layer!
  - How?

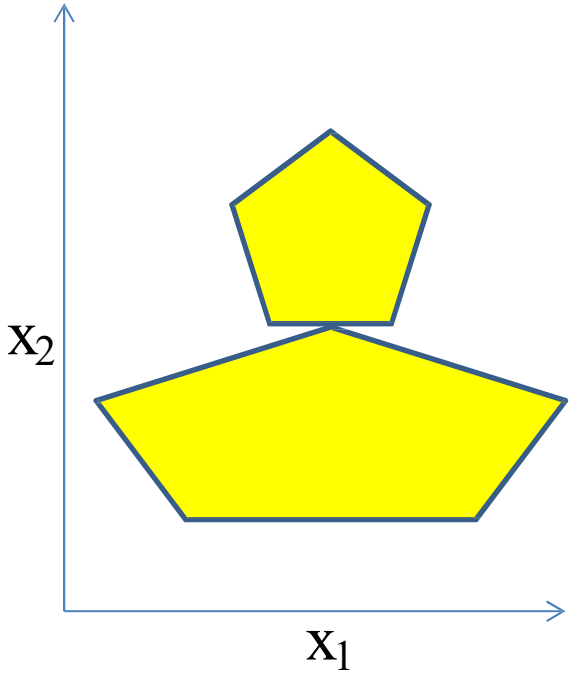
MLP with Different Number of Layers

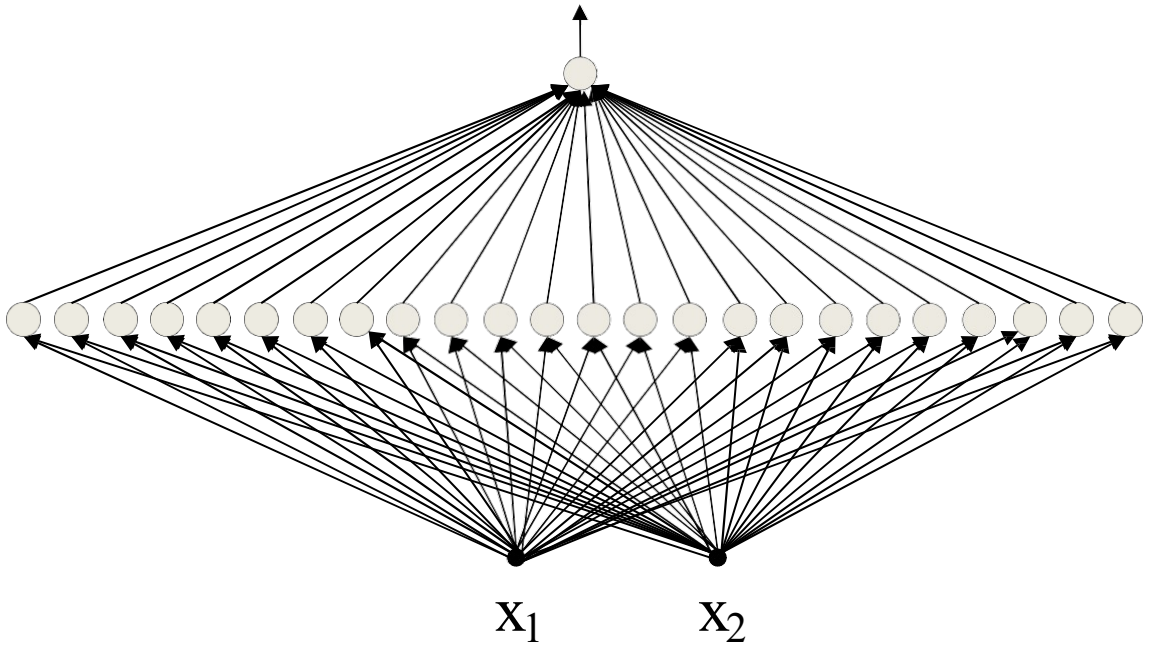
MLP with unit step activation function

Decision region found by an output unit.

Structure	Type of Decision Regions	Interpretation	Example of region
Single Layer (no hidden layer)	Half space	Region found by a hyper-plane	
Two Layer (one hidden layer)	Polyhedral (open or closed) region	Intersection of half spaces	
Three Layer (two hidden layers)	Arbitrary regions	Union of polyhedrals	

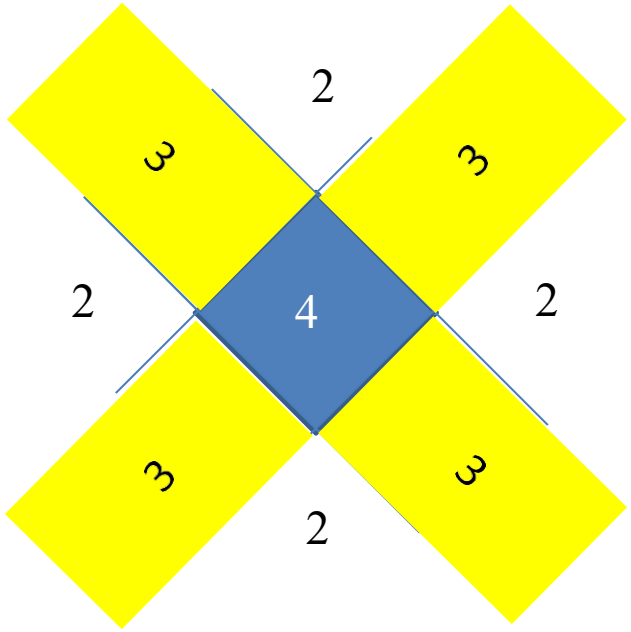
Exercise: compose this with one hidden layer



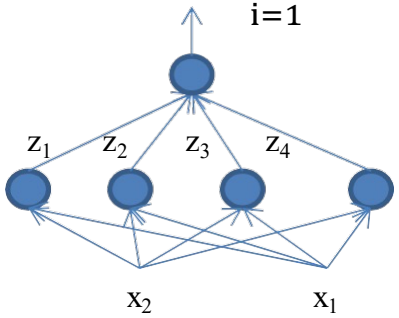


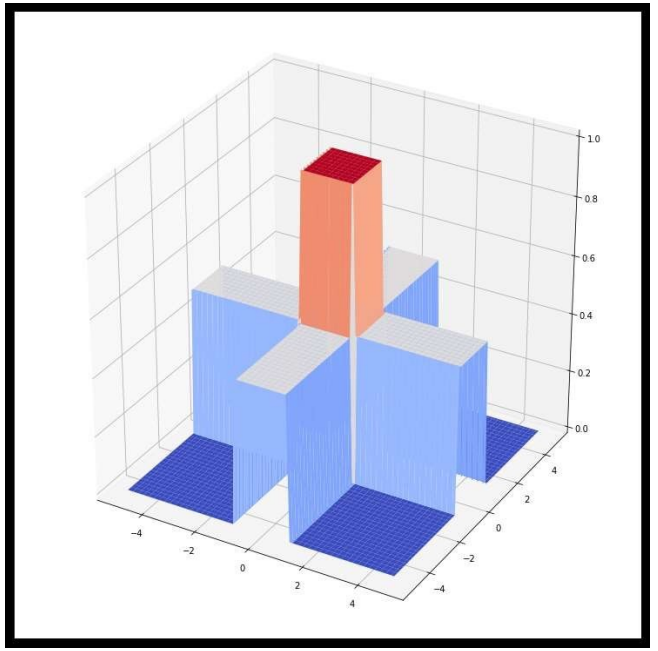
- How would you compose the decision boundary to the left with only one hidden layer?

Composing a square decision boundary



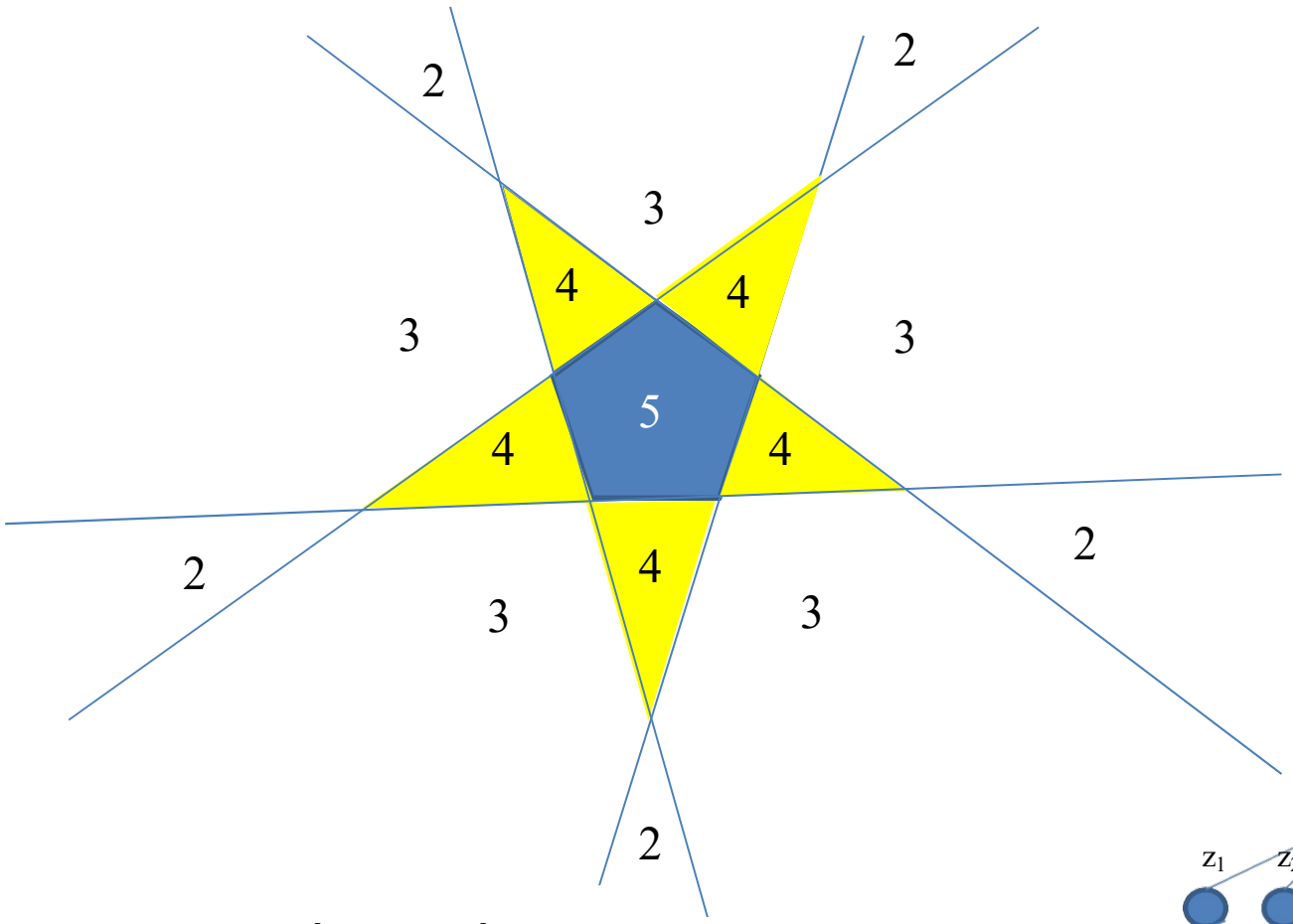
$$\sum_{i=1}^{4} z_i \geq 4 \; ?$$

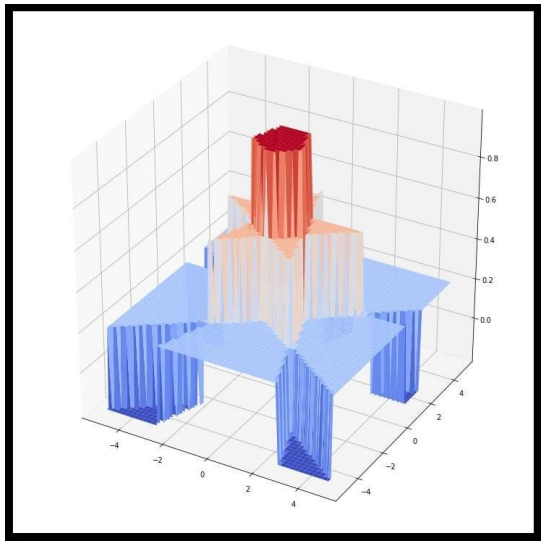


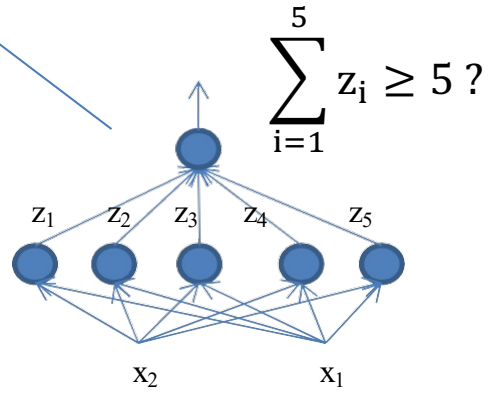


- The polygon net

Composing a square decision boundary

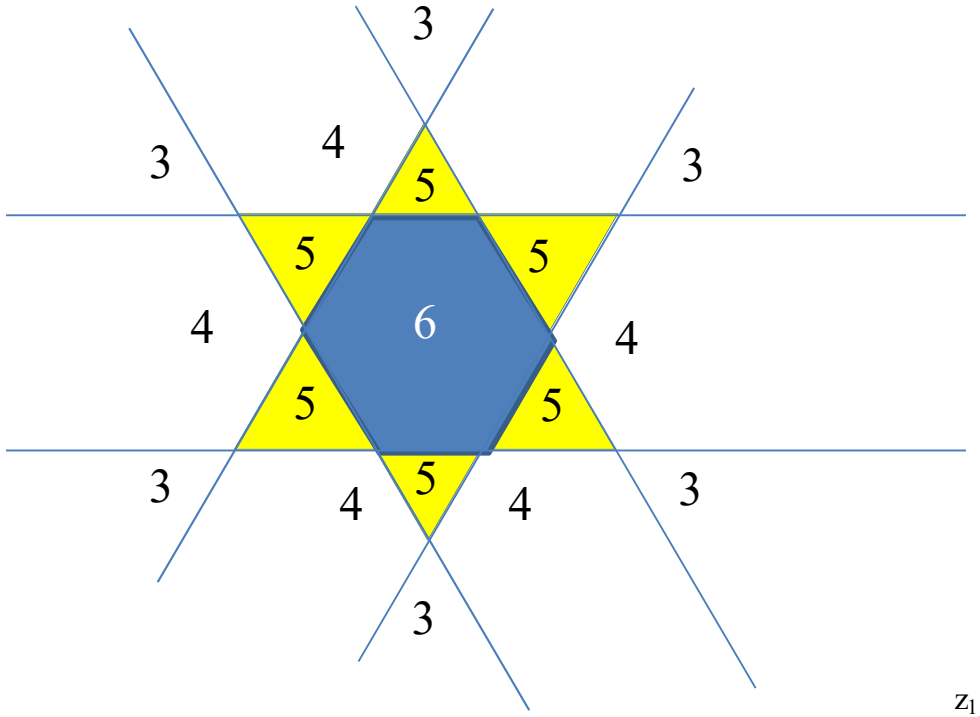


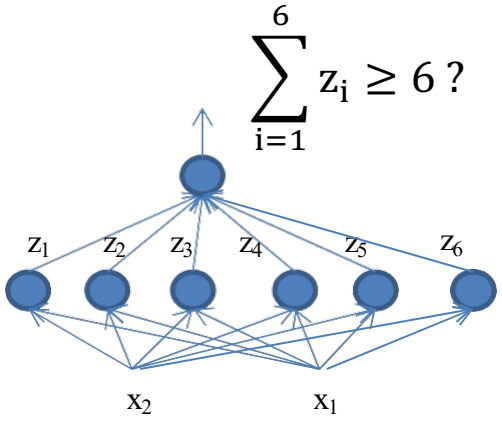


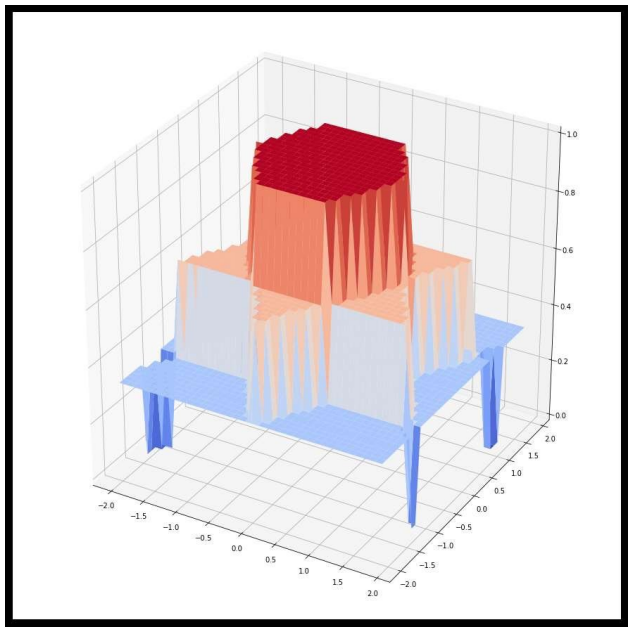


- The polygon net

Composing a pentagon

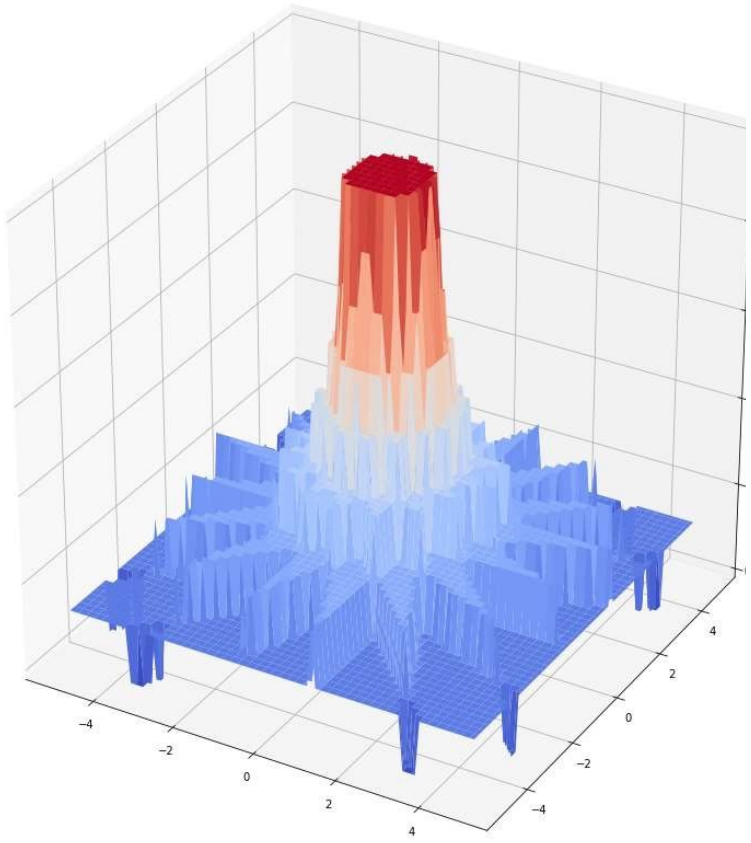






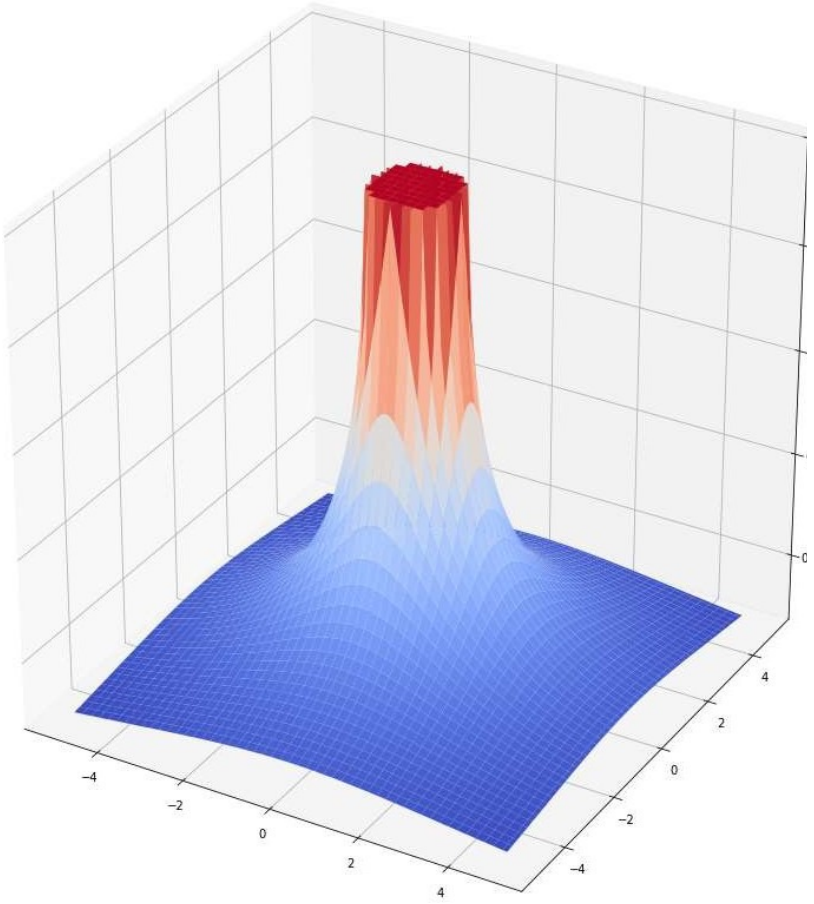
- The polygon net

16 sides



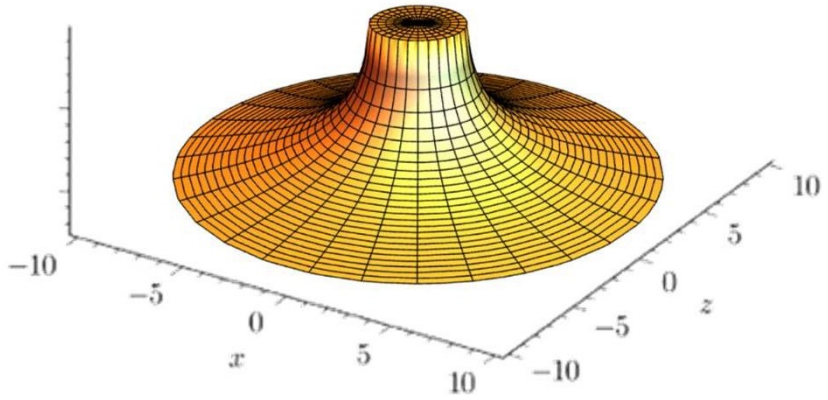
- What are the sums in the different regions?

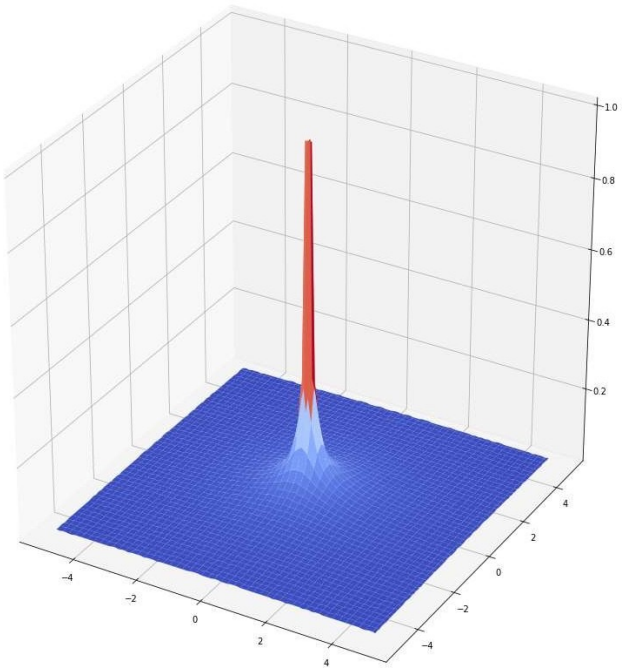
Polygon net



- Increasing the number of sides M reduces the area outside the polygon that have M/2 < Sum < M

In the limit

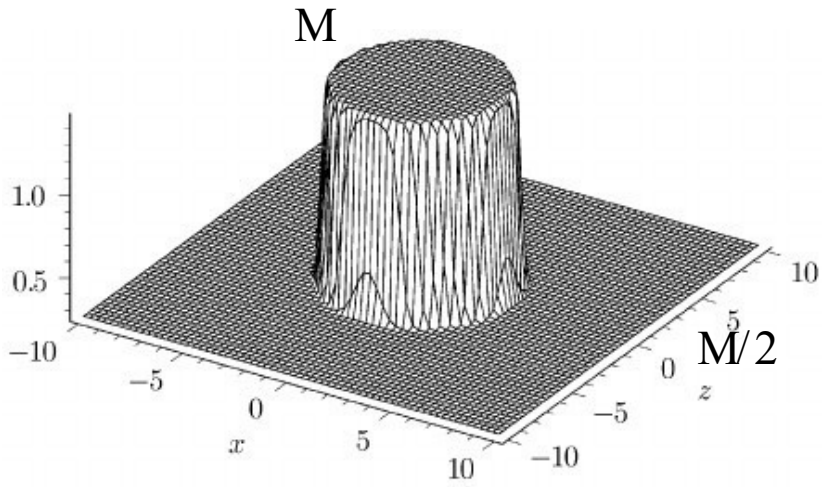


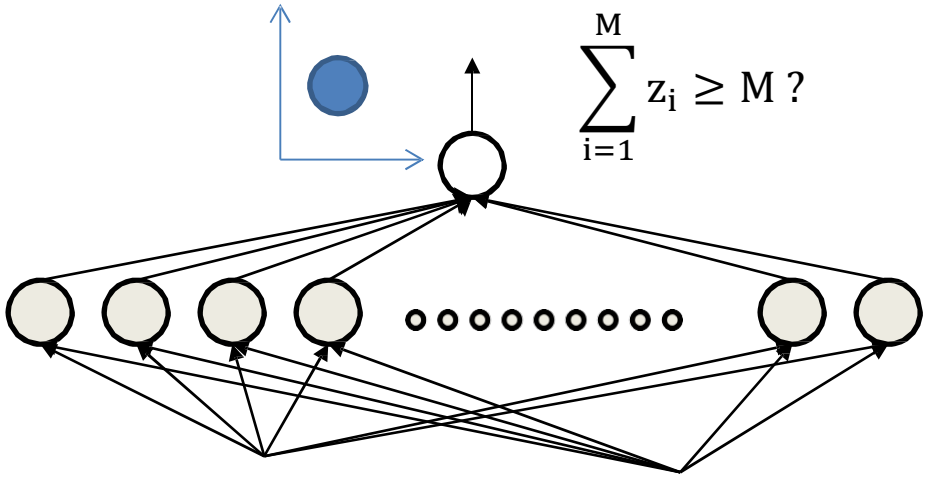


$$\sum_i z_i = M\left(1 - \frac{1}{\pi}\arccos\left(\min(1, \frac{radius}{|x - cent|})\right)\right)$$

- For small radius, it's a near perfect cylinder
  - M in the cylinder, M/2 outside

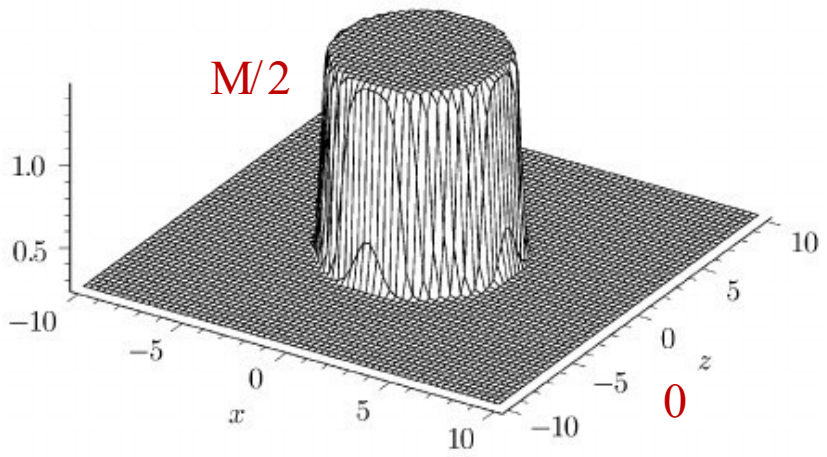
Composing a circle

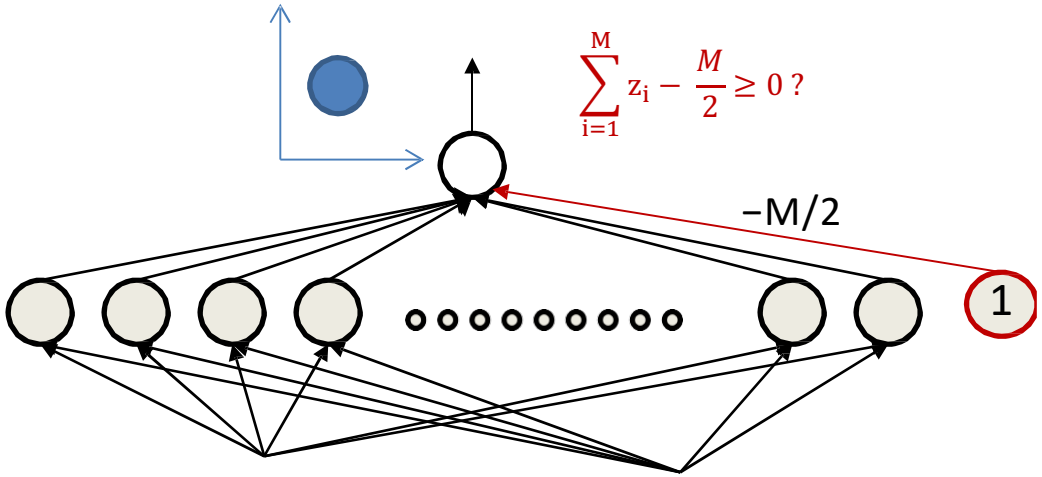




- The circle net
  - Very large number of neurons
  - Sum is M inside the circle, M/2 outside almost everywhere
  - Circle can be at any location

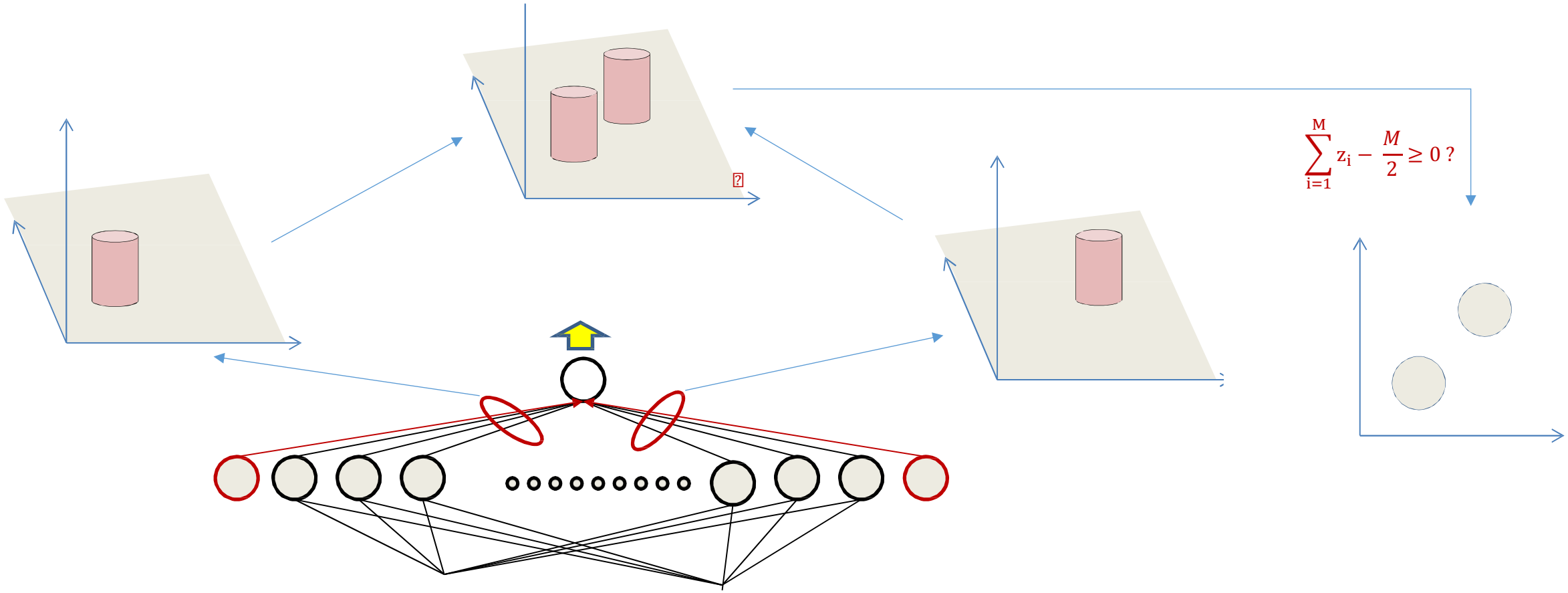
Composing a circle





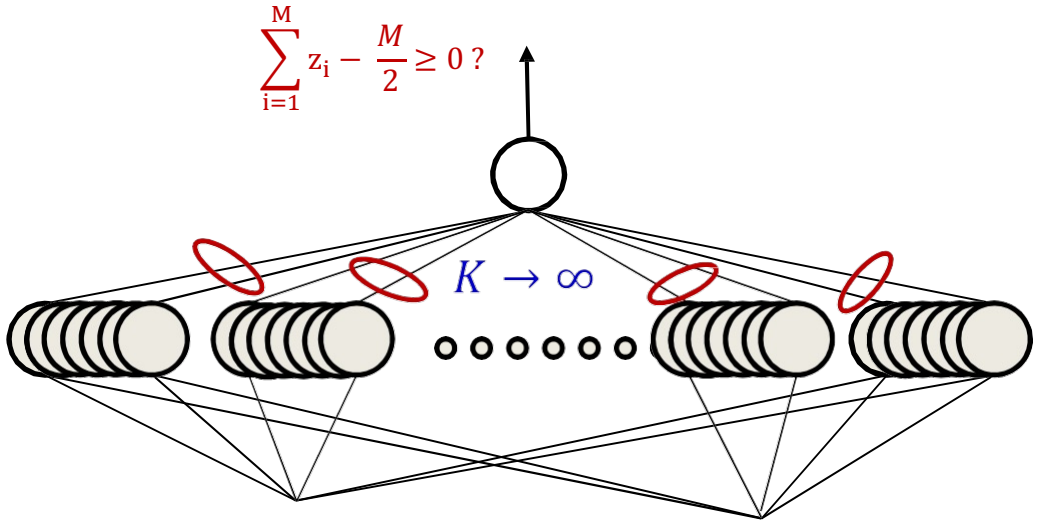
- The circle net
  - Very large number of neurons
  - Sum is M/2 inside the circle, 0 outside almost everywhere
  - Circle can be at any location

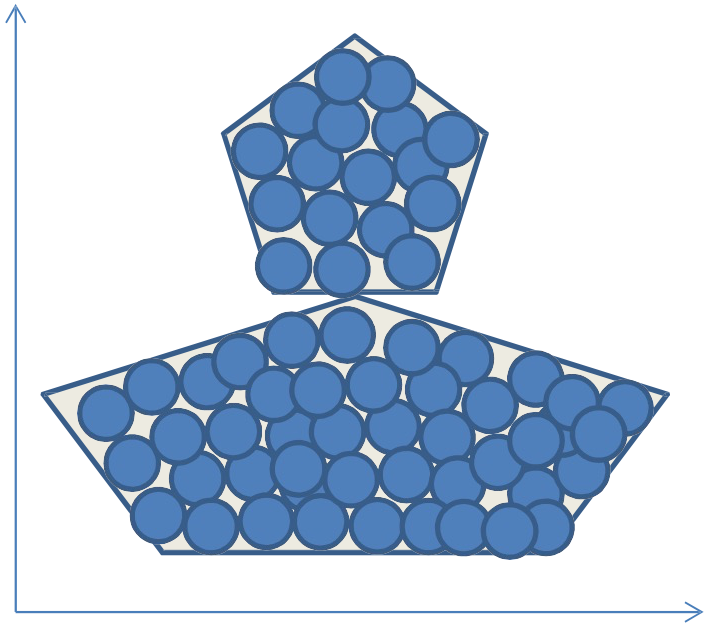
Adding circles



- The “sum” of two circles sub nets is exactly M/2 inside either circle, and 0 almost everywhere outside

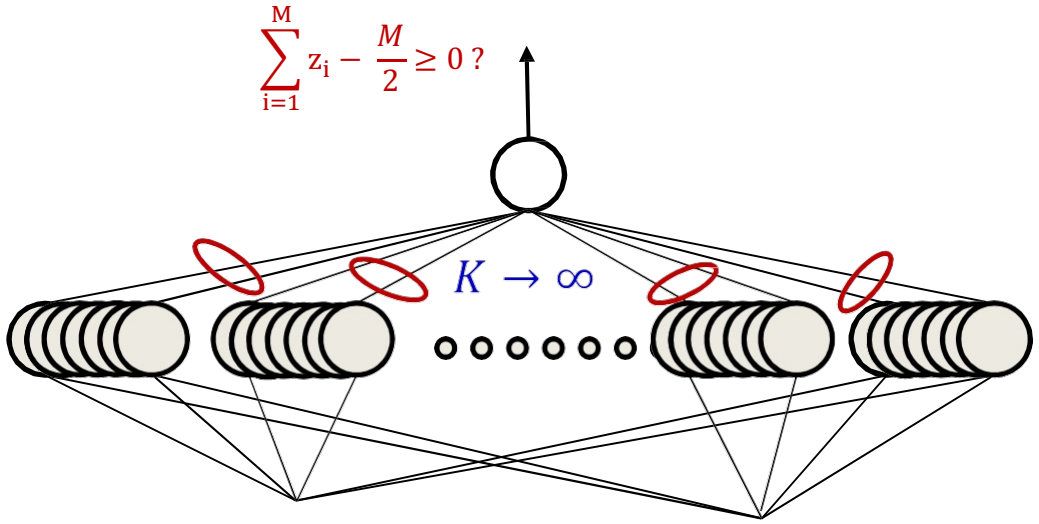
Composing an arbitrary figure

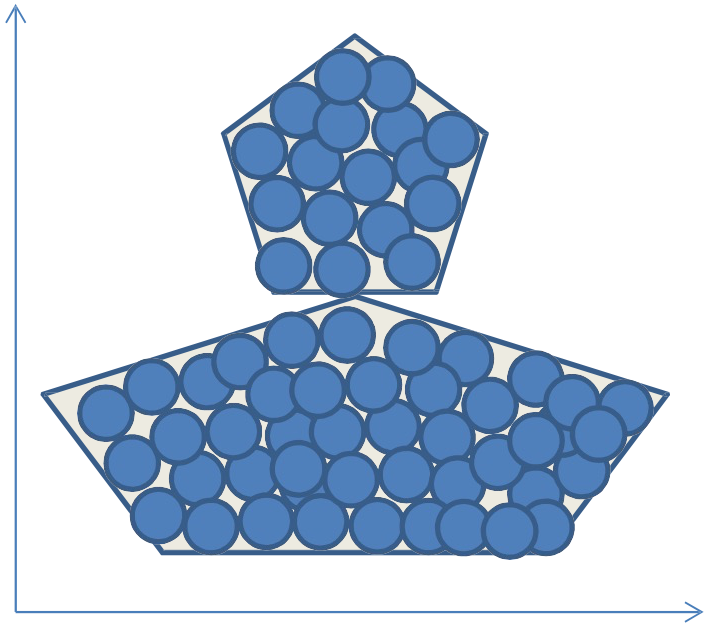




- Just fit in an arbitrary number of circles
  - More accurate approximation with greater number of smaller circles
  - Can achieve arbitrary precision

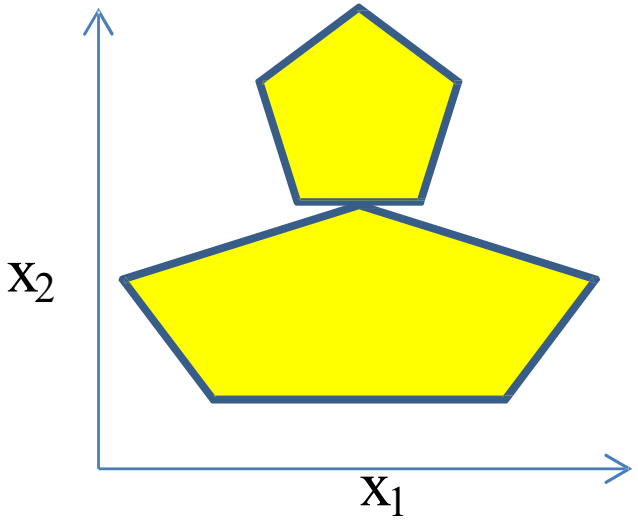
MLP: Universal classifier

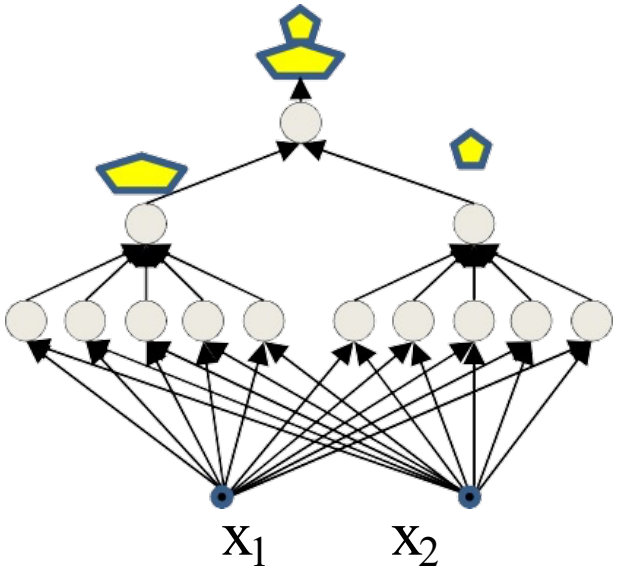


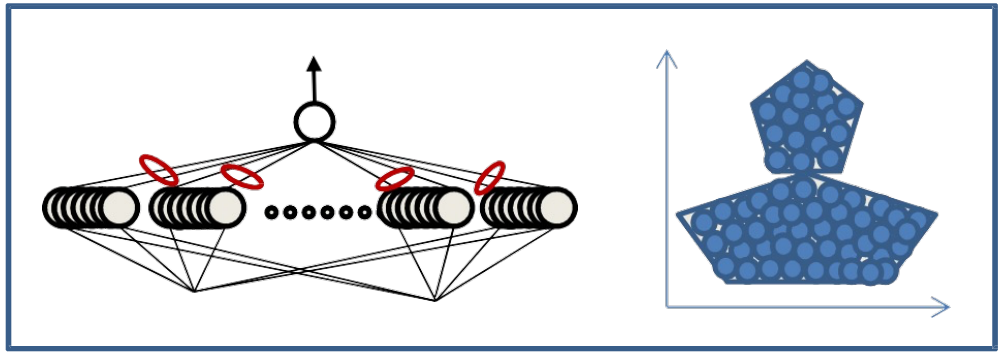


- MLPs can capture any classification boundary
- A one-layer MLP can model any classification boundary
- MLPs are universal classifiers

Depth and the universal classifier







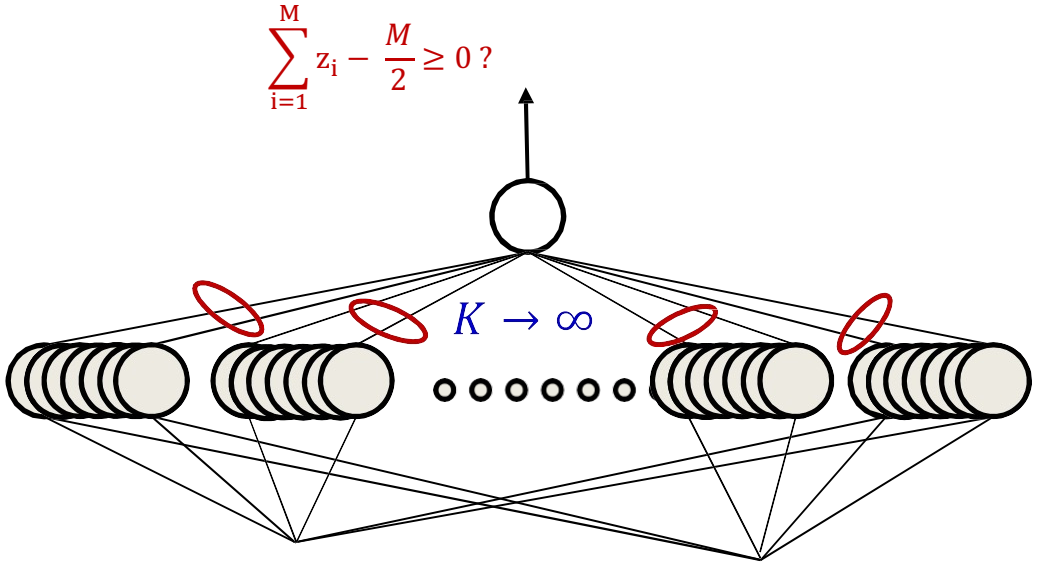
- Deeper networks can require far fewer neurons

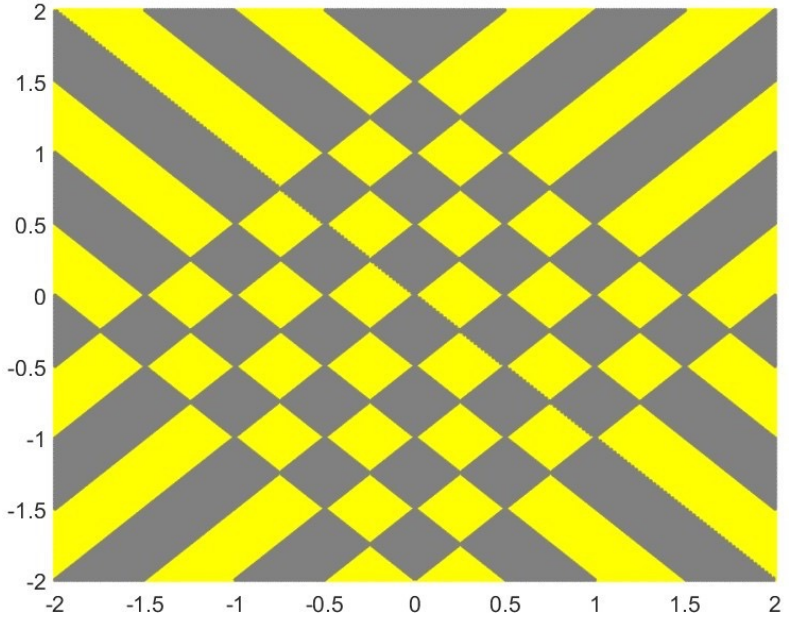
Optimal depth in generic nets

- We look at a different pattern:
  - “worst case” decision boundaries

- For threshold-activation networks
  - Generalizes to other nets

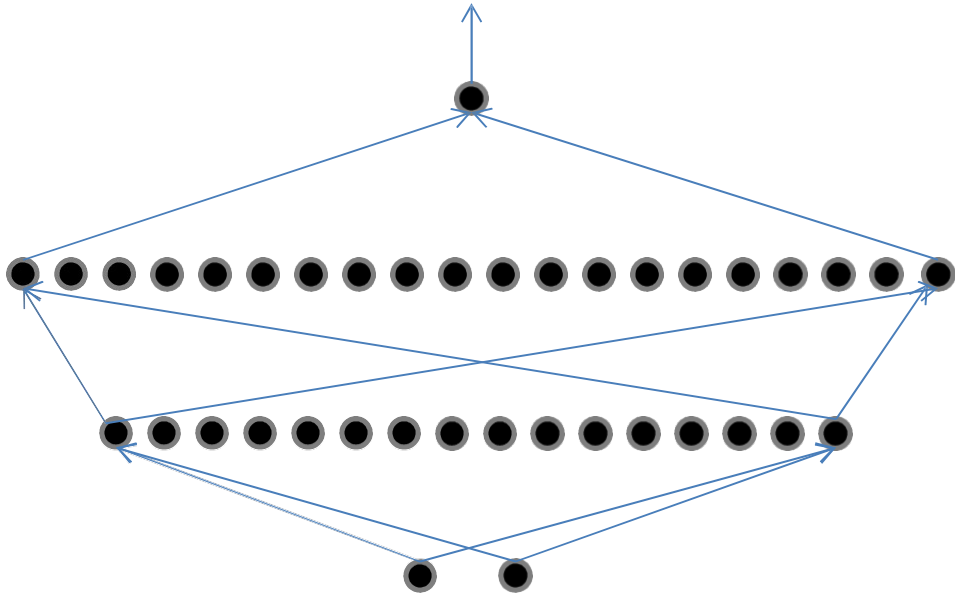
Optimal depth

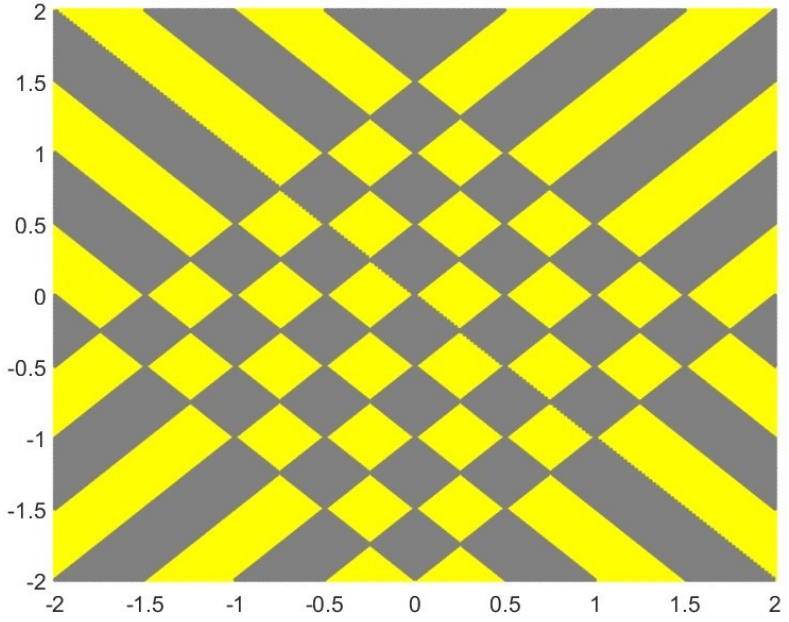




- A naïve one-hidden-layer neural network will required infinite hidden neurons

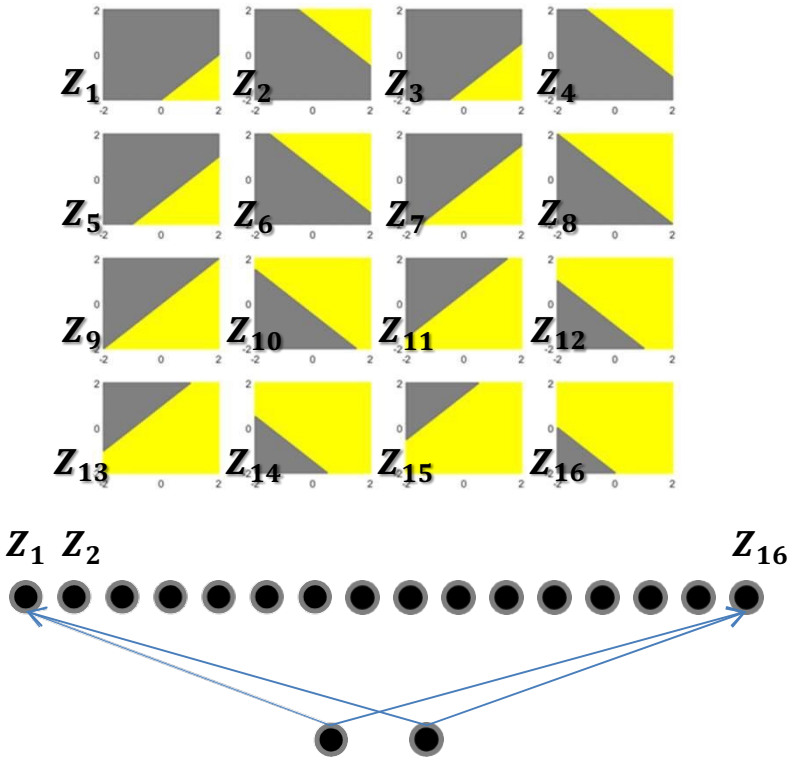
Optimal depth

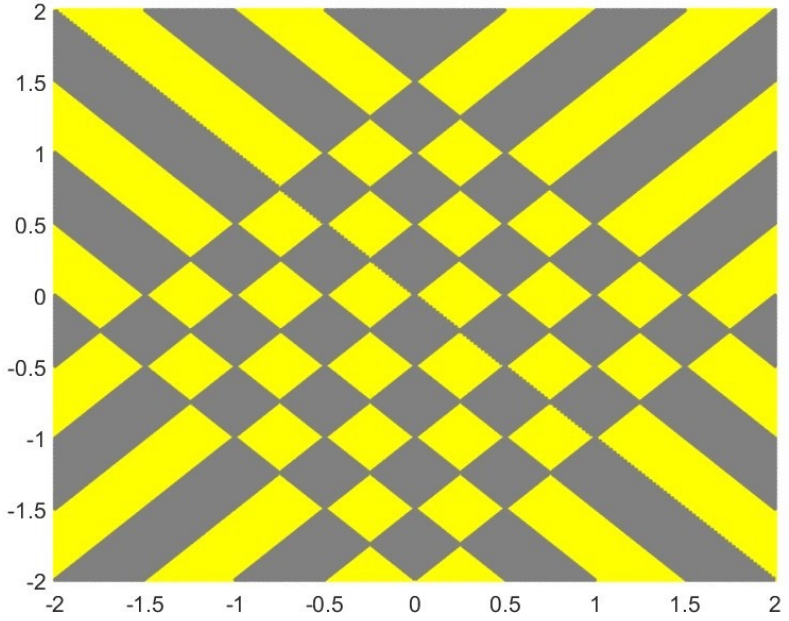




- Two hidden-layer network: 56 hidden neurons

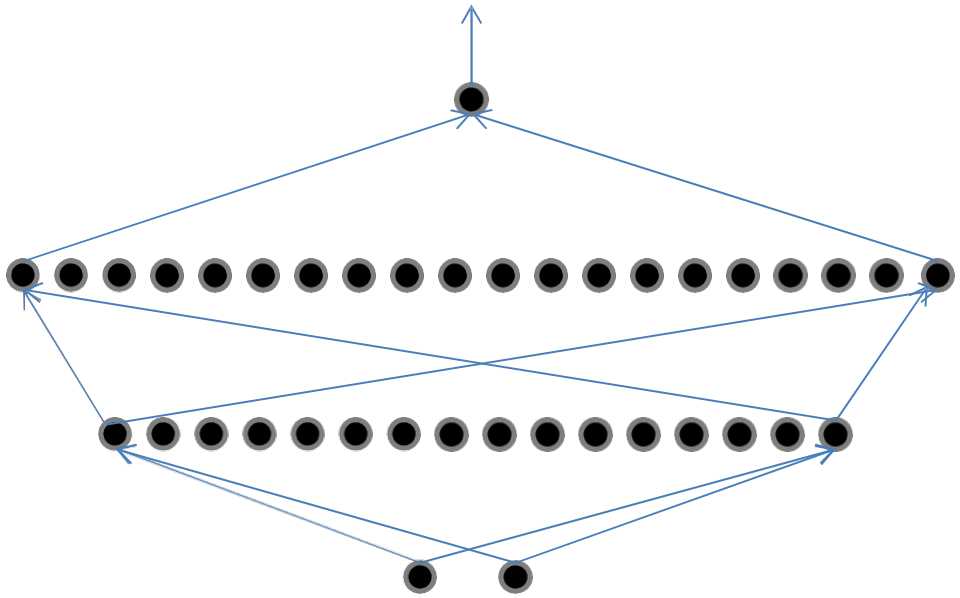
Optimal depth

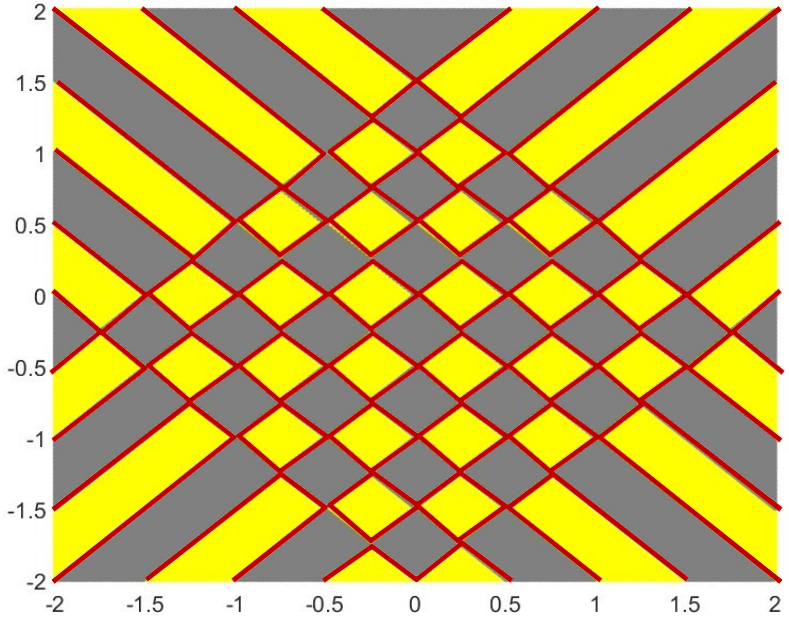




- Two layer network: 56 hidden neurons
  - 16 neurons in hidden layer 1

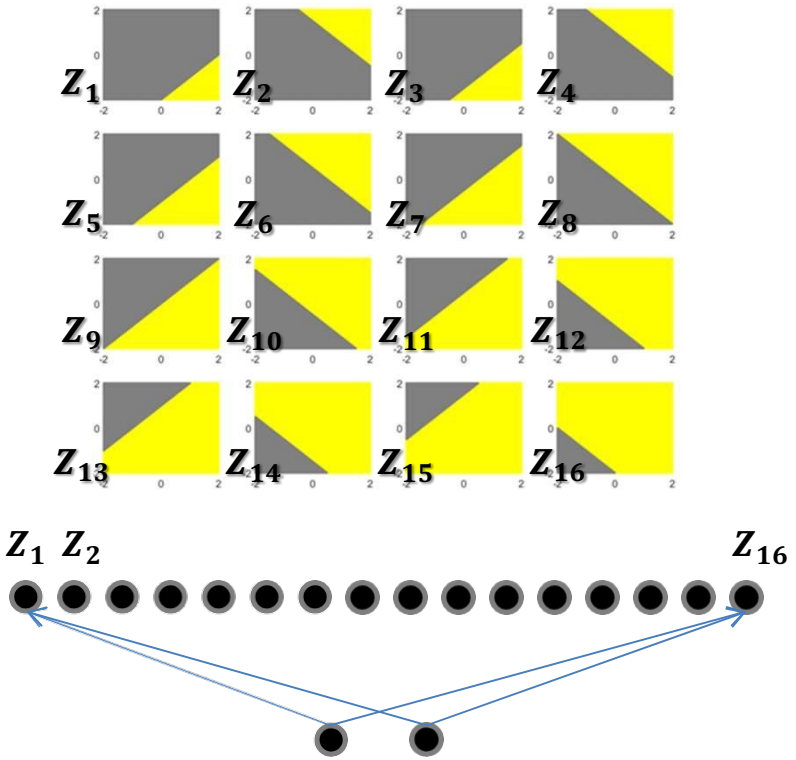
Optimal depth

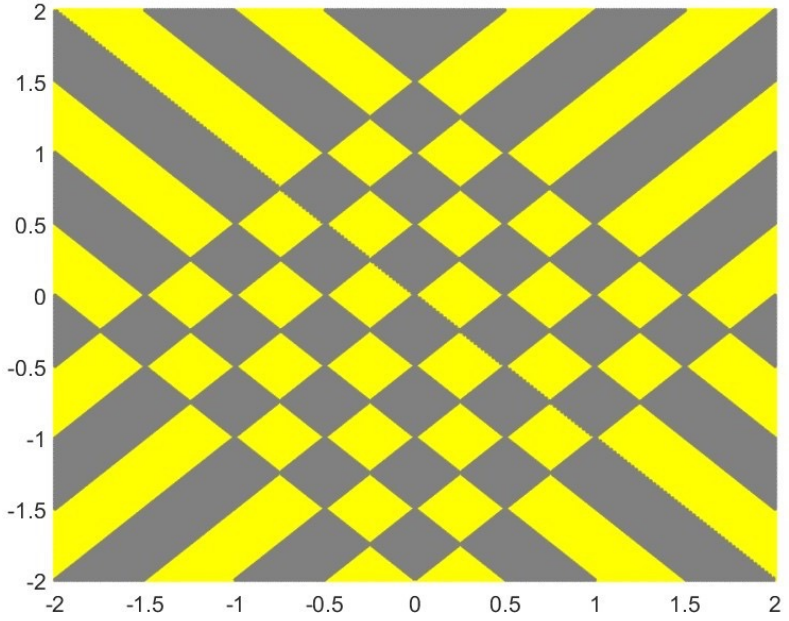




- Two-layer network: 56 hidden neurons
  - 16 in hidden layer 1
  - 40 in hidden layer 2
  - 57 total neurons, including output neuron

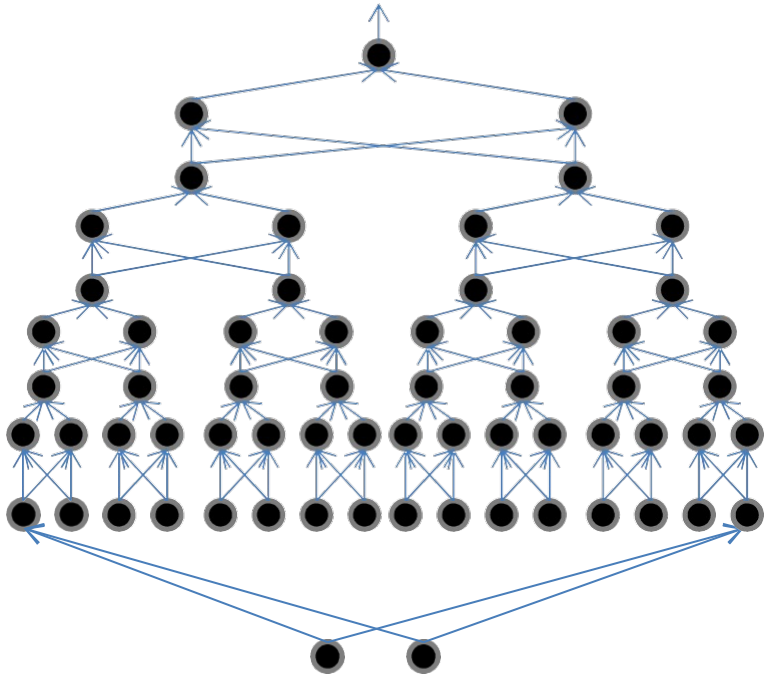
Optimal depth

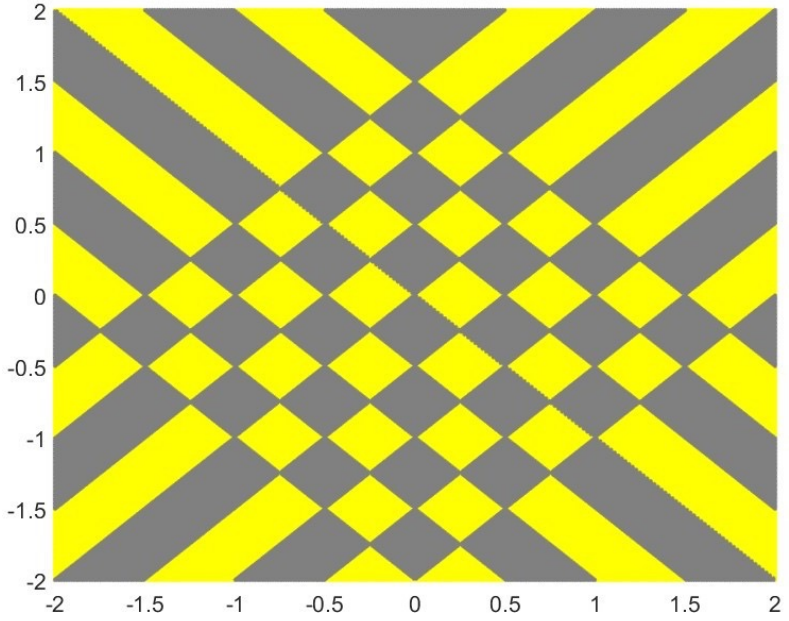




- But this isjust $Z_1 \oplus Z_2 \oplus \cdots \oplus Z_{16}$

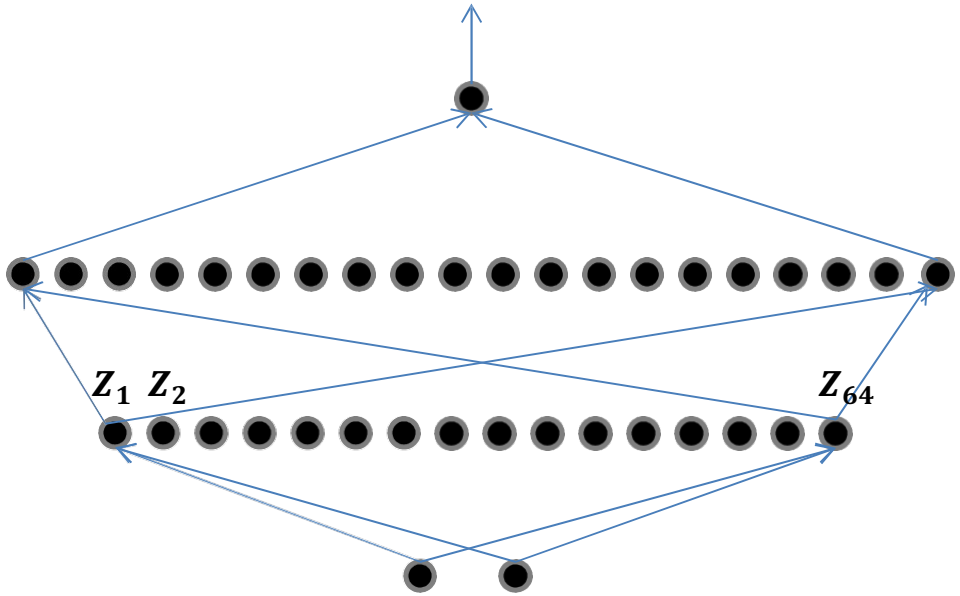
Optimal depth

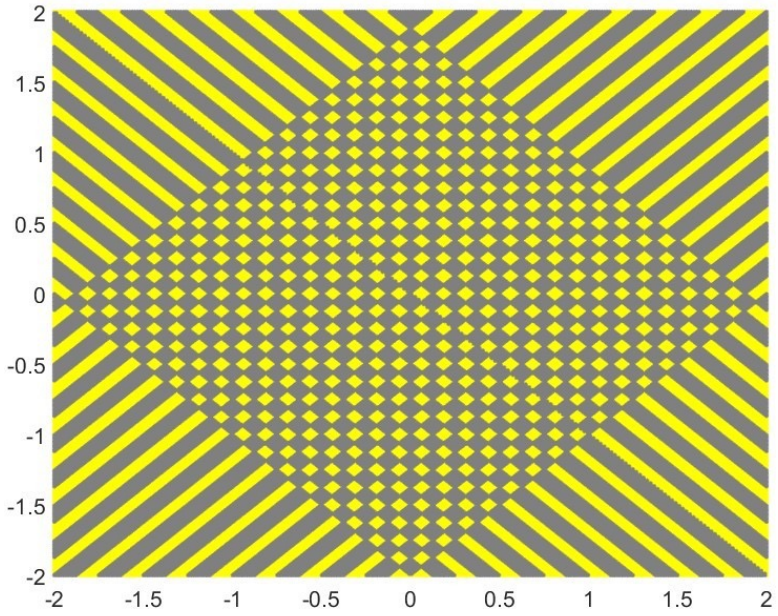




- But this is just $Z_1 \oplus Z_2 \oplus \cdots \oplus Z_{16}$
  - The XOR net will require 16+15×3 = 61 neurons
    - 46 neurons if we use a two-gate XOR

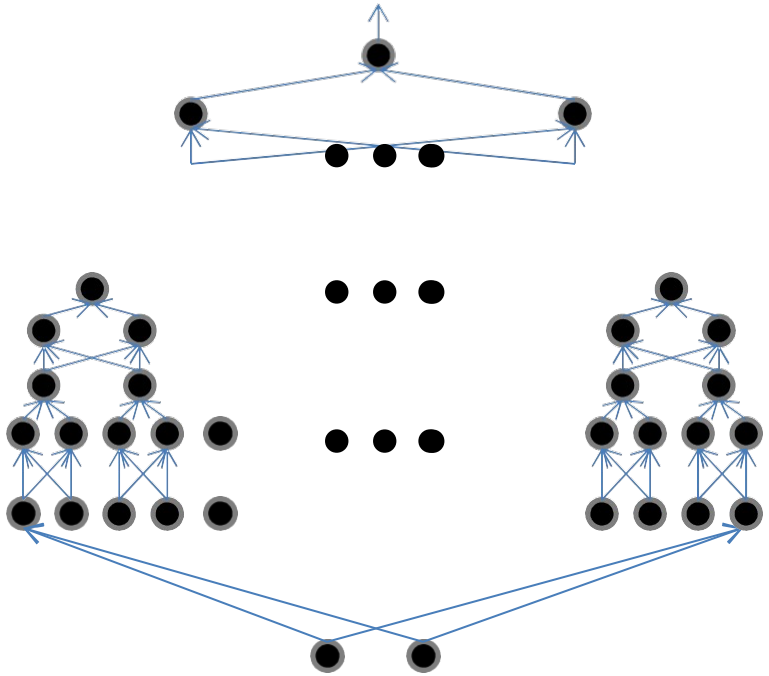
Optimal depth

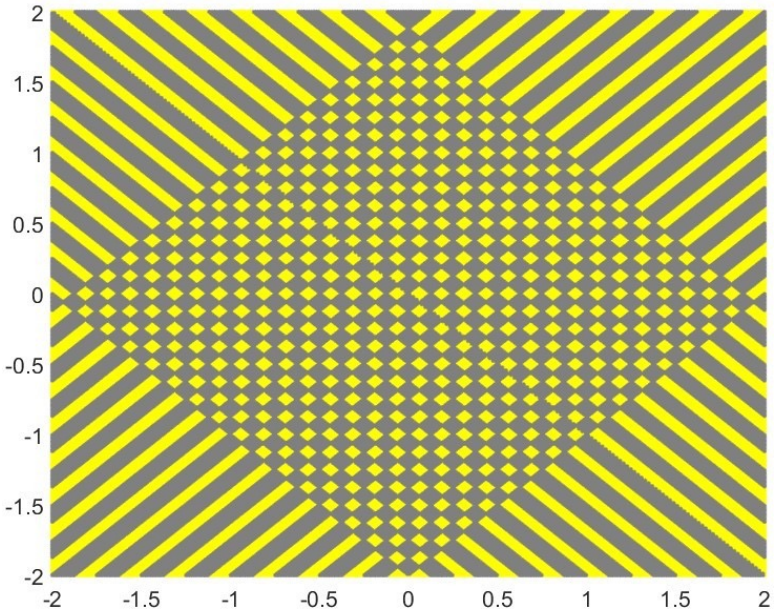




- Two hidden layers: 608 hidden neurons
  - 64 in layer 1
  - 544 in layer 2
- 609 total neurons (including output neuron)

Optimal depth

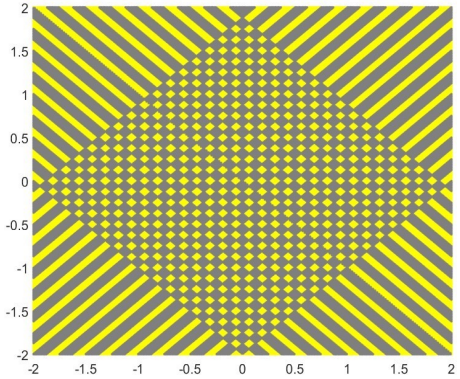




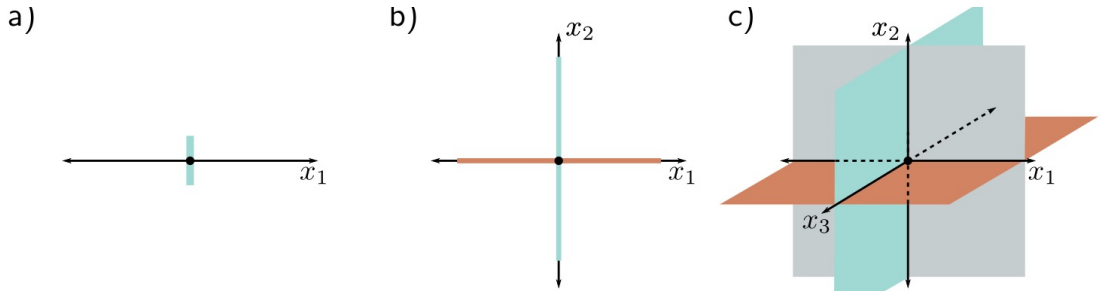
- XOR network (12 hidden layers): 253 neurons
  - 190 neurons with 2-gate XOR
- The difference in size between the deeper optimal (XOR) net and shallower nets increases with increasing pattern complexity and input dimension

Network size?

- In this problem the 2-layer net was quadratic in the no of neurons in 1st hidden layer
  - $O(M^2)$ neurons in second hidden layer
  - Not exponential even though the pattern is an XOR
  - Why?
    - The data are two-dimensional and its exponential w.r.t. $D = 2$



- For general case of M mutually intersecting hyperplanes in D dimensions, we will need $O\left(\frac{M^D}{(D-1)!}\right)$ weights (assuming M>>D).
  - Increasing input dimensions can increase the worst-case size of the shallower network exponentially, but not the XOR net
    - The size of the XOR net depends only on the number of first-level linear detectors (M)

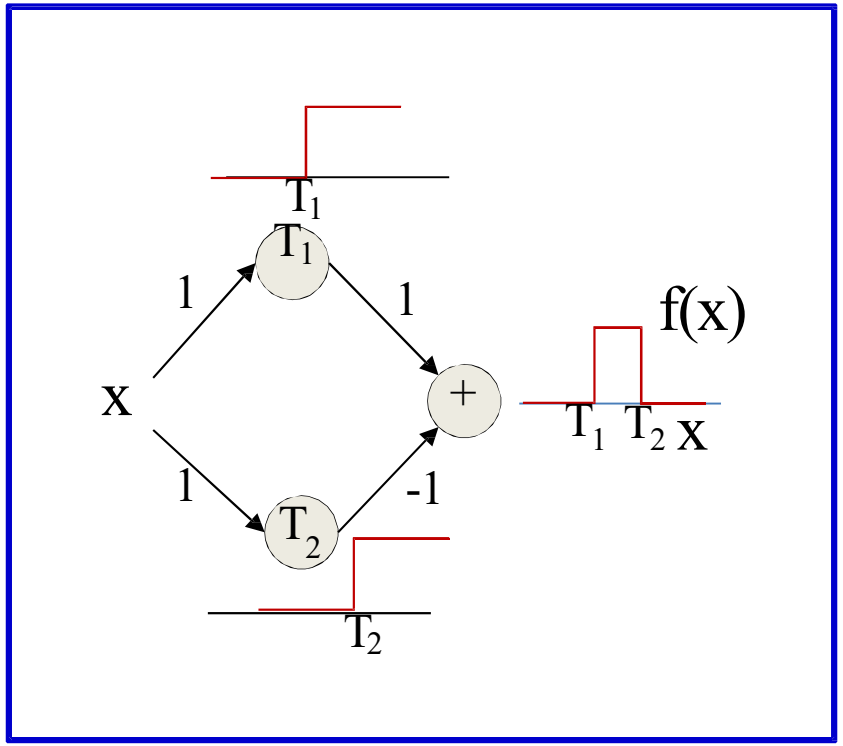


Summary

- Multi-layer perceptrons are Universal Boolean Machines
  - Even a network with a single hidden layer is a universal Boolean machine
- Multi-layer perceptrons are Universal Classification Functions
  - Even a network with a single hidden layer is a universal classifier
- But a single-layer network may require an exponentially large number of perceptrons than a deep one
- Deeper networks may require far fewer neurons than shallower networks to express the same function
  - Could be exponentially smaller
  - Deeper networks are more expressive

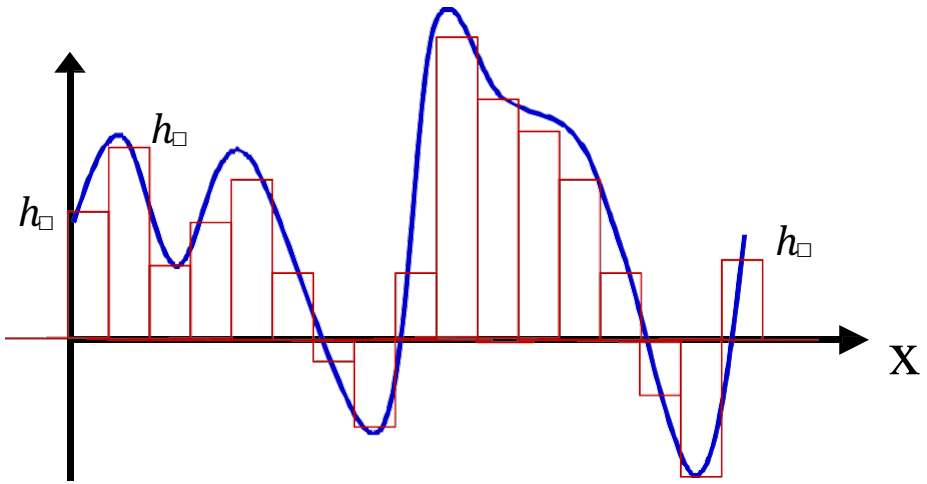
MLPs as universal approximators

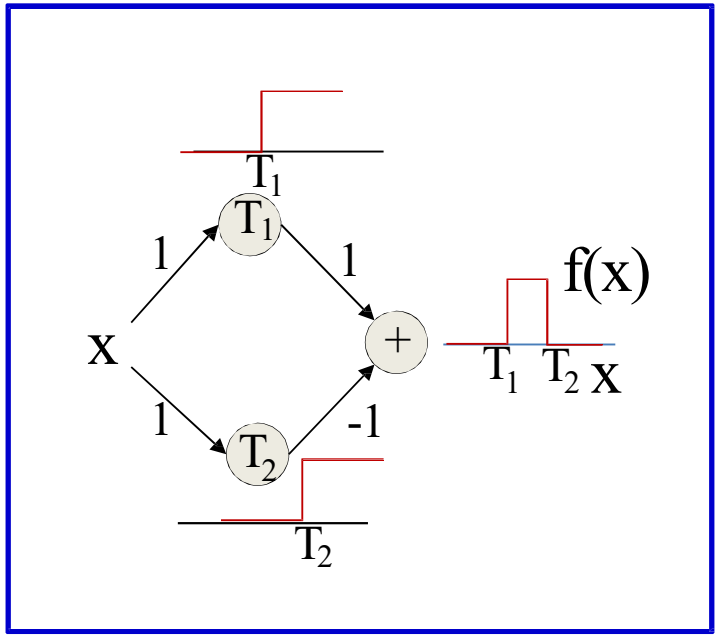
MLP as a continuous-valued regression



- A simple 3-unit MLP with a "summing" output unit can generate a "square pulse" over an input
  - Output is 1 only if the input lies between T_1 and T_2
  - T_1 and T_2 can be arbitrarily specified

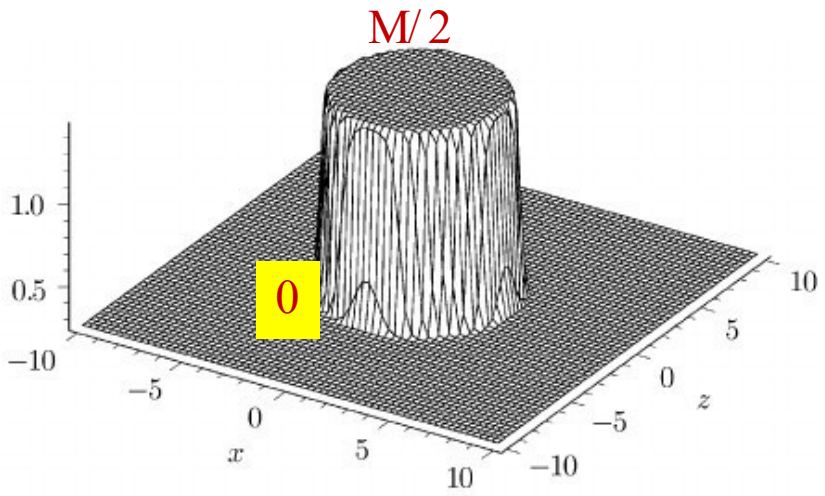
MLP as a continuous-valued regression

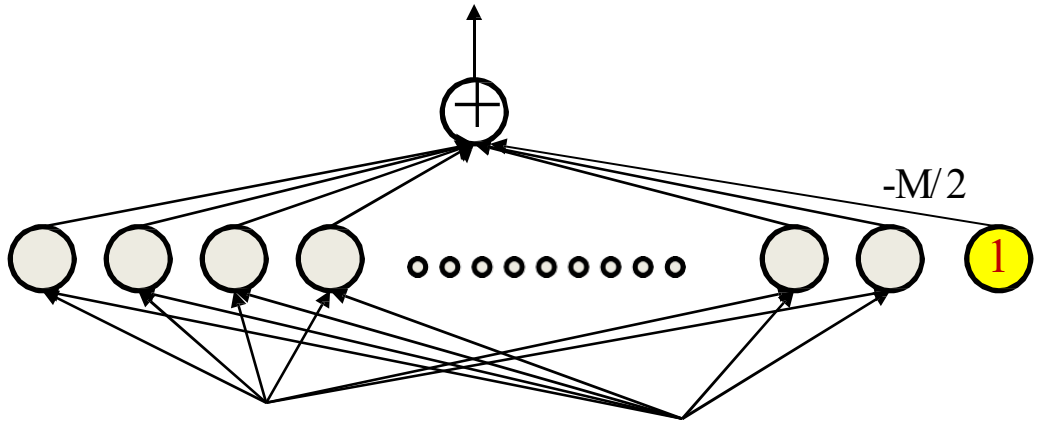




- A simple 3-unit MLP can generate a “square pulse” over an input
- An MLP with many units can model an arbitrary function over an input
  - To arbitrary precision
    - Simply make the individual pulses narrower
- A one-layer MLP can model an arbitrary function of a single input

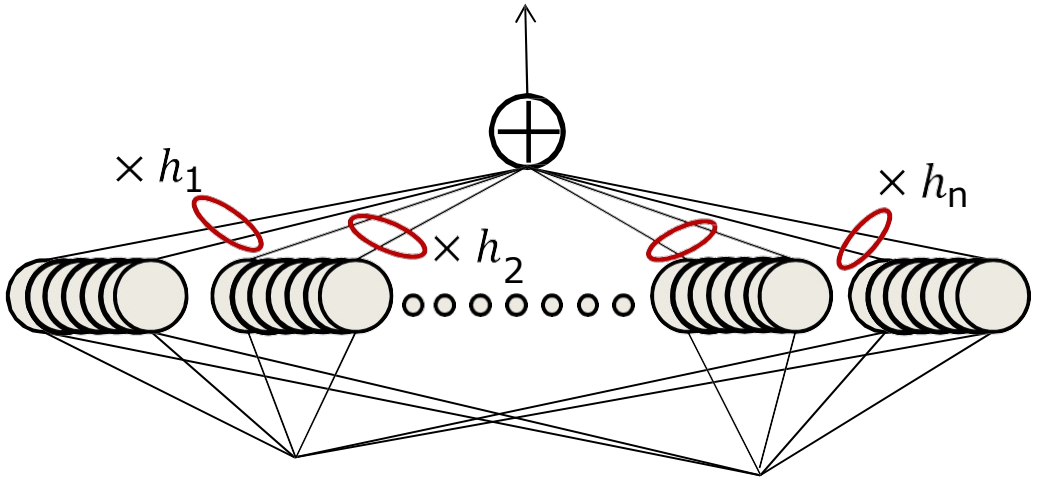
For higher dimensions

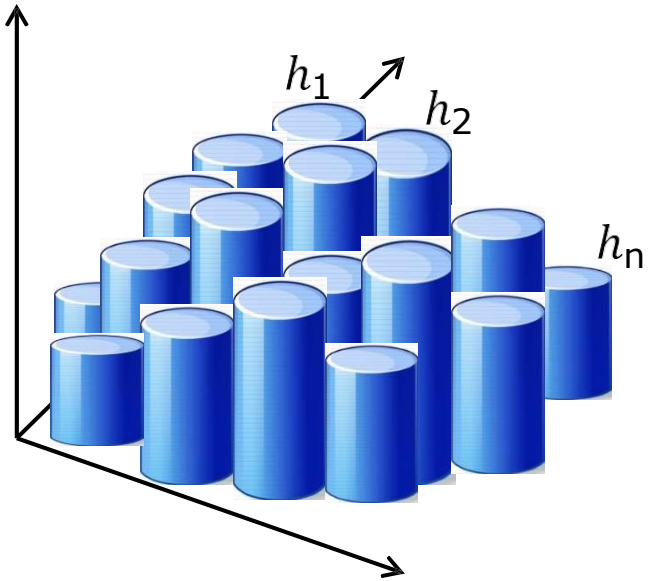




- An MLP can compose a cylinder
  - $\frac{M}{2}$ in the circle, 0 outside

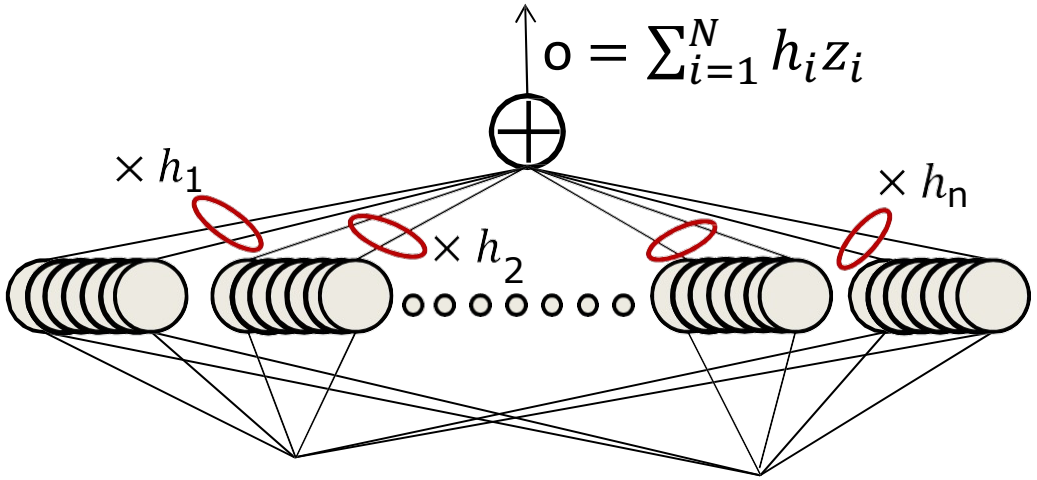
MLP as a continuous-valued function

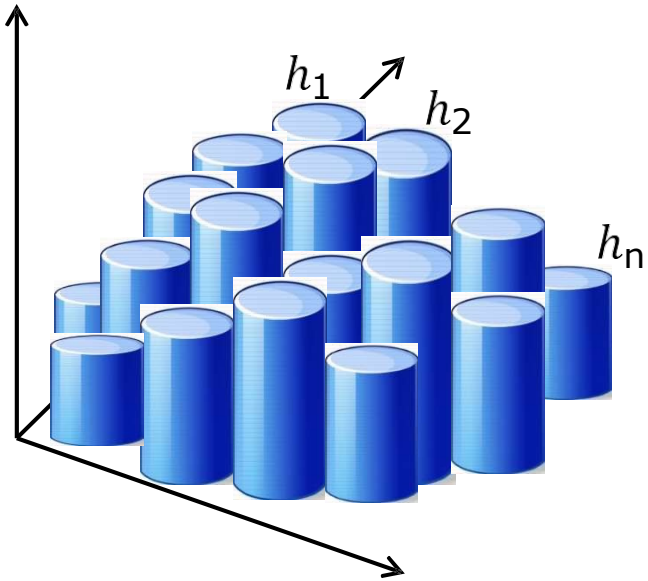




- MLPs can actually compose arbitrary functions in any number of dimensions!
  - Even with only one layer
    - As sums of scaled and shifted cylinders
  - To arbitrary precision
    - By making the cylinders thinner
  - The MLP is a universal approximator!

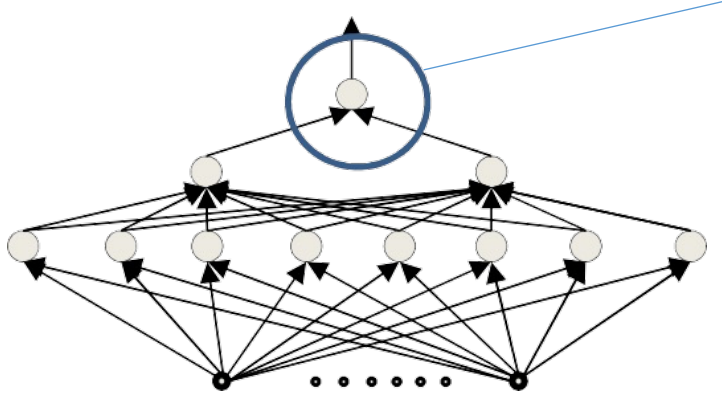
Caution: MLPs with additive output units are universal approximators

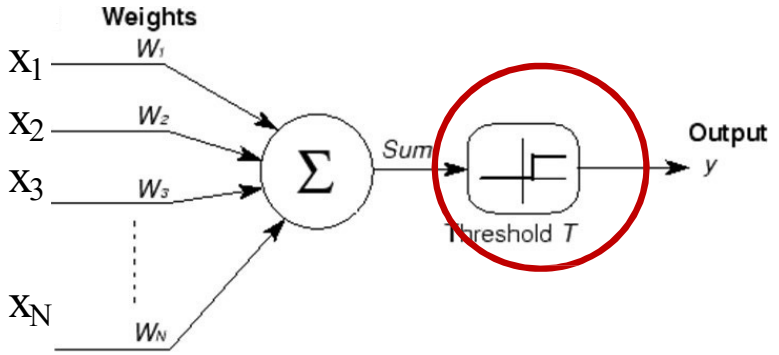


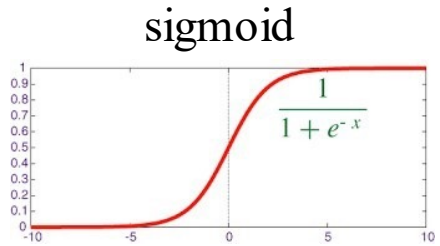


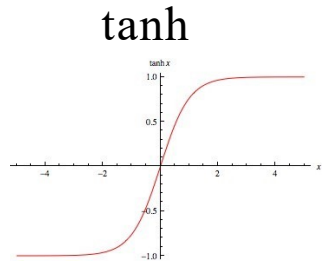
- MLPs can actually compose arbitrary functions in any number of dimensions!
- But explanation so far only holds if the output unit only performs summation
  - i.e. does not have an additional “activation”

“Proper” networks: Outputs with activations

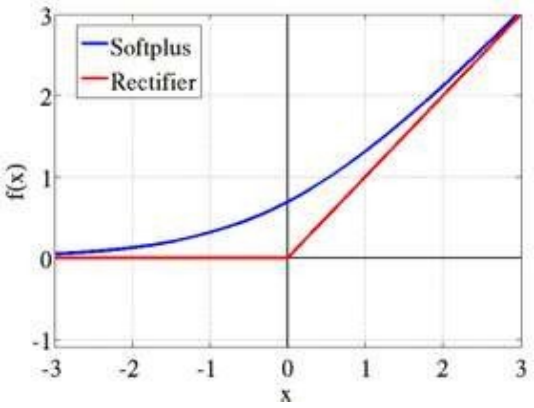






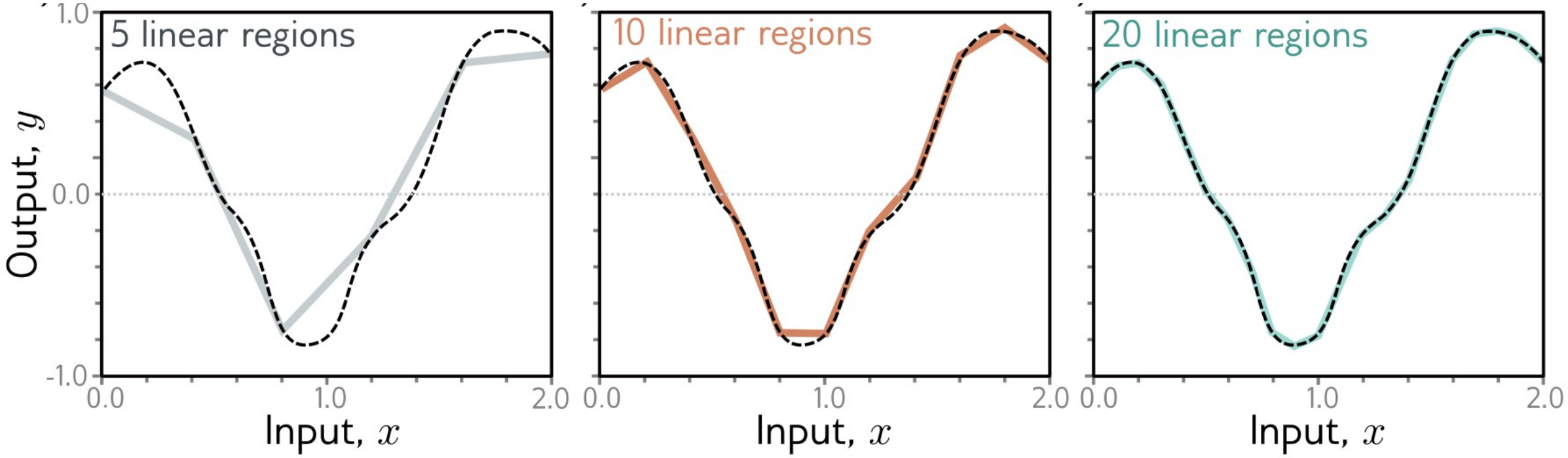


- Output neuron may have actual “activation”
  - Threshold, sigmoid, tanh, softplus, rectifier, etc.
- What is the property of such networks?

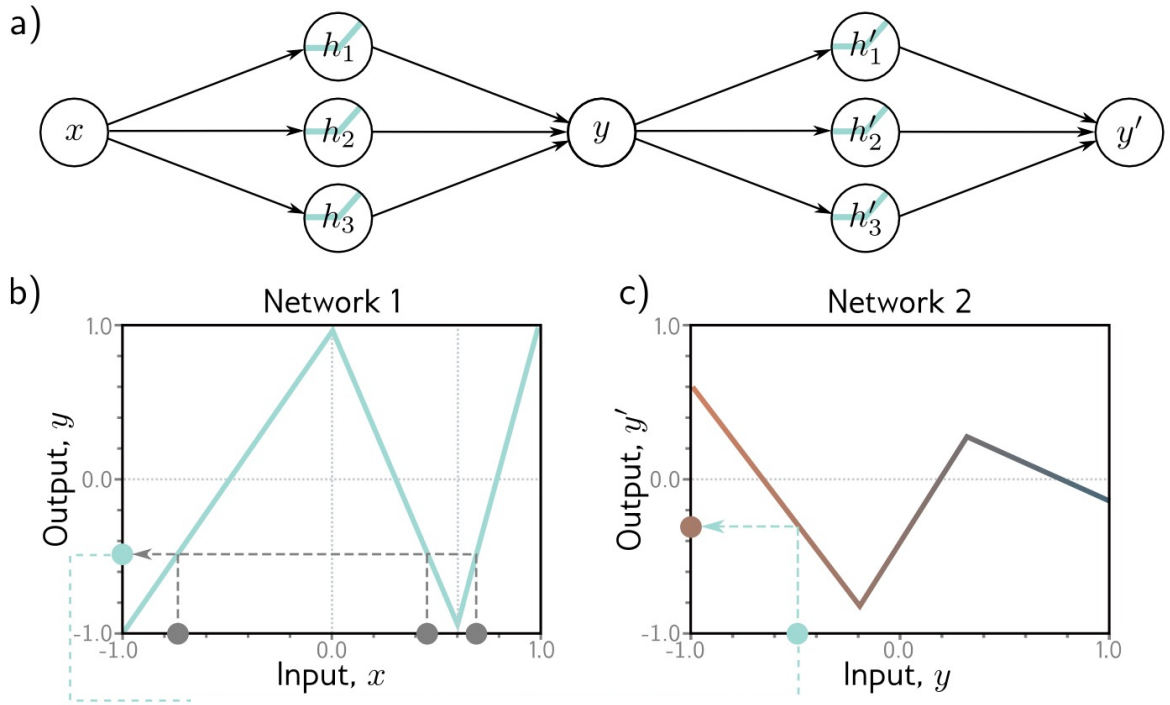


Approximating by MLP with ReLUs

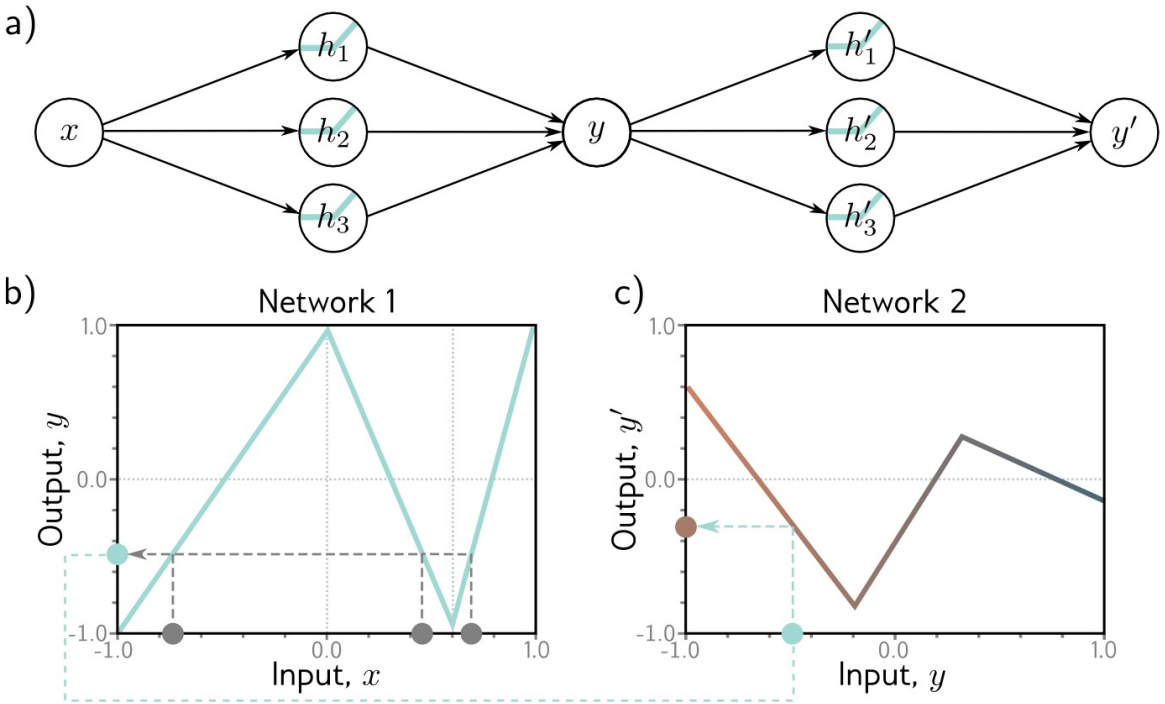
- Approximation by piecewise linear functions

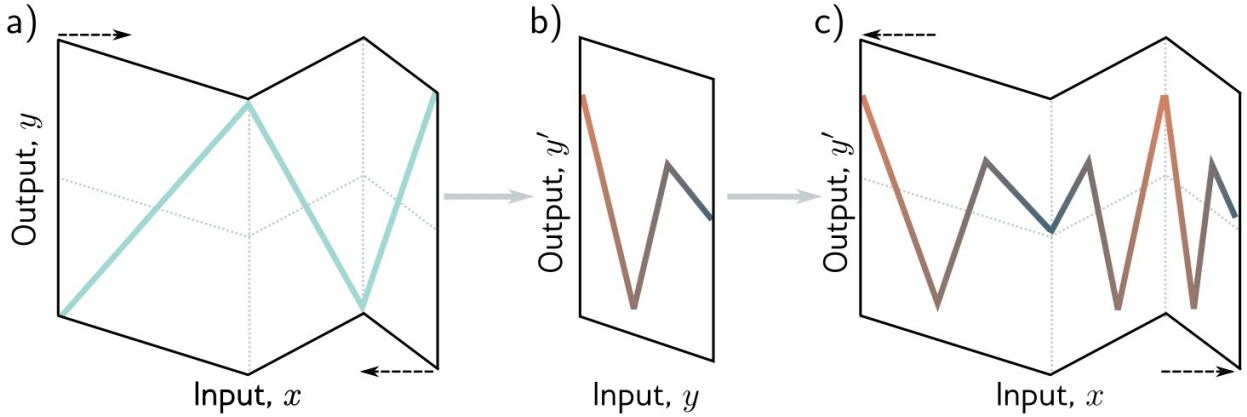


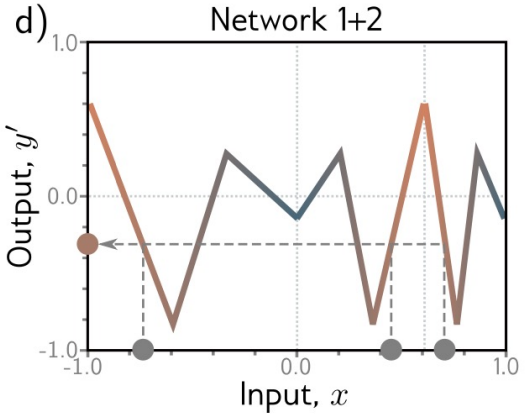
Composing Networks



Composing Networks



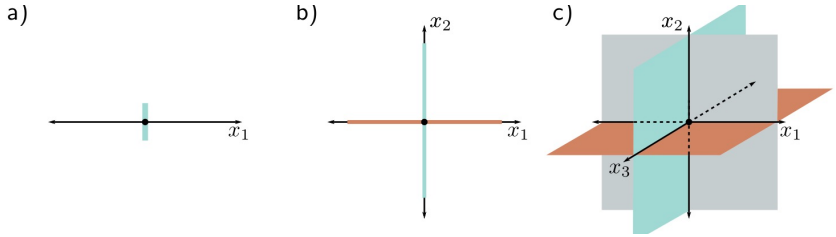




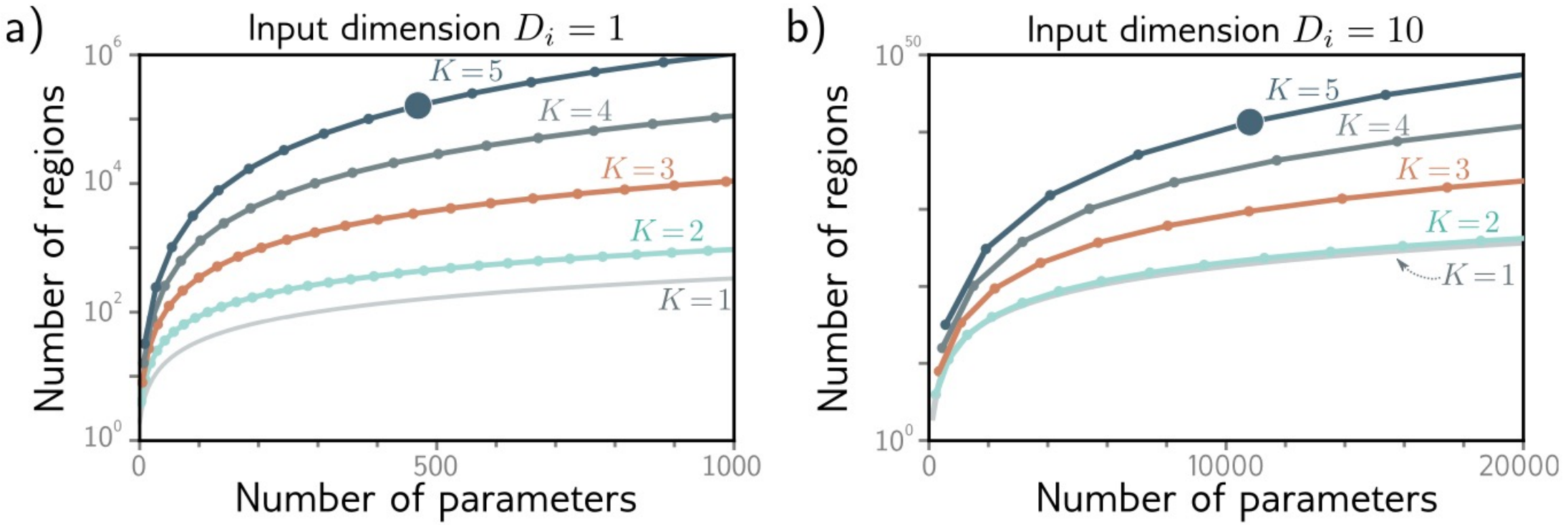
[Understanding Deep Learning, 2023]

Max no of Regions

- Max number of linear regions increases as a function of the number of parameters (scalar output)



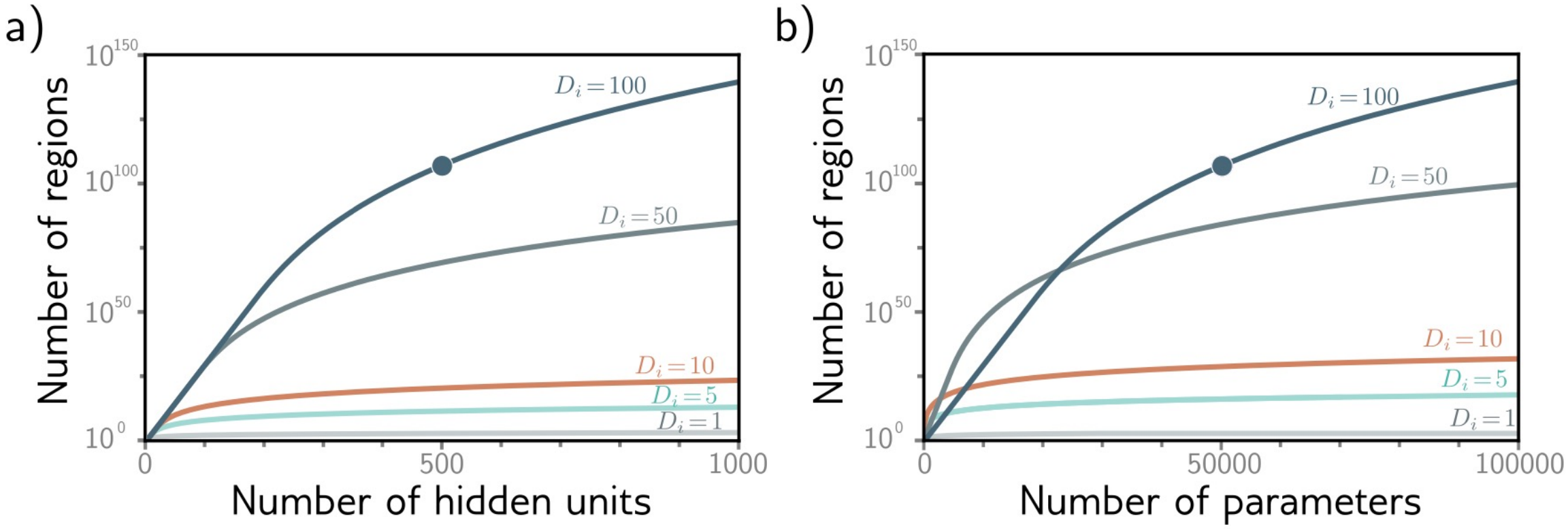
K layers



Understanding Deep Learning, 2023

Max no of Regions

- Maximum possible regions as a function of the number of hidden units and the number of parameters for five different input dimensions



Summary

- MLPs are universal Boolean function
- MLPs are universal classifiers
- MLPs are universal function approximators

- A single-layer MLP can approximate anything to arbitrary precision
  - But could be exponentially or even infinitely wide in its inputs size
- Deeper MLPs can achieve the same precision with far fewer neurons
  - Deeper networks are more expressive