Neural Networks: What can a network represent

Deep Learning, Fall 2017

Projects

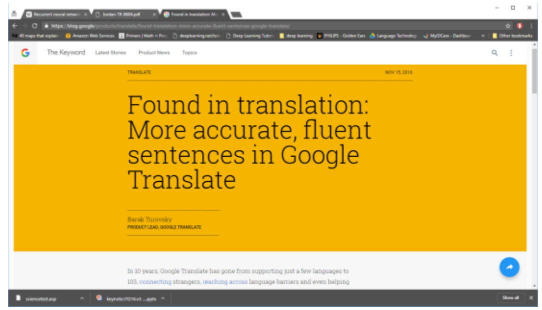
- Everyone must do a project
  - Teams of two
- Projects must
  - Use neural networks
  - Address a well-defined problem
  - Outcomes must be objectively or subjectively evaluateable
- Quality:
  - May simply revisit already published literature
    - E.g. obtain near-state-of-art on imagenet, or speech recognition
  - Existing solutions, new problems
    - MT for a new language
  - Propose new designs or learning methods
    - E.g. use LSTMs for image recognition
  - Be entirely novel
- Objective: Demonstrate ability to implement a complex solution using neural networks

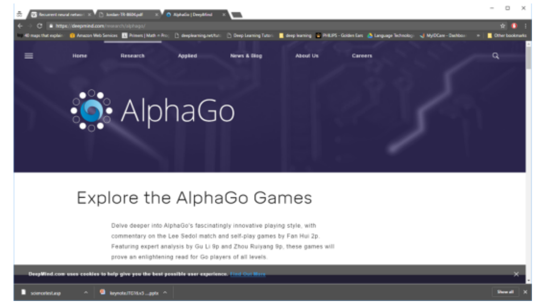
Projects

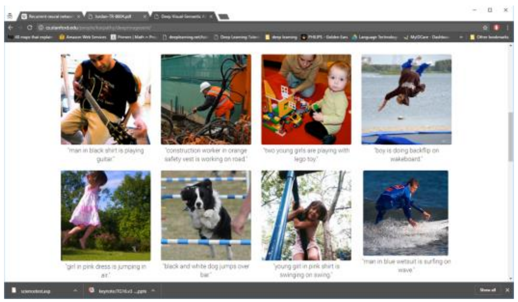
- Schedule:
  - Announce teams to TAs/myself by 15 Sep
  - Send project proposals by 21 Sep
  - Finalize project by 28 Sep

- Poster presentation: Between Dec 7 and Dec 10th

Recap : Neural networks have taken over AI





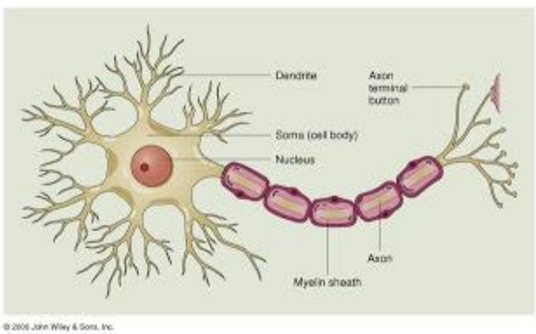


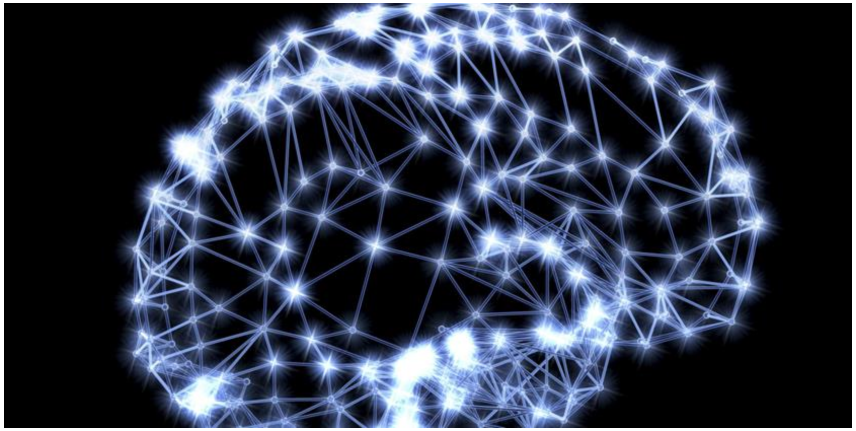
- Tasks that are made possible by NNs, aka deep learning

Recap : NNets and the brain

- In their basic form, NNets mimic the networked structure in the brain

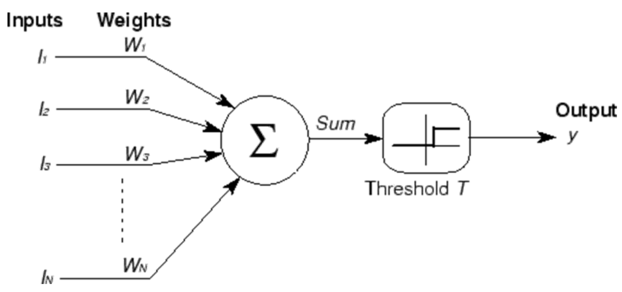
Recap : The brain

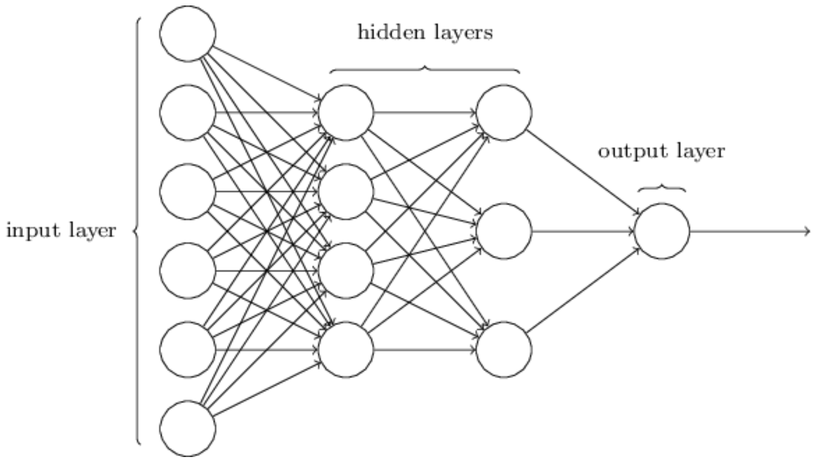




- The Brain is composed of networks of neurons

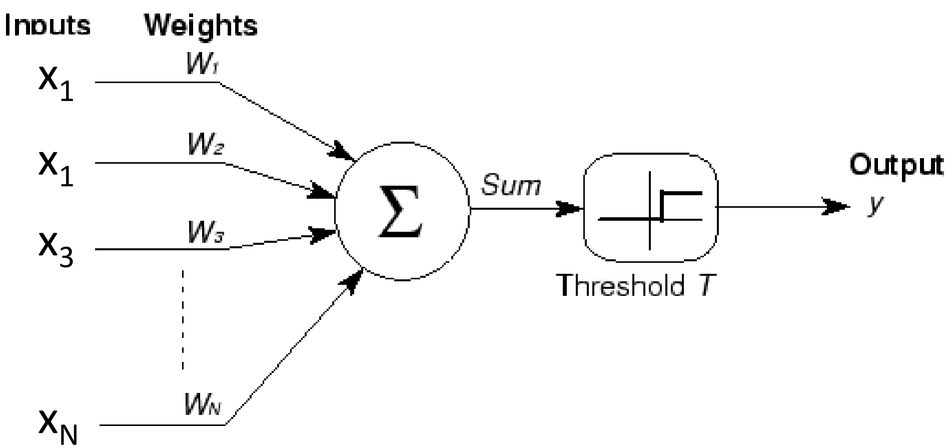
Recap : Nnets and the brain





- Neural nets are composed of networks of computational models of neurons called perceptrons

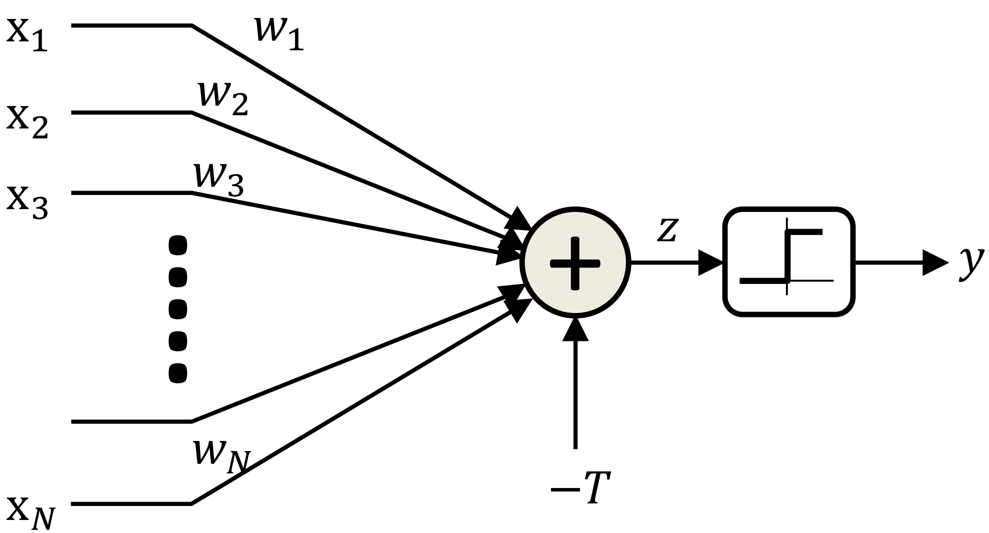
Recap: the perceptron



$$y = \begin{cases} 1 \; if \; \sum_i w_i x_i \geq T \\ 0 \; else \end{cases}$$

- A threshold unit
  - "Fires" if the weighted sum of inputs exceeds a threshold

A better figure

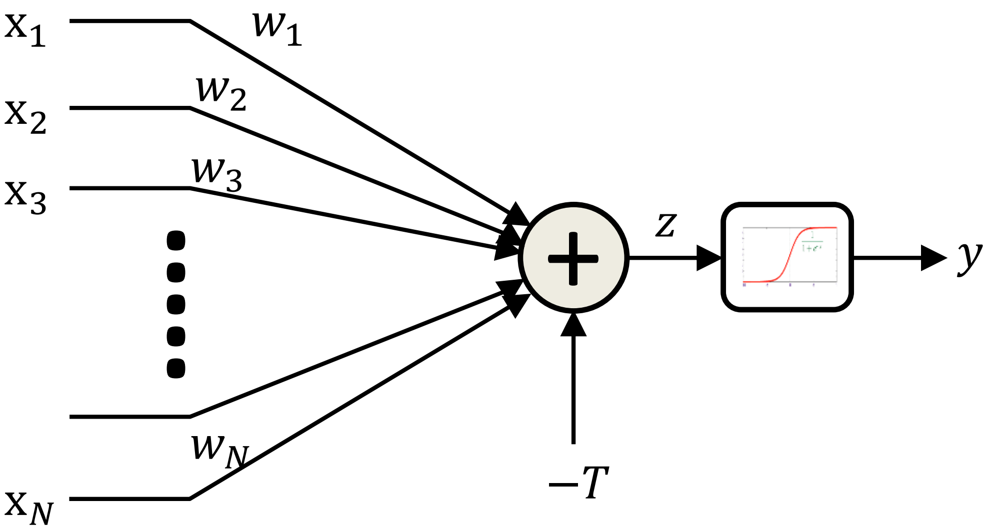


$$z = \sum_i w_i x_i - T$$

$$y = \begin{cases} 1 \; if \; z \geq 0 \\ 0 \; else \end{cases}$$

- A threshold unit
  - "Fires" if the weighted sum of inputs and the "bias" T is positive

The “soft” perceptron

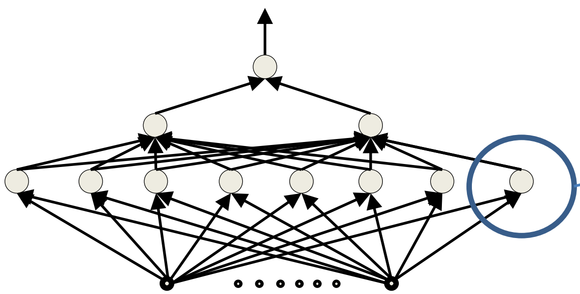


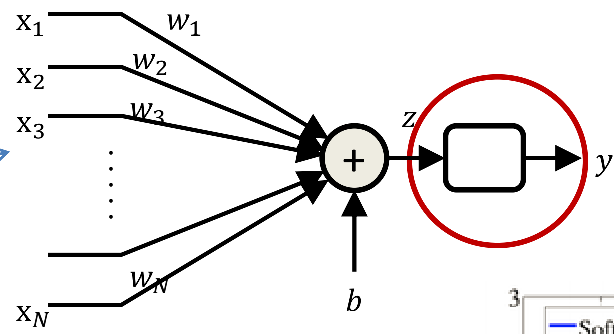
$$z = \sum_i w_i x_i - T$$

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

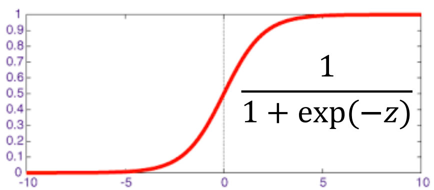
- A “squashing” function instead of a threshold at the output
  - The sigmoid “activation” replaces the threshold
    - **Activation:** The function that acts on the weighted combination of inputs (and threshold)

Other "activations"

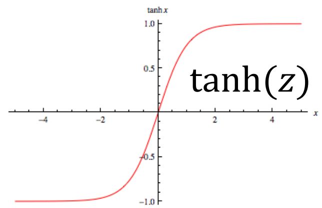


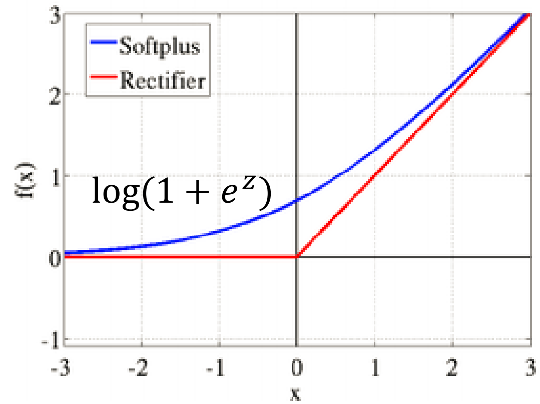


sigmoid



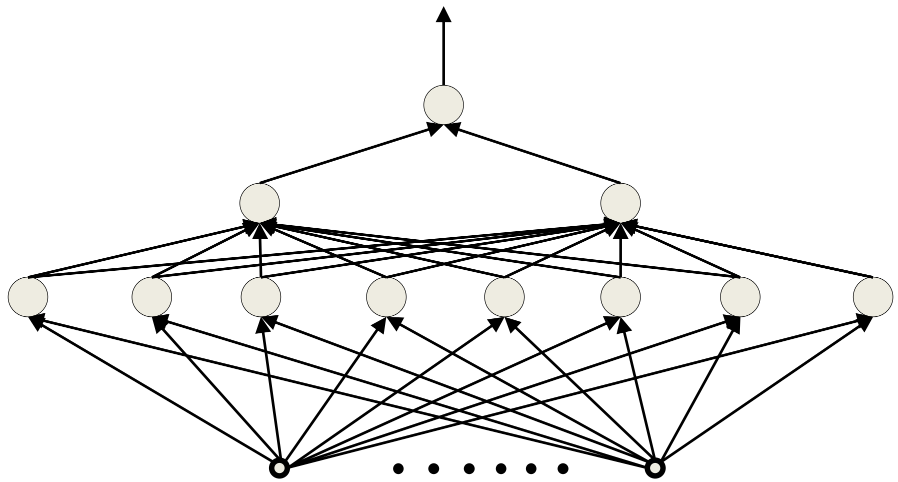
tanh

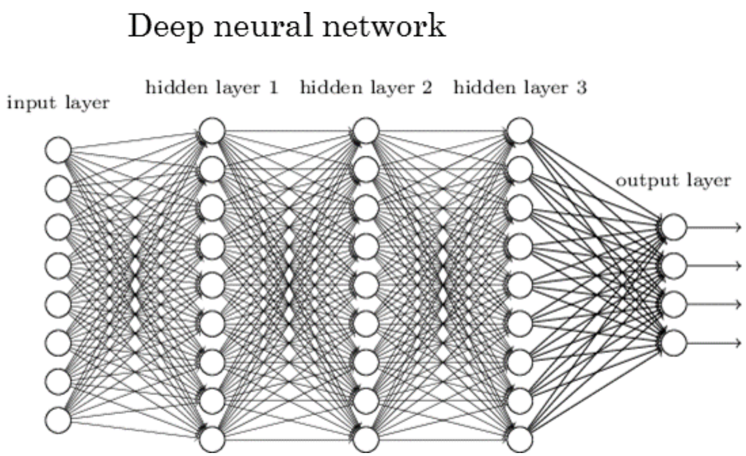




- Does not always have to be a squashing function
  - We will hear more about activations later
- We will continue to assume a "threshold" activation in this lecture

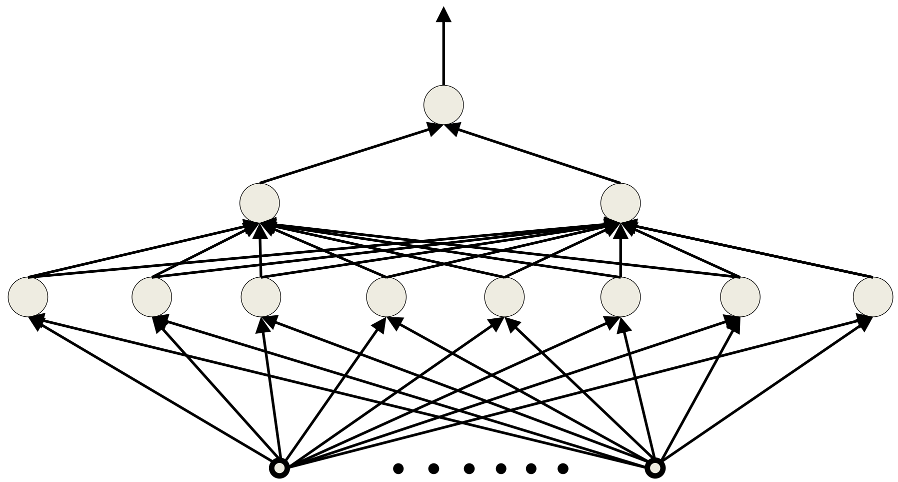
Recap: the multi-layer perceptron

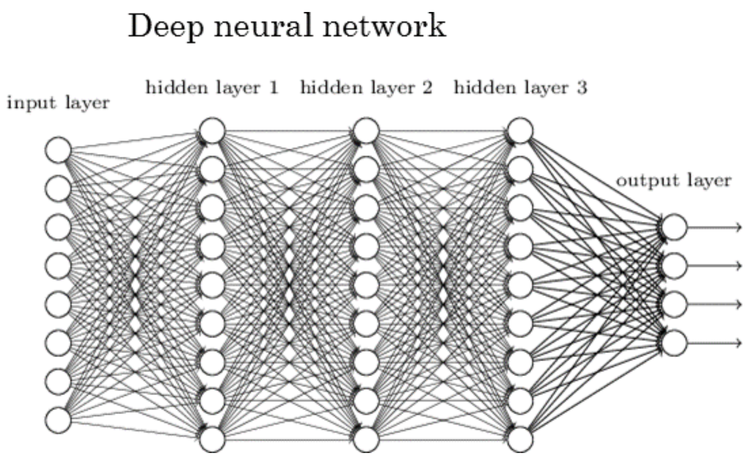




- A network of perceptrons
  - Generally "layered"

Defining "depth"

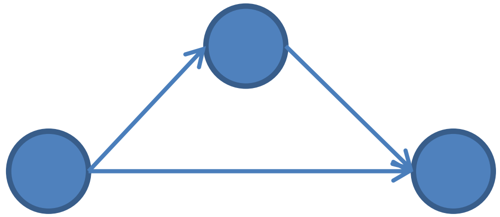


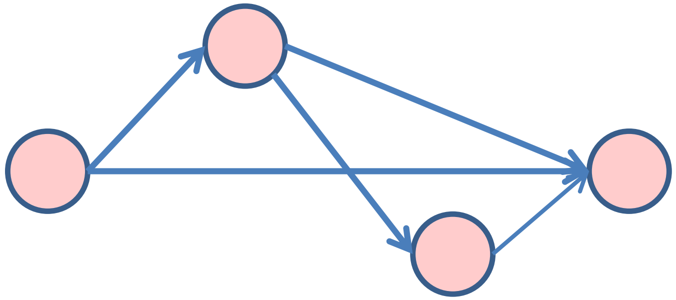


- What is a "deep" network

Deep Structures

- In any directed network of computational elements with input source nodes and output sink nodes, "depth" is the length of the longest path from a source to a sink

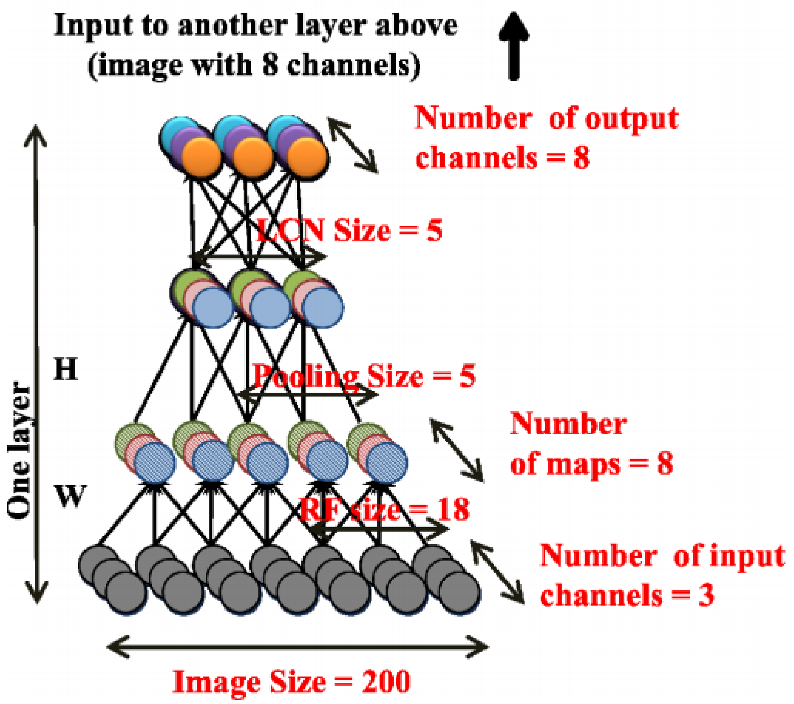




- Left: Depth = 2. Right: Depth = 3

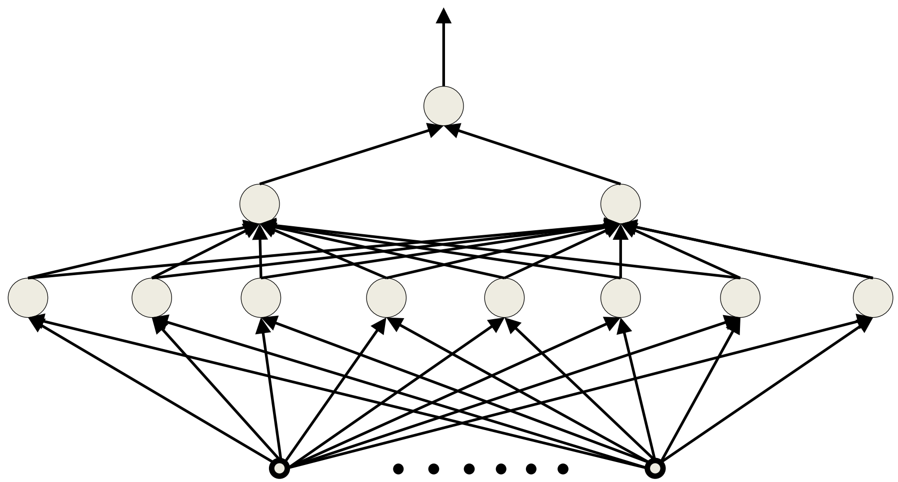
Deep Structures

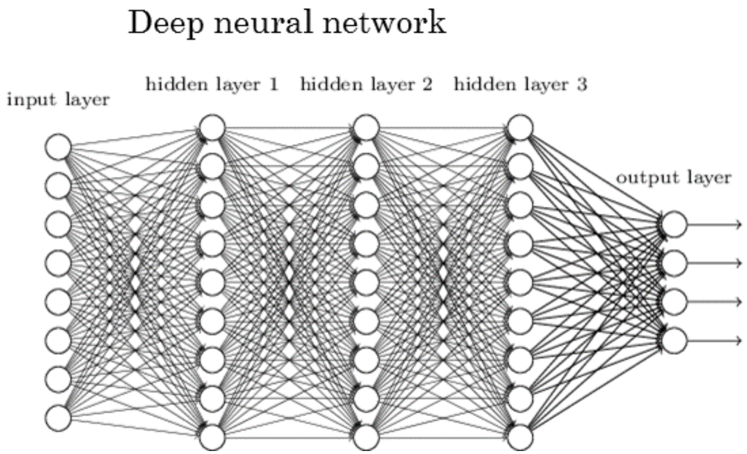
- *Layered* deep structure



- "Deep" → Depth > 2

The multi-layer perceptron

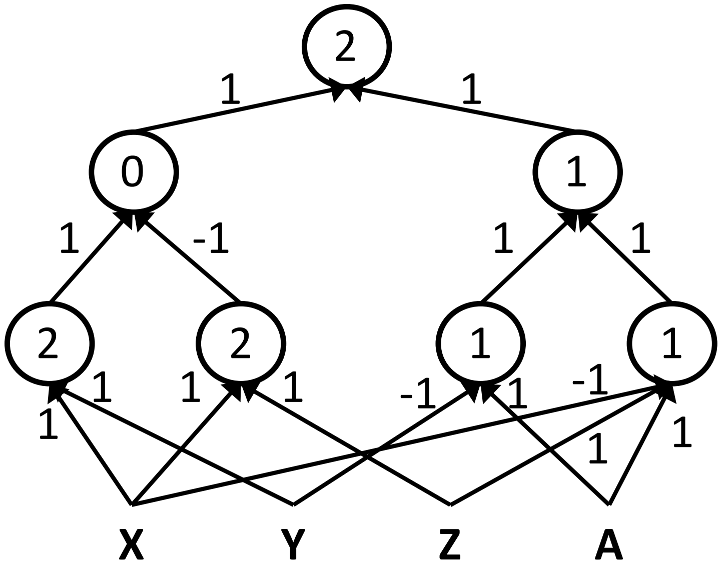


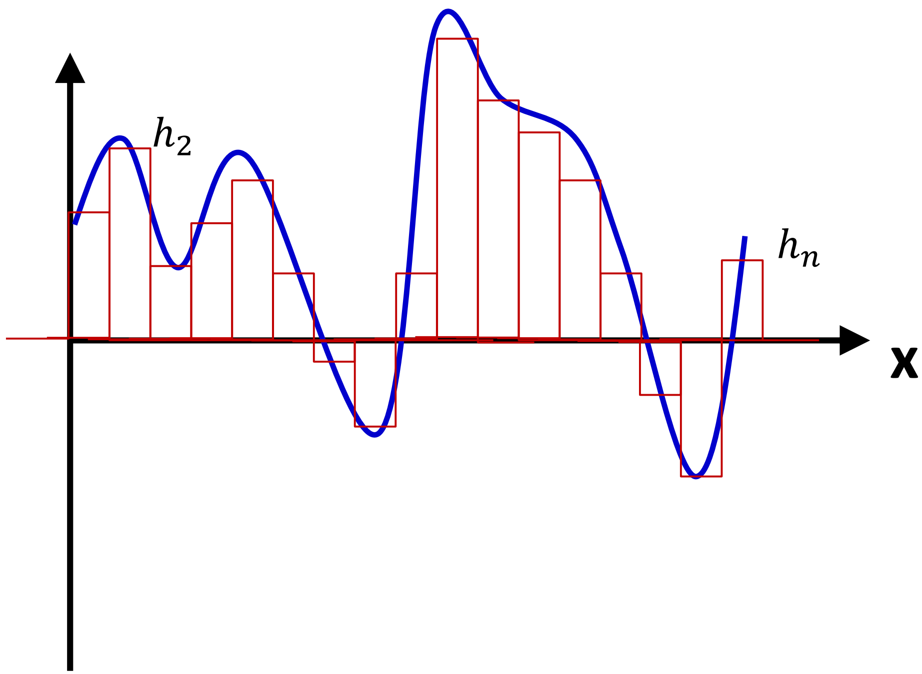


- Inputs are real or Boolean stimuli
- Outputs are real or Boolean values
  - Can have multiple outputs for a single input
- **What can this network compute?**
  - **What kinds of input/output relationships can it model?**

MLPs approximate functions

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





- MLPs can compose Boolean functions
- MLPs can compose real-valued functions
- What are the limitations?

Today

- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
- MLPs as universal classifiers
  - The need for depth
- MLPs as universal approximators
- A discussion of optimal depth and width
- Brief segue: RBF networks

Today

- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
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  - The need for depth
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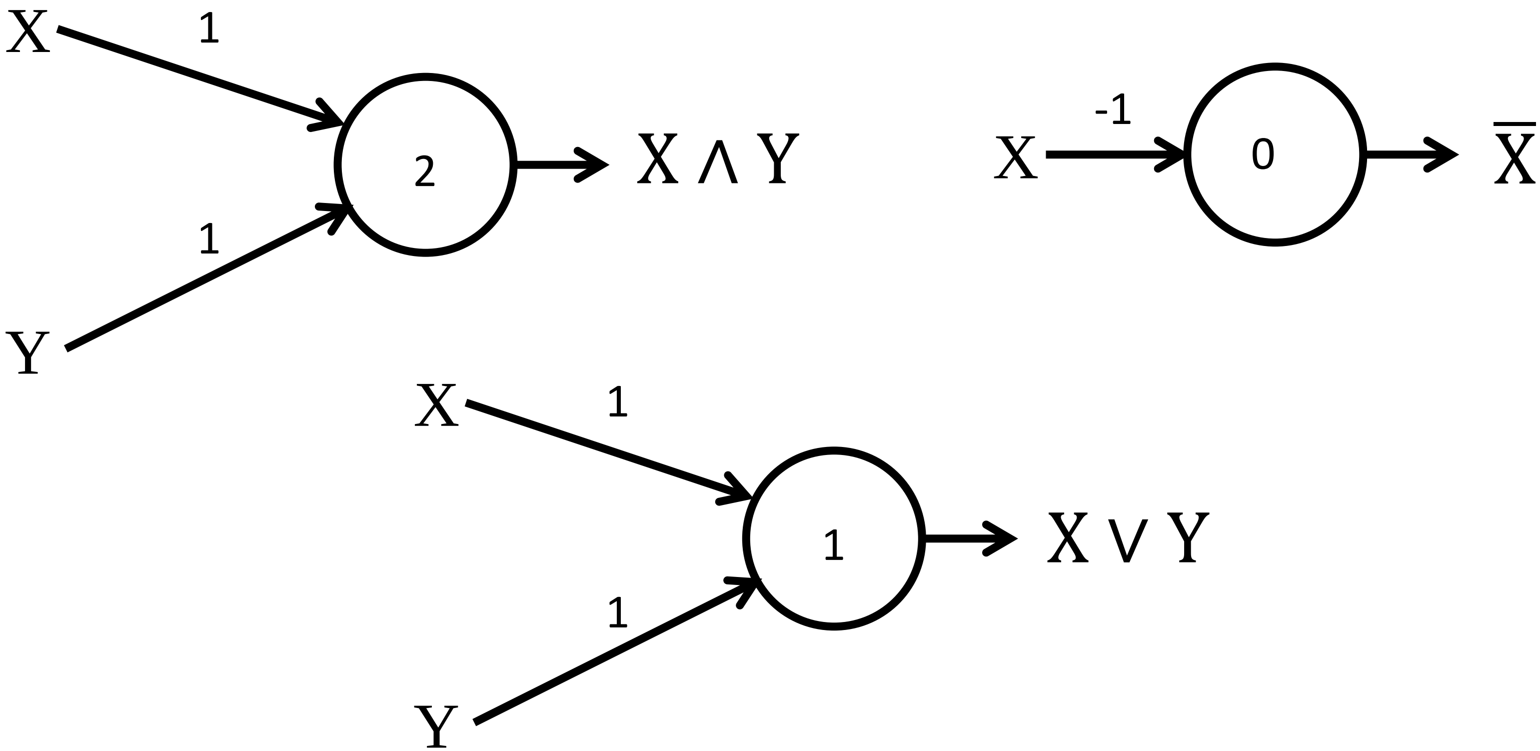
- A discussion of optimal depth and width
- Brief segue: RBF networks

The MLP as a Boolean function

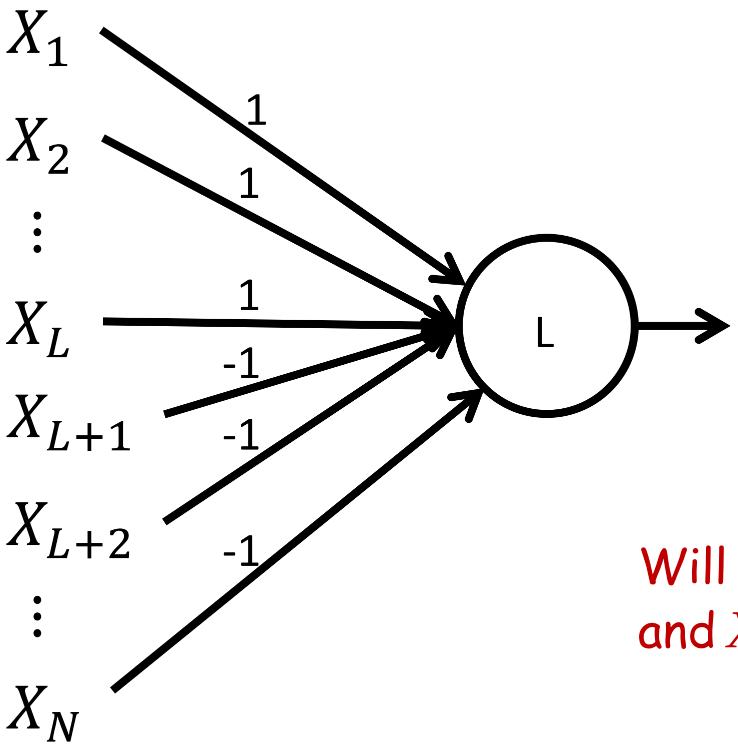
- How well do MLPs model Boolean functions?

The perceptron as a Boolean gate



- A perceptron can model any simple binary Boolean gate

Perceptron as a Boolean gate

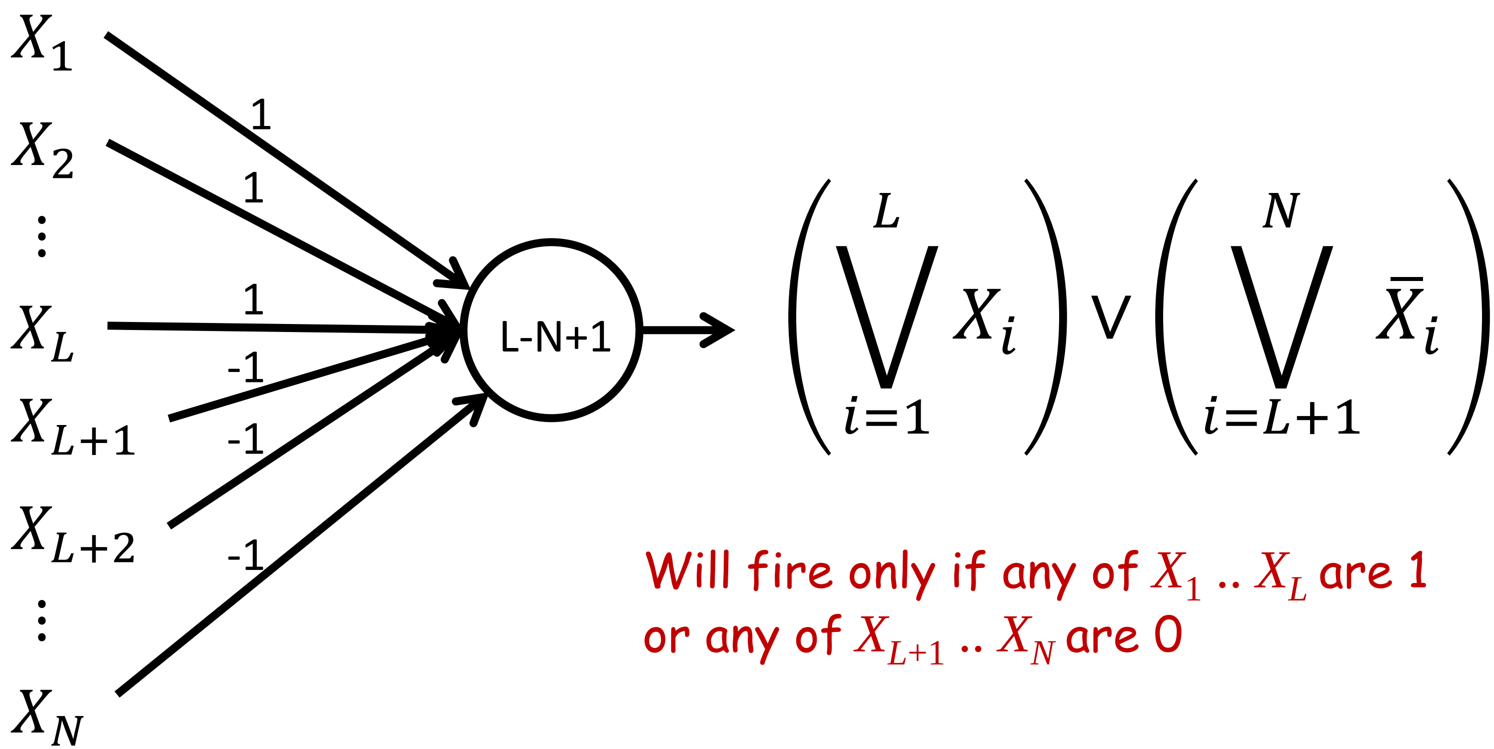


$$\left(\bigwedge_{i=1}^{L} X_i\right) \wedge \left(\bigwedge_{i=L+1}^{N} \bar{X}_i\right)$$

Will fire only if X_1 .. X_L are all 1 and X_{L+1} .. X_N are all 0

- The universal AND gate
  - AND any number of inputs
    - Any subset of who may be negated

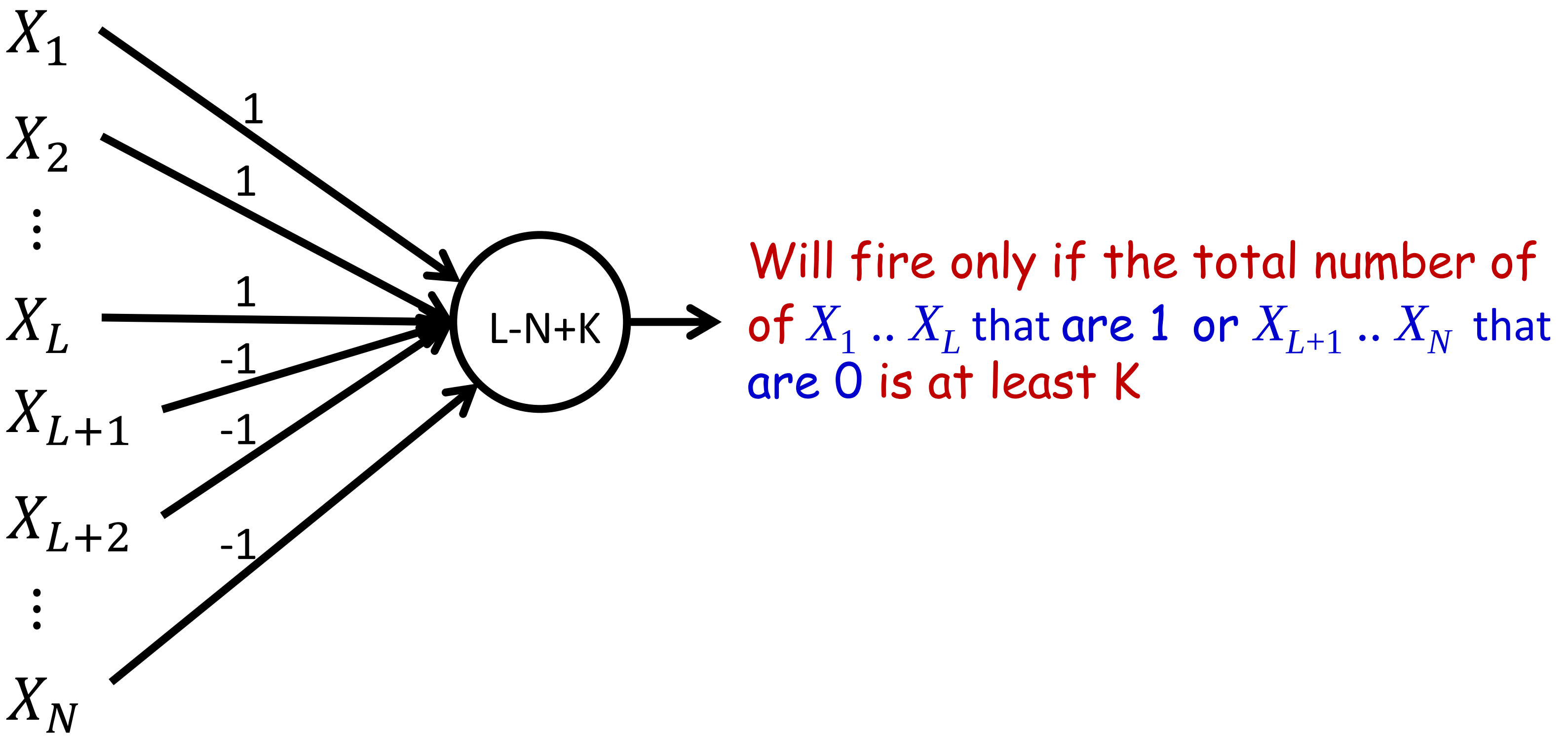
Perceptron as a Boolean gate



Will fire only if any of X_1 .. X_L are 1 or any of X_{L+1} .. X_N are 0

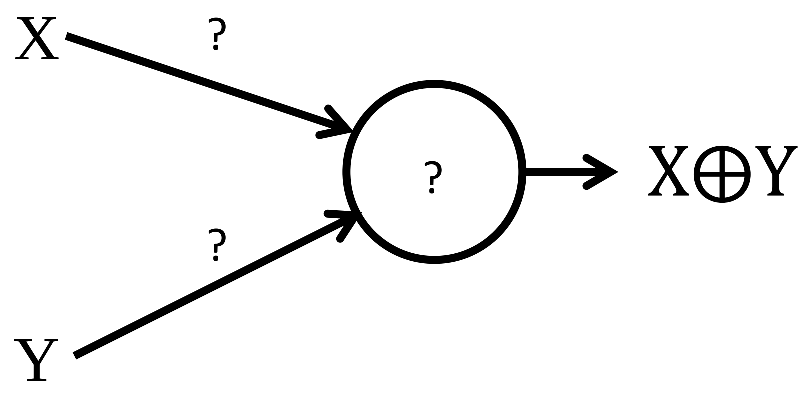
- The universal OR gate
  - OR any number of inputs
    - Any subset of who may be negated

Perceptron as a Boolean Gate



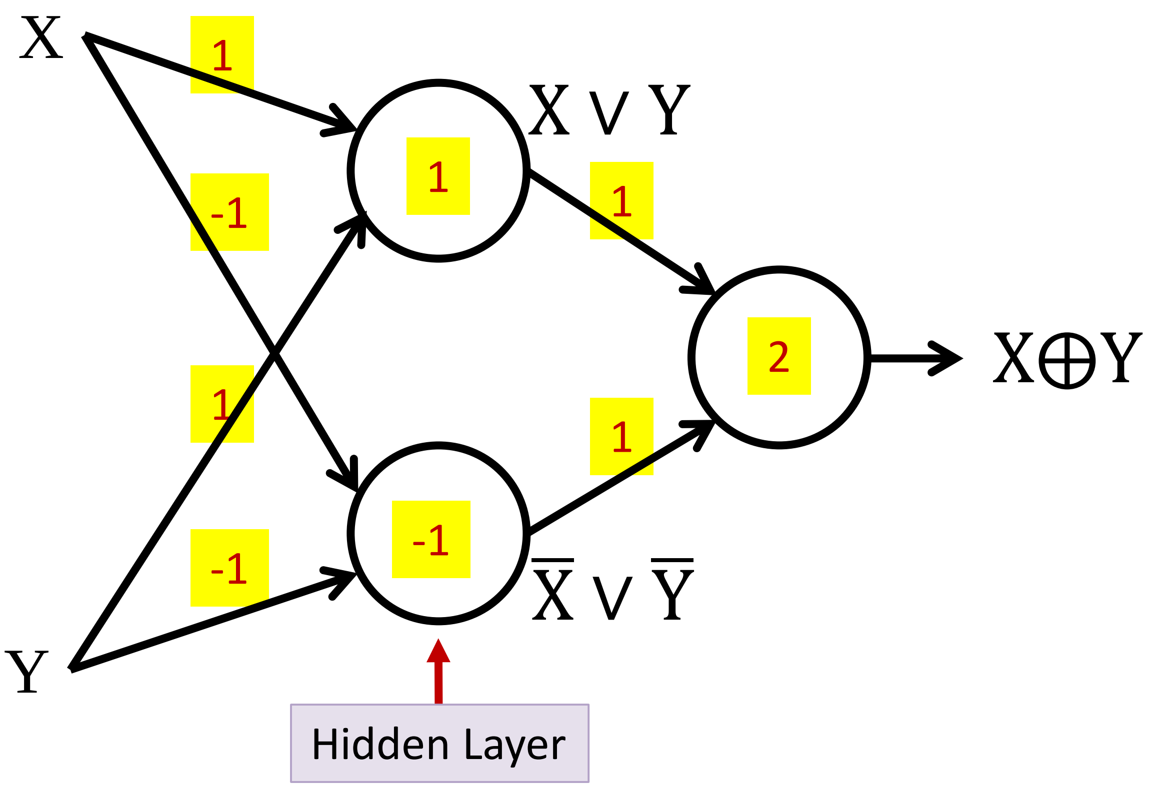
- Universal OR:
  - Fire if any K-*subset* of inputs is "ON"

The perceptron is not enough



- Cannot compute an XOR

Multi-layer perceptron



- MLPs can compute the XOR

Multi-layer perceptron

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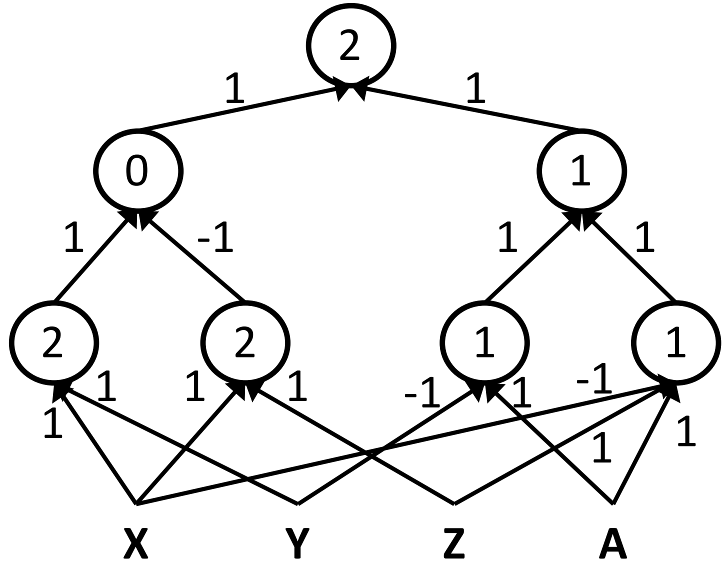

- MLPs can compute more complex Boolean functions
- MLPs can compute *any* Boolean function
  - Since they can emulate individual gates
- **MLPs are *universal Boolean functions***

MLP as Boolean Functions

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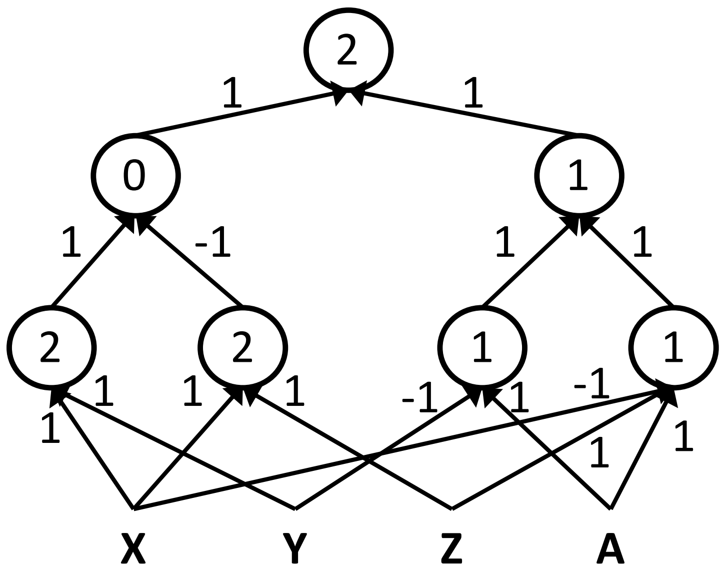

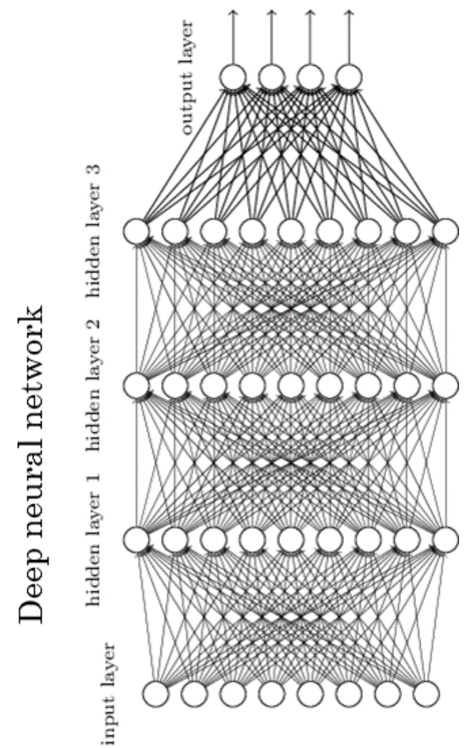

- MLPs are universal Boolean functions
  - Any function over any number of inputs and any number of outputs
- But how many "layers" will they need?

How many layers for a Boolean MLP?

Truth table shows *all* input combinations for which output is 1

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
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- Expressed in disjunctive normal form

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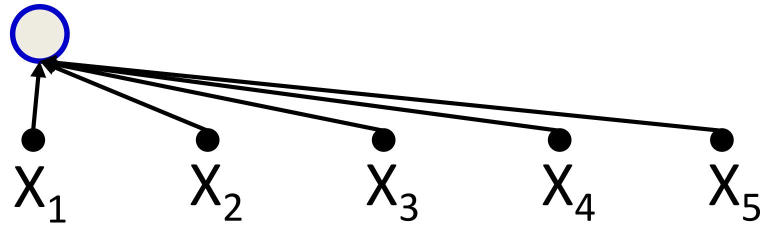

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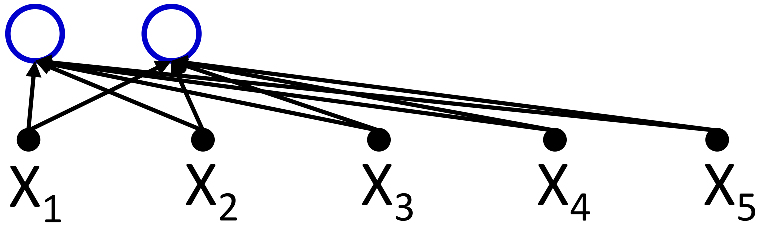

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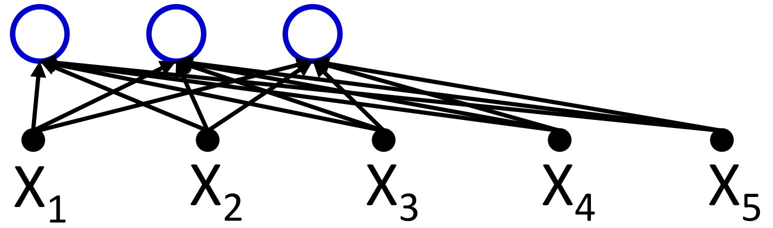

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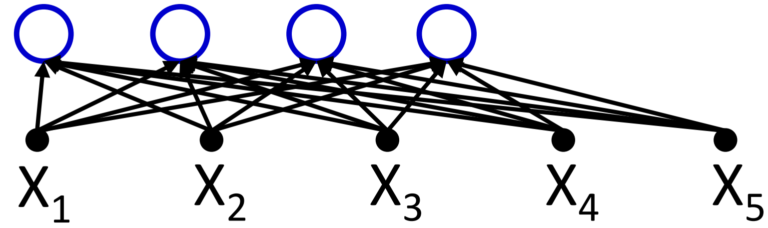

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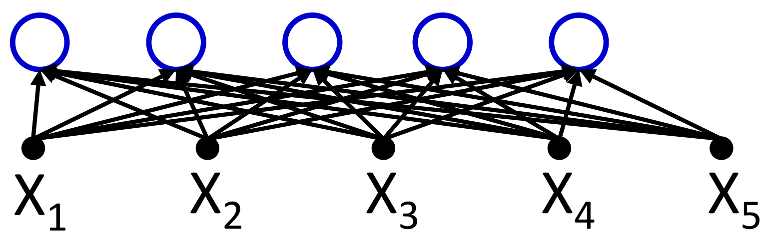

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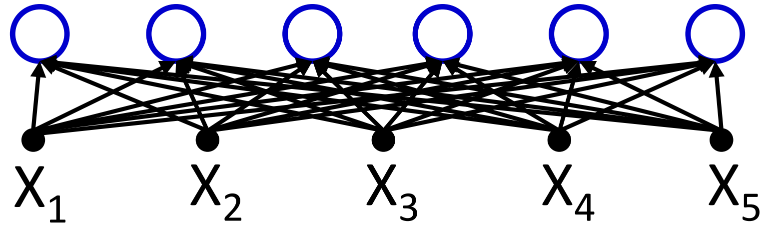

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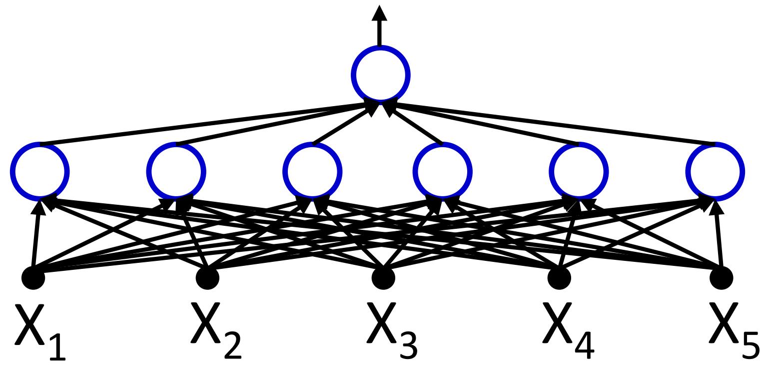
1	1	0	0	1	1

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

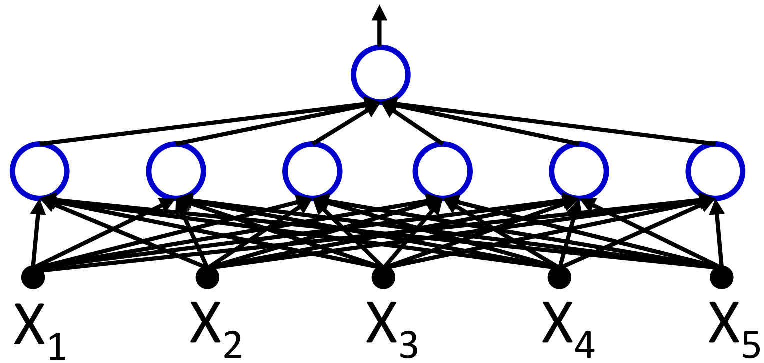
How many layers for a Boolean MLP?

Truth table shows *all* input combinations for which output is 1

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

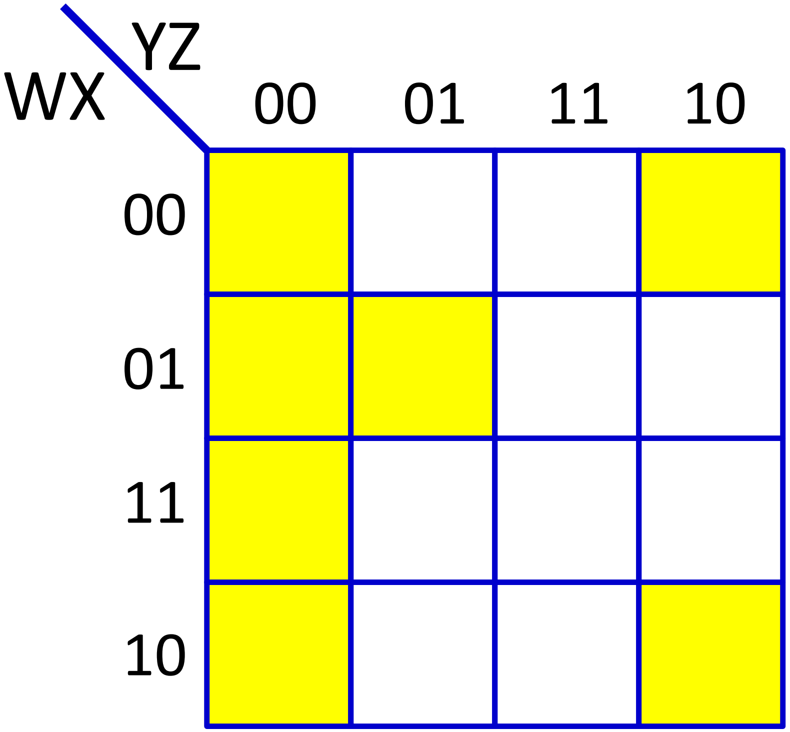
$$Y = \bar{X}_1\bar{X}_2X_3X_4\bar{X}_5 + \bar{X}_1X_2\bar{X}_3X_4X_5 + \bar{X}_1X_2X_3\bar{X}_4\bar{X}_5 + X_1\bar{X}_2\bar{X}_3\bar{X}_4X_5 + X_1\bar{X}_2X_3X_4X_5 + X_1X_2\bar{X}_3\bar{X}_4X_5$$



- *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?

Reducing a Boolean Function



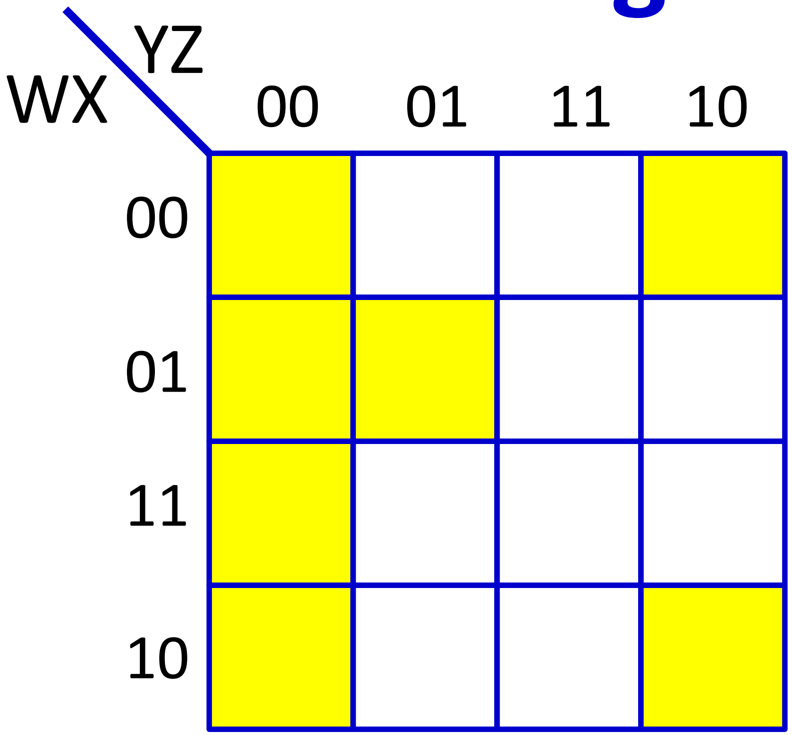
This is a "Karnaugh Map"

It represents a truth table as a grid
Filled boxes represent input combinations for which output is 1; blank boxes have output 0

Adjacent boxes can be "grouped" to reduce the complexity of the DNF formula for the table

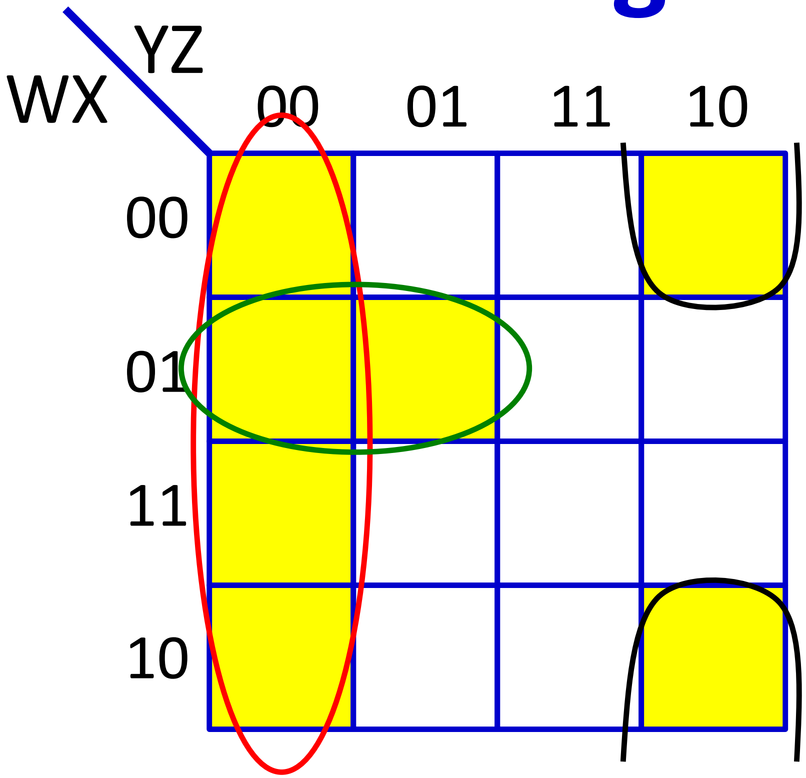
- DNF form:
  - Find groups
  - Express as reduced DNF

Reducing a Boolean Function



Basic DNF formula will require 7 terms

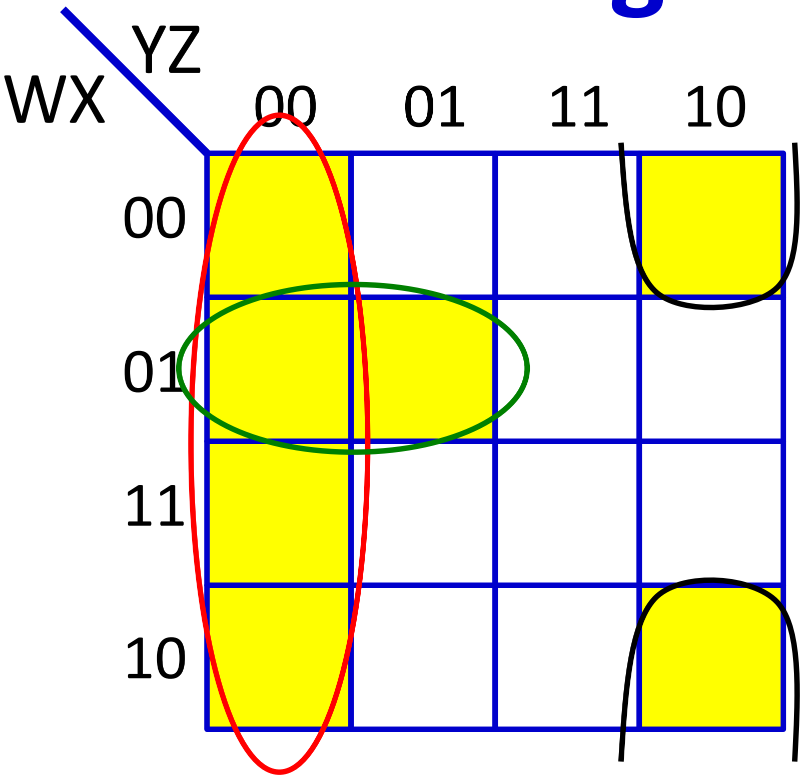
Reducing a Boolean Function



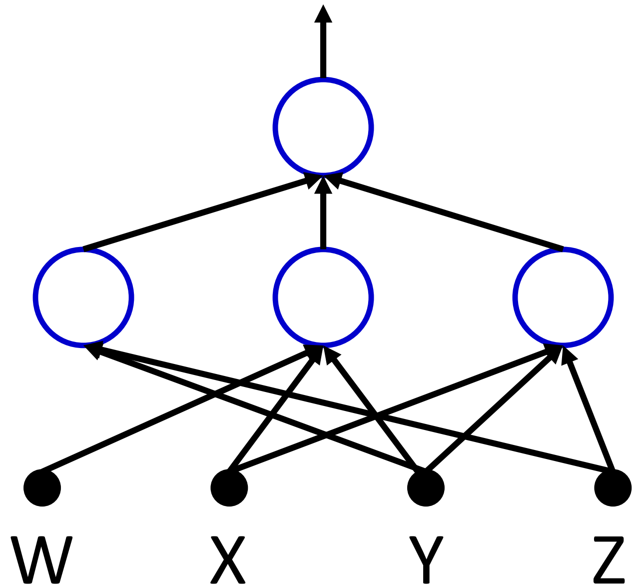
$$O = \bar{Y}\bar{Z} + \bar{W}X\bar{Y} + \bar{X}Y\bar{Z}$$

- *Reduced* DNF form:
  - Find groups
  - Express as reduced DNF

Reducing a Boolean Function

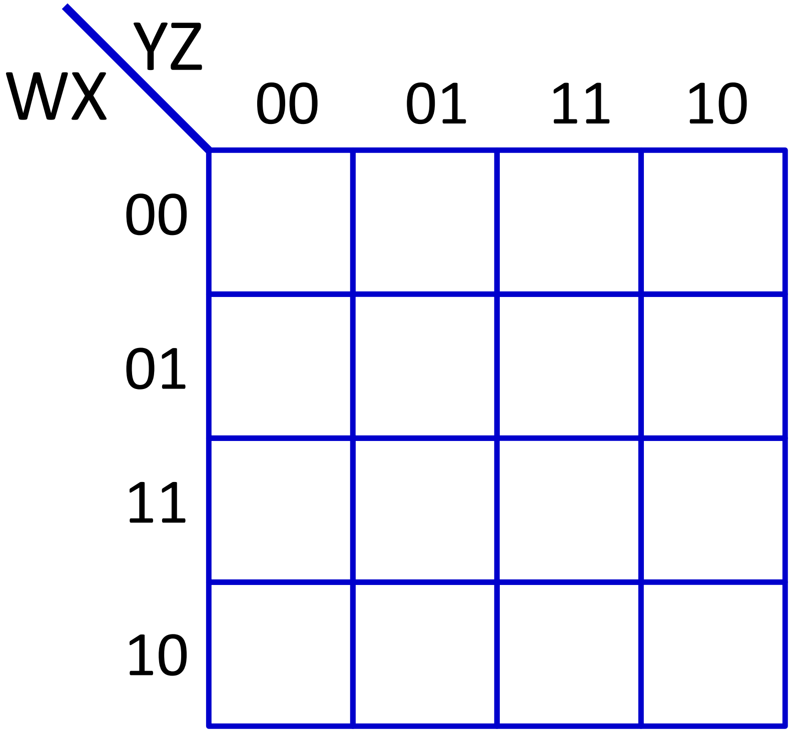


$$O = \bar{Y}\bar{Z} + \bar{W}X\bar{Y} + \bar{X}Y\bar{Z}$$



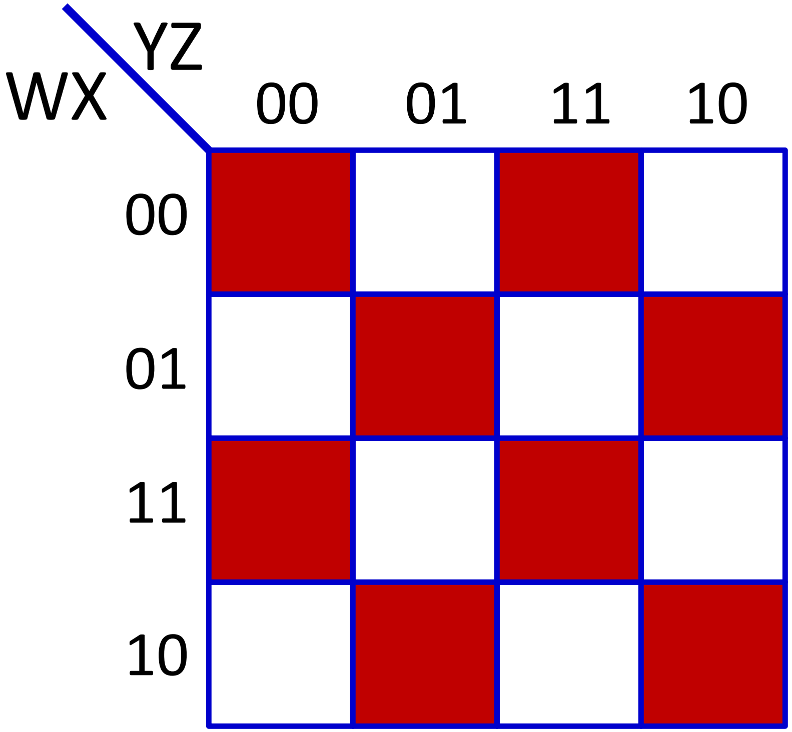
- *Reduced* DNF form:
  - Find groups
  - Express as reduced DNF

Largest irreducible DNF?



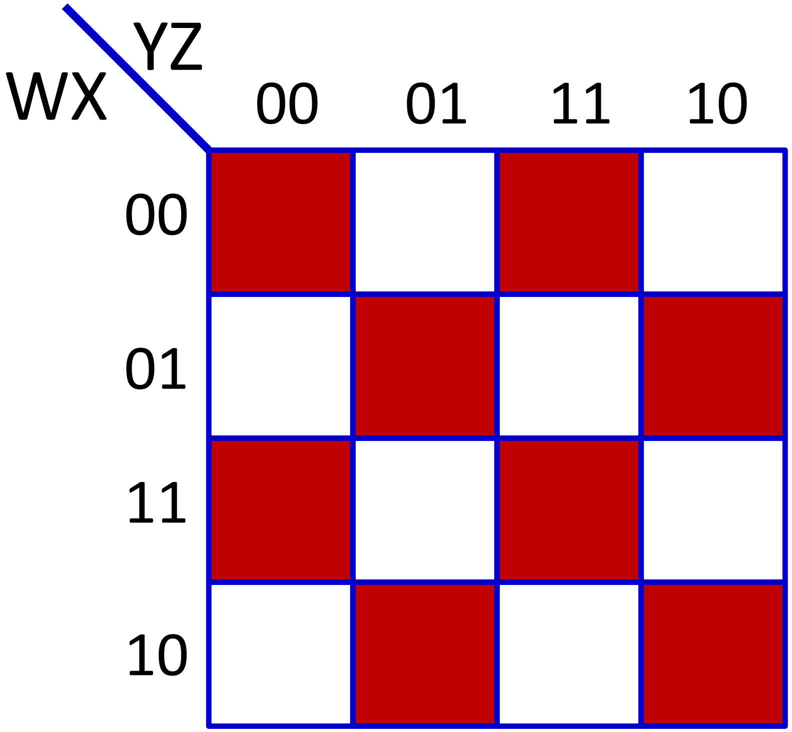
- What arrangement of ones and zeros simply cannot be reduced further?

Largest irreducible DNF?



- What arrangement of ones and zeros simply cannot be reduced further?

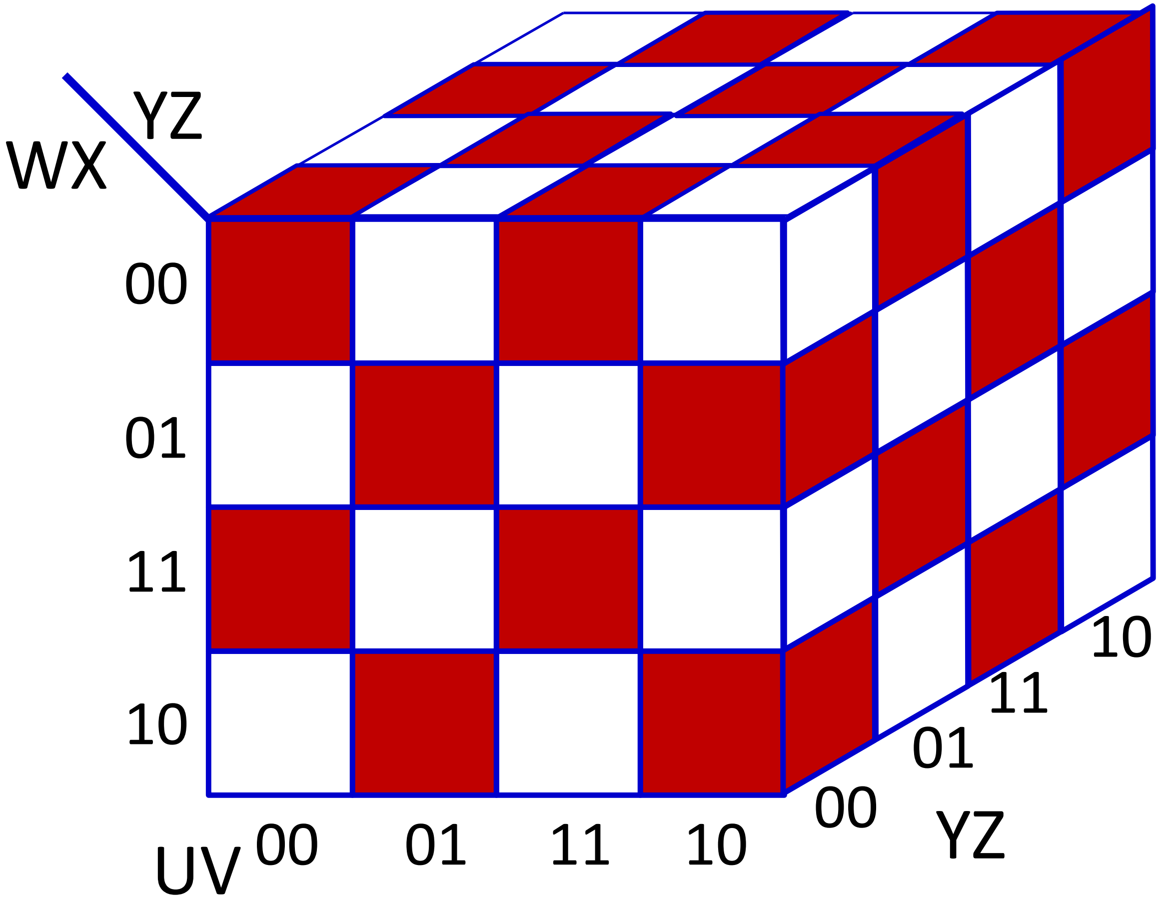
Largest irreducible DNF?



How many neurons in a DNF (one-hidden-layer) MLP for this Boolean function?

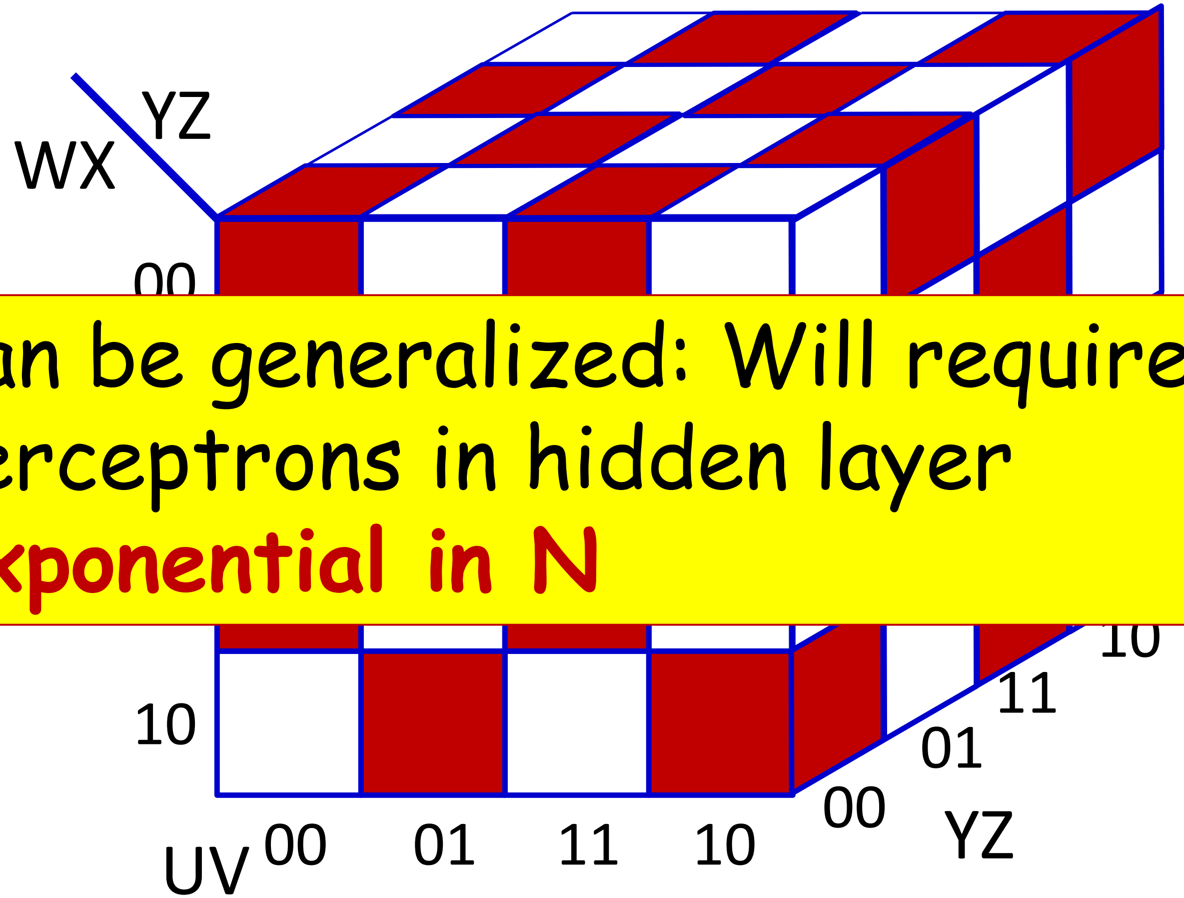
- What arrangement of ones and zeros simply cannot be reduced further?

Width of a single-layer Boolean MLP



- How many neurons in a DNF (one-hidden-layer) MLP for this Boolean function of 6 variables?

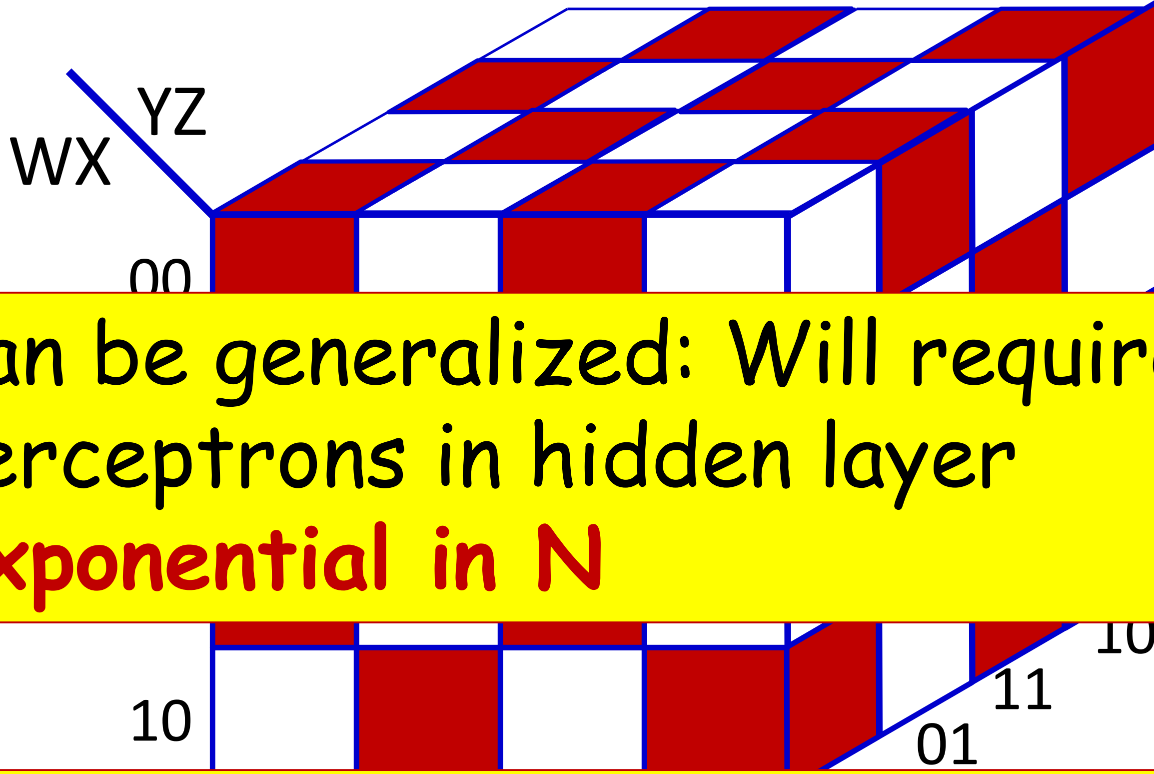
Width of a single-layer Boolean MLP



Can be generalized: Will require 2^{N-1} perceptrons in hidden layer
Exponential in N

- How many neurons in a DNF (one-hidden-layer) MLP for this Boolean function

Width of a single-layer Boolean MLP



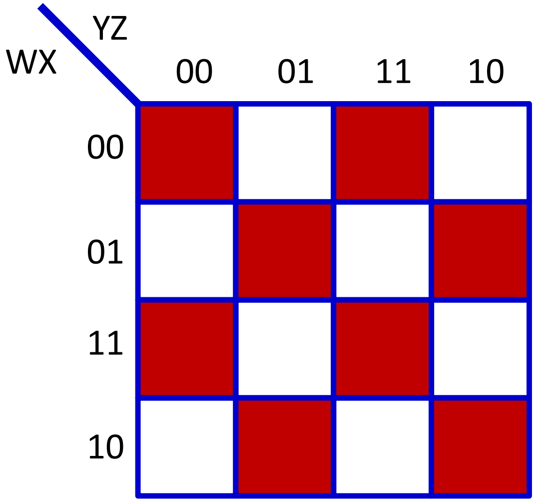
Can be generalized: Will require 2^{N-1} perceptrons in hidden layer

Exponential in N

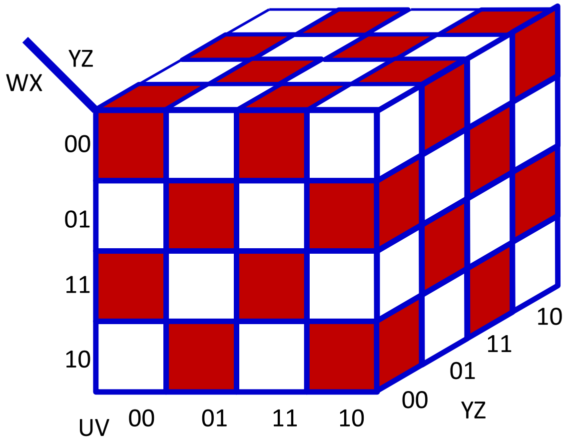
How many units if we use multiple layers?

- How many neurons in a DNF (one-hidden-layer) MLP for this Boolean function

Width of a deep MLP

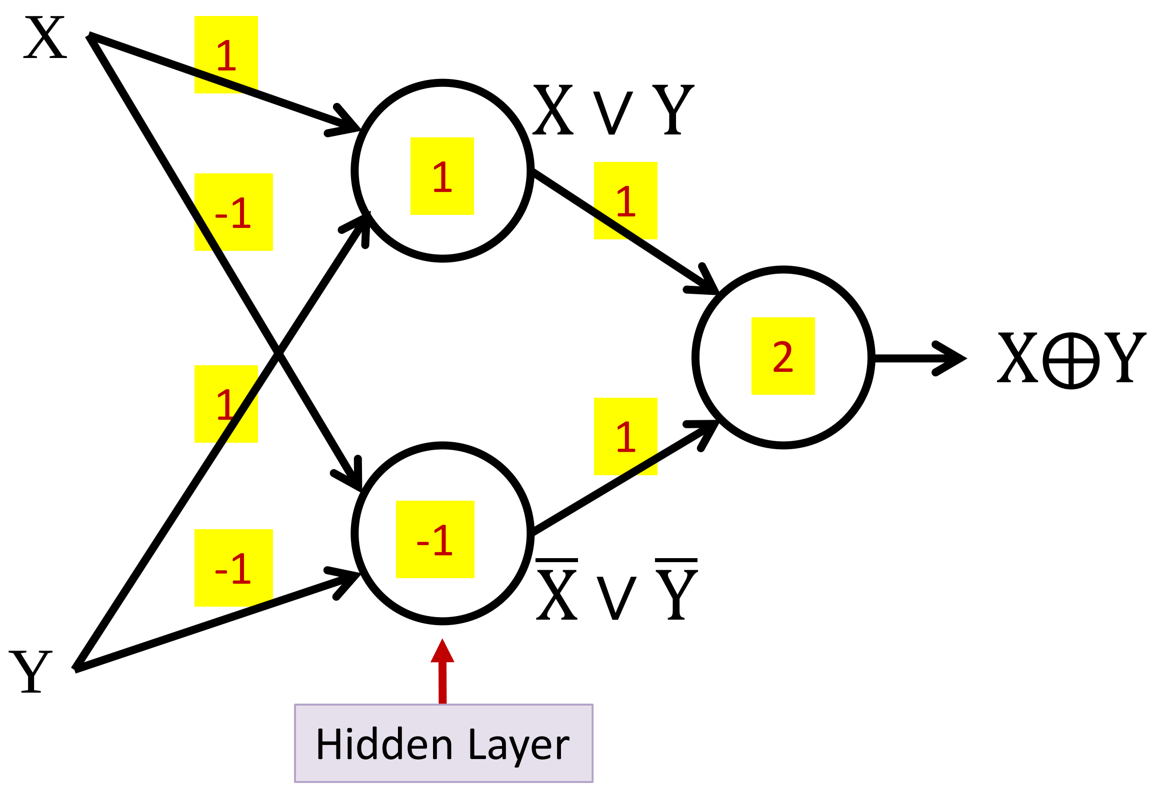


$$O = W \oplus X \oplus Y \oplus Z$$



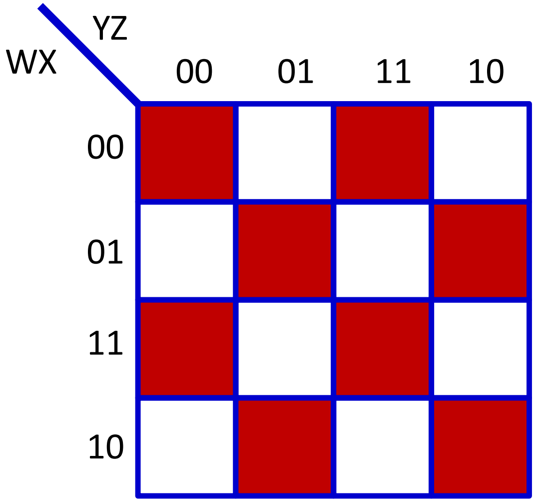
$$O = U \oplus V \oplus W \oplus X \oplus Y \oplus Z$$

Multi-layer perceptron XOR

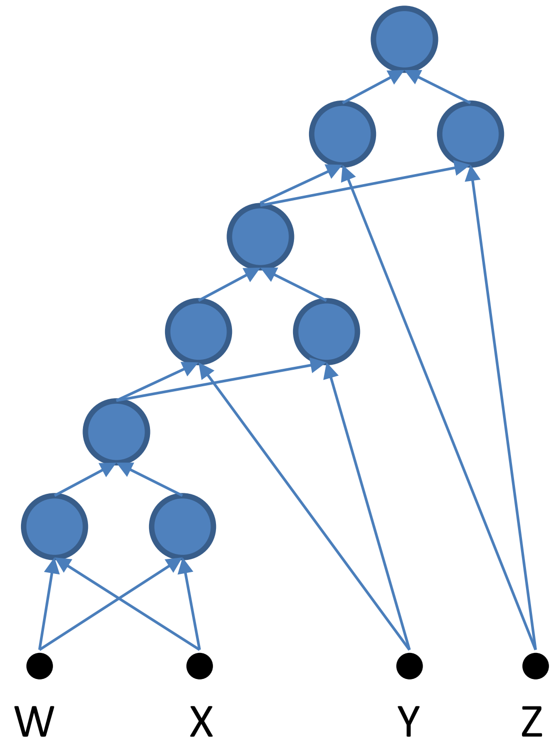


- An XOR takes three perceptrons

Width of a deep MLP



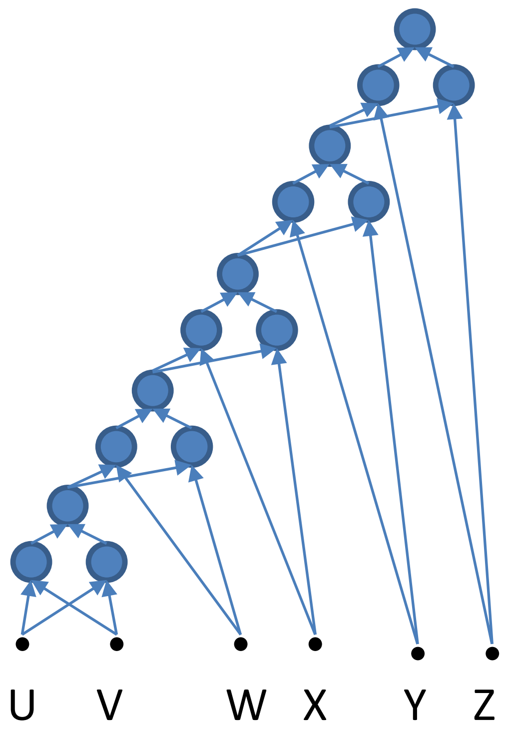
$$O = W \oplus X \oplus Y \oplus Z$$

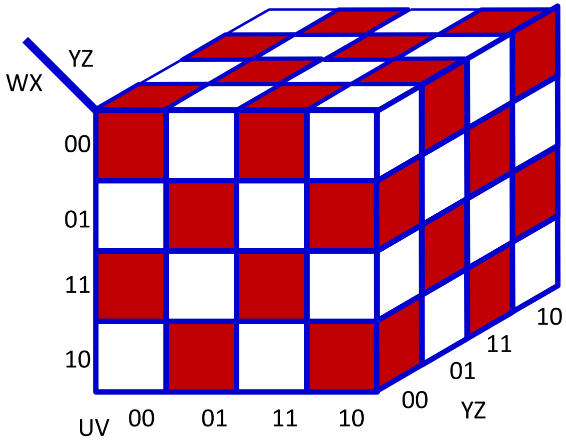


9 perceptrons

- An XOR needs 3 perceptrons
- This network will require 3x3 = 9 perceptrons

Width of a deep MLP



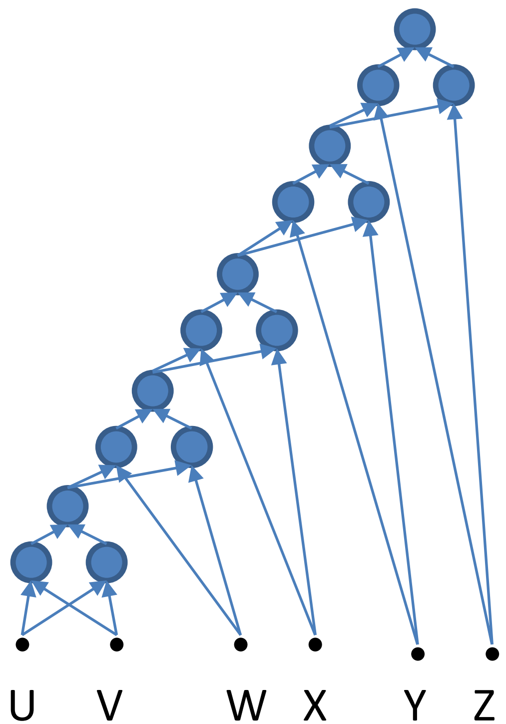


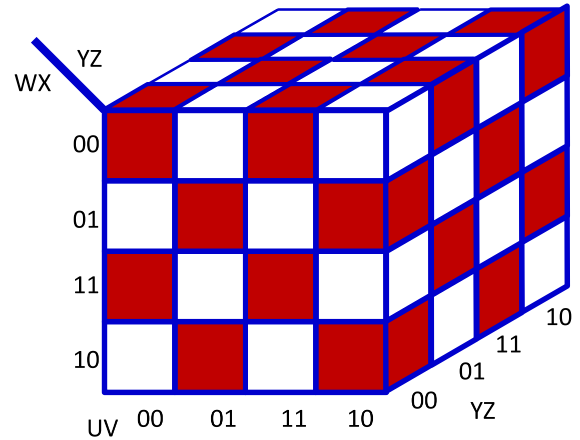
$$O = U \oplus V \oplus W \oplus X \oplus Y \oplus Z$$

15 perceptrons

- An XOR needs 3 perceptrons
- This network will require 3x5 = 15 perceptrons

Width of a deep MLP



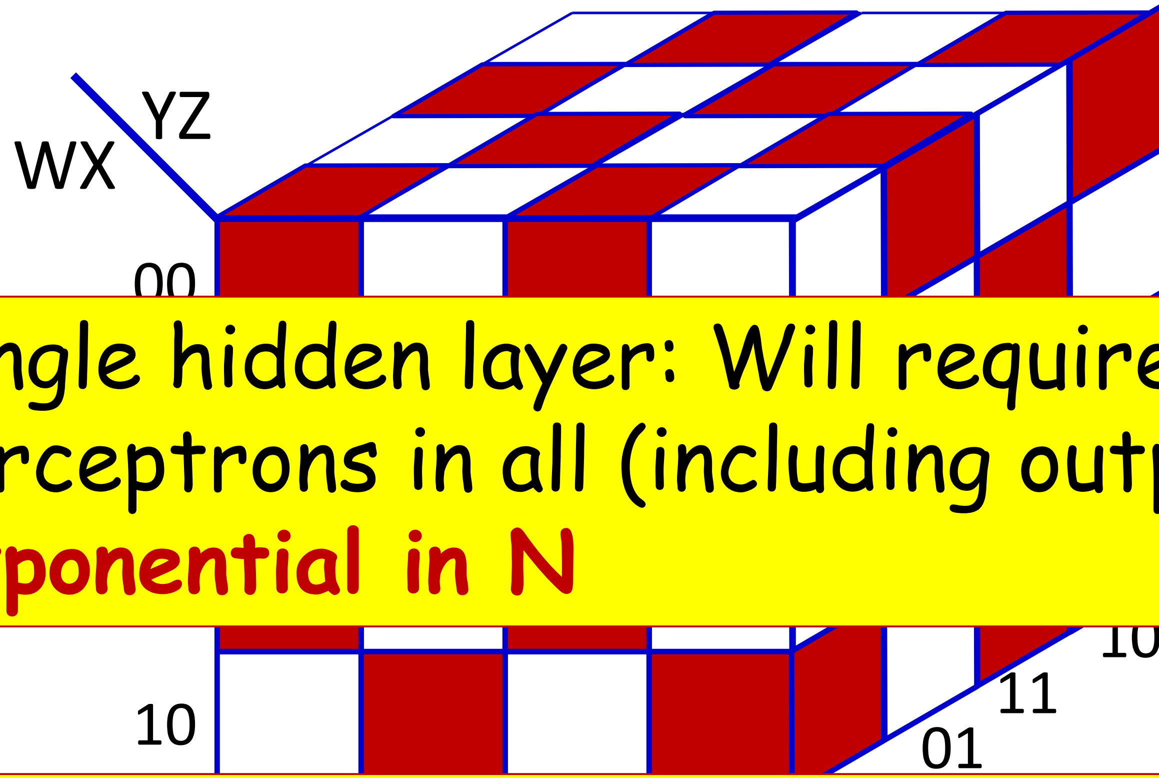


$$O = U \oplus V \oplus W \oplus X \oplus Y \oplus Z$$

More generally, the XOR of N variables will require 3(N-1) perceptrons!!

- An XOR needs 3 perceptrons
- This network will require 3x5 = 15 perceptrons

Width of a single-layer Boolean MLP



Single hidden layer: Will require $2^{N-1}+1$ perceptrons in all (including output unit)

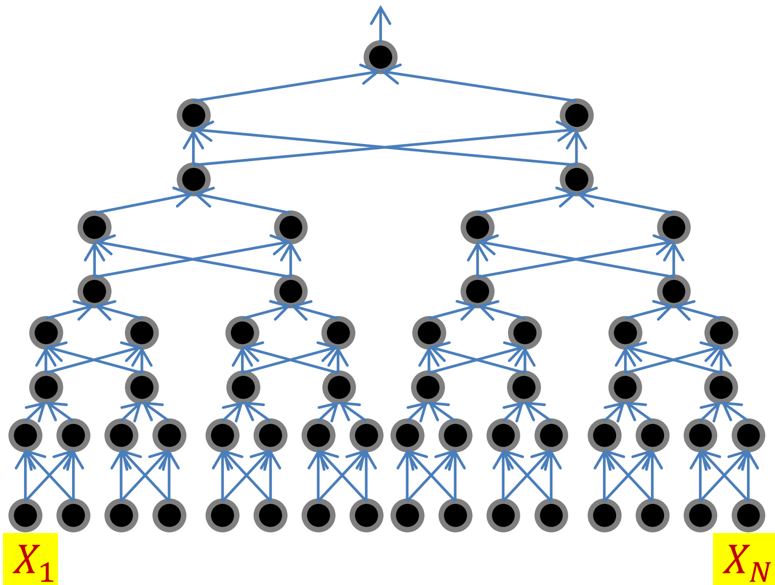
Exponential in N

Will require 3(N-1) perceptrons in a deep network

Linear in N!!!

Can be arranged in only $2\log_2(N)$ layers

A better representation

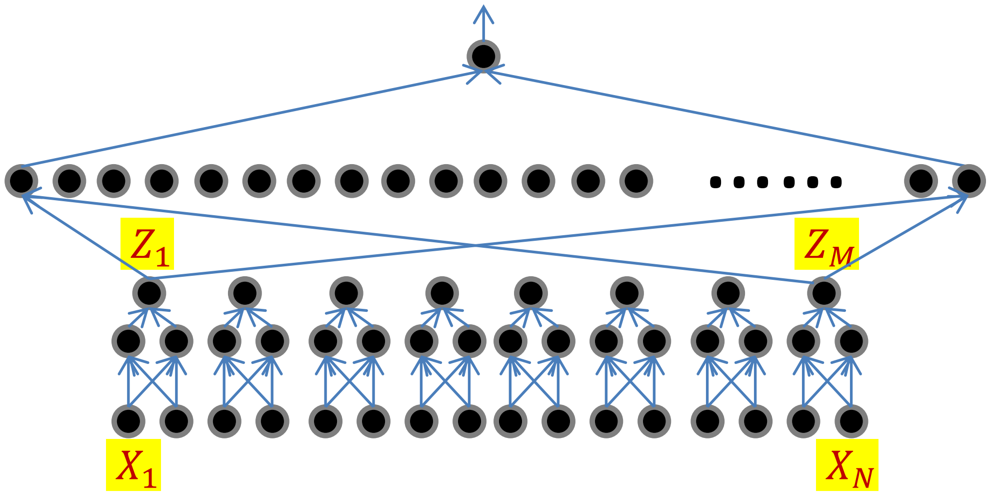


$$O = X_1 \oplus X_2 \oplus \cdots \oplus X_N$$

- Only $2\log_2 N$ layers
  - By pairing terms
  - 2 layers per XOR

$$O = (((((X_1 \oplus X_2) \oplus (X_1 \oplus X_2)) \oplus ((X_5 \oplus X_6) \oplus (X_7 \oplus X_8))) \oplus (((\ldots$$

The challenge of depth



$$O = X_1 \oplus X_2 \oplus \cdots \oplus X_N$$
$$= Z_1 \oplus Z_2 \oplus \cdots \oplus Z_M$$

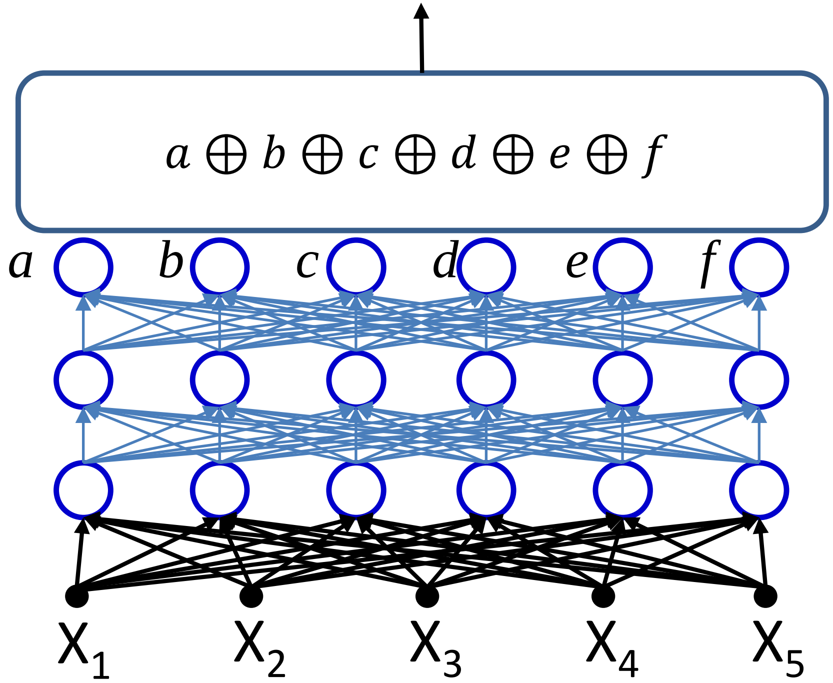
- Using only K hidden layers will require $O(2^{(N-K/2)})$ neurons in the Kth layer
  - Because the output can be shown to be the XOR of all the outputs of the K-1th hidden layer
  - **I.e. reducing the number of layers below the minimum will result in an exponentially sized network to express the function fully**
  - **A network with fewer than the required number of neurons *cannot* model the function**

Recap: The need for depth

- *Deep* Boolean MLPs that scale *linearly* with the number of inputs …
- … can become exponentially large if recast using only one layer

- It gets worse..

The need for depth



- The wide function can happen at any layer
- Having a few extra layers can greatly reduce network size

Network size: summary

- An MLP is a universal Boolean function

- But can represent a given function only if
  - It is sufficiently wide
  - It is sufficiently deep
  - Depth can be traded off for (sometimes) exponential growth of the width of the network

- 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

Story so far

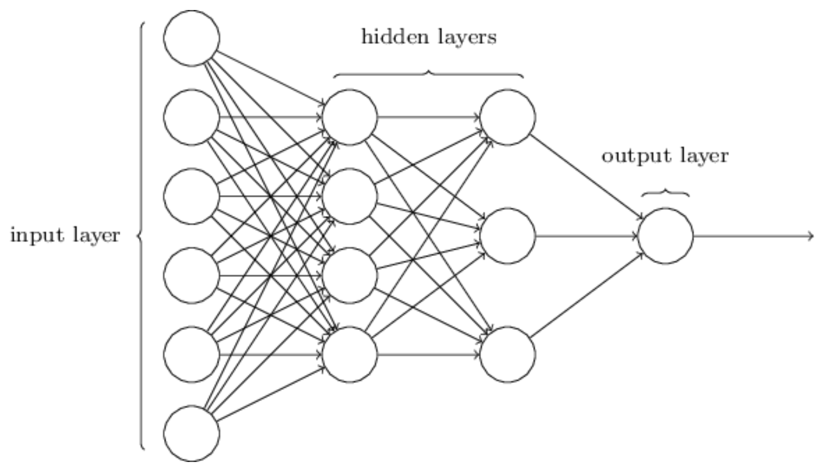
- Multi-layer perceptrons are *Universal Boolean Machines*
- Even a network with a *single* hidden layer is a universal Boolean machine
  - But a single-layer network may require an exponentially large number of perceptrons
- Deeper networks may require far fewer neurons than shallower networks to express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

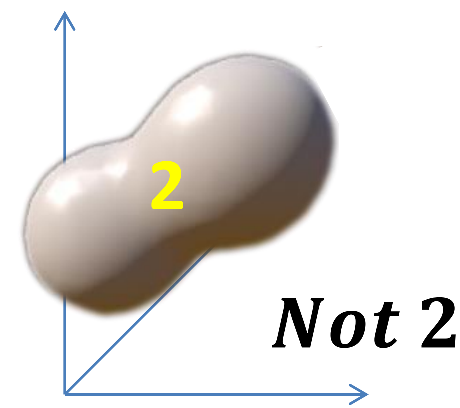
Today

- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
- MLPs as universal classifiers
  - The need for depth
- MLPs as universal approximators
- A discussion of optimal depth and width
- Brief segue: RBF networks

The MLP as a classifier

784 dimensions
(MNIST)

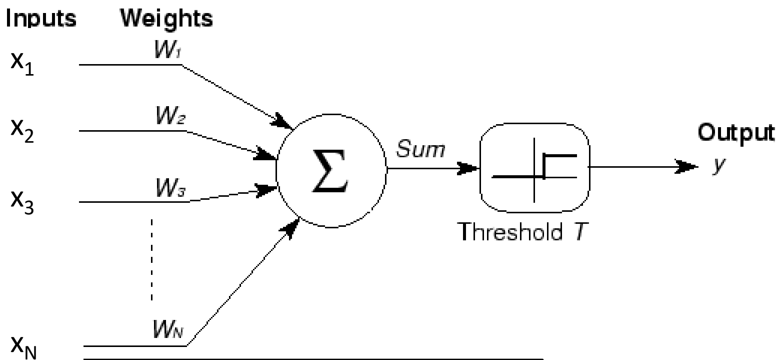




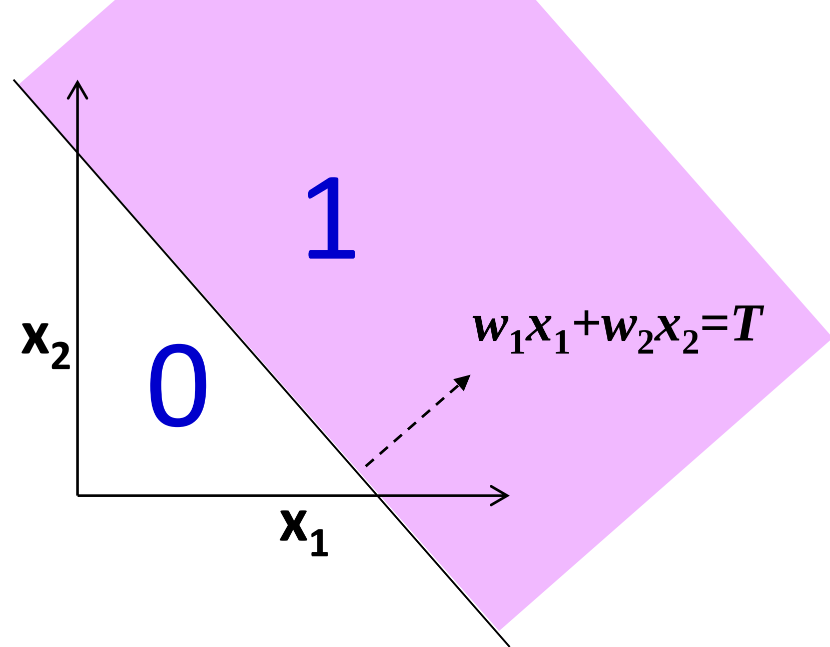
784 dimensions

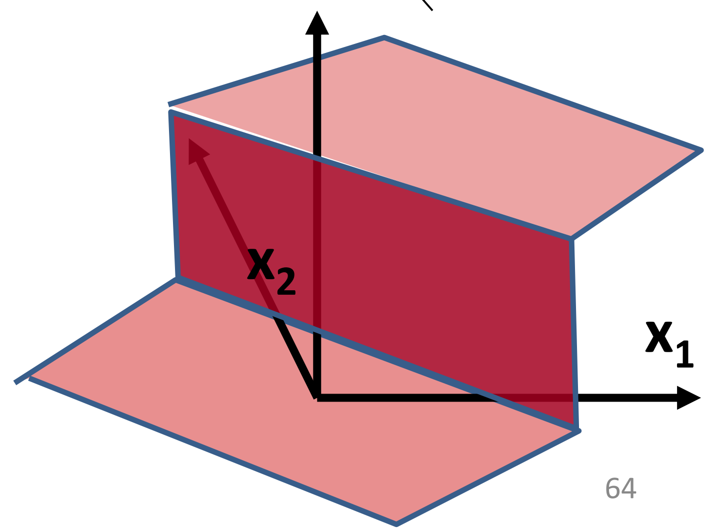
- MLP as a function over real inputs
- MLP as a function that finds a complex "decision boundary" over a space of *reals*

A Perceptron on Reals



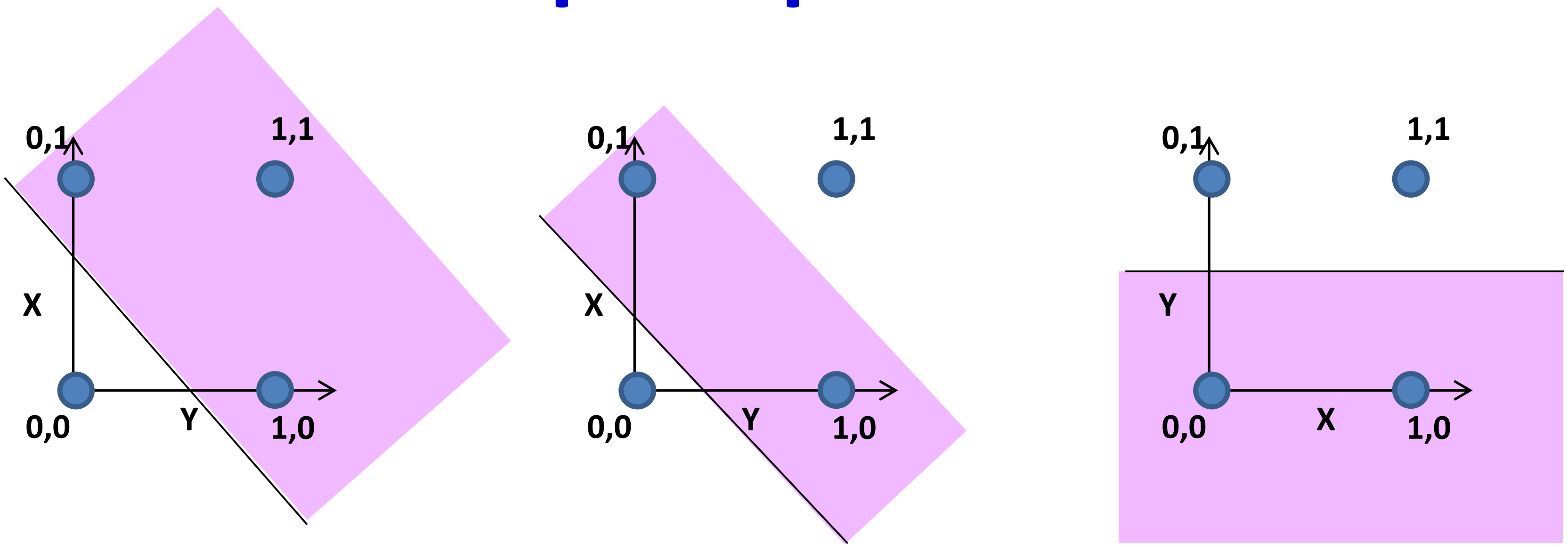
$$y = \begin{cases} 1 \; if \; \sum_i w_i x_i \geq T \\ 0 \; else \end{cases}$$





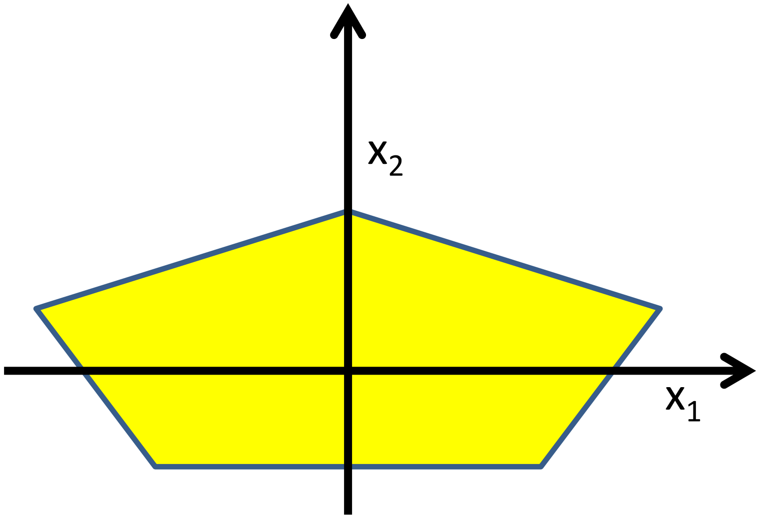
- A perceptron operates on *real*-valued vectors
  - **This is a *linear classifier***

Boolean functions with a real perceptron



- Boolean perceptrons are also linear classifiers
  - Purple regions are 1

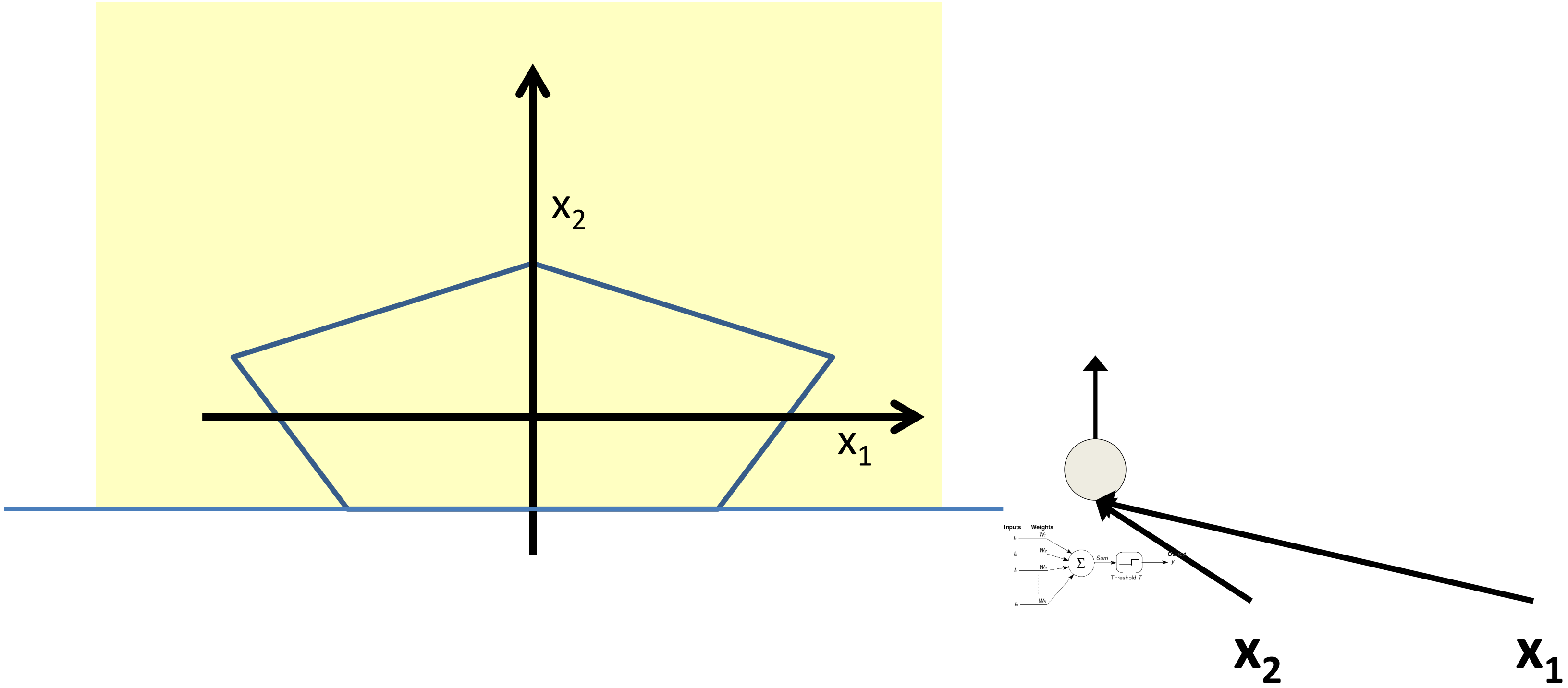
Composing complicated "decision" boundaries



Can now be composed into "networks" to compute arbitrary classification "boundaries"

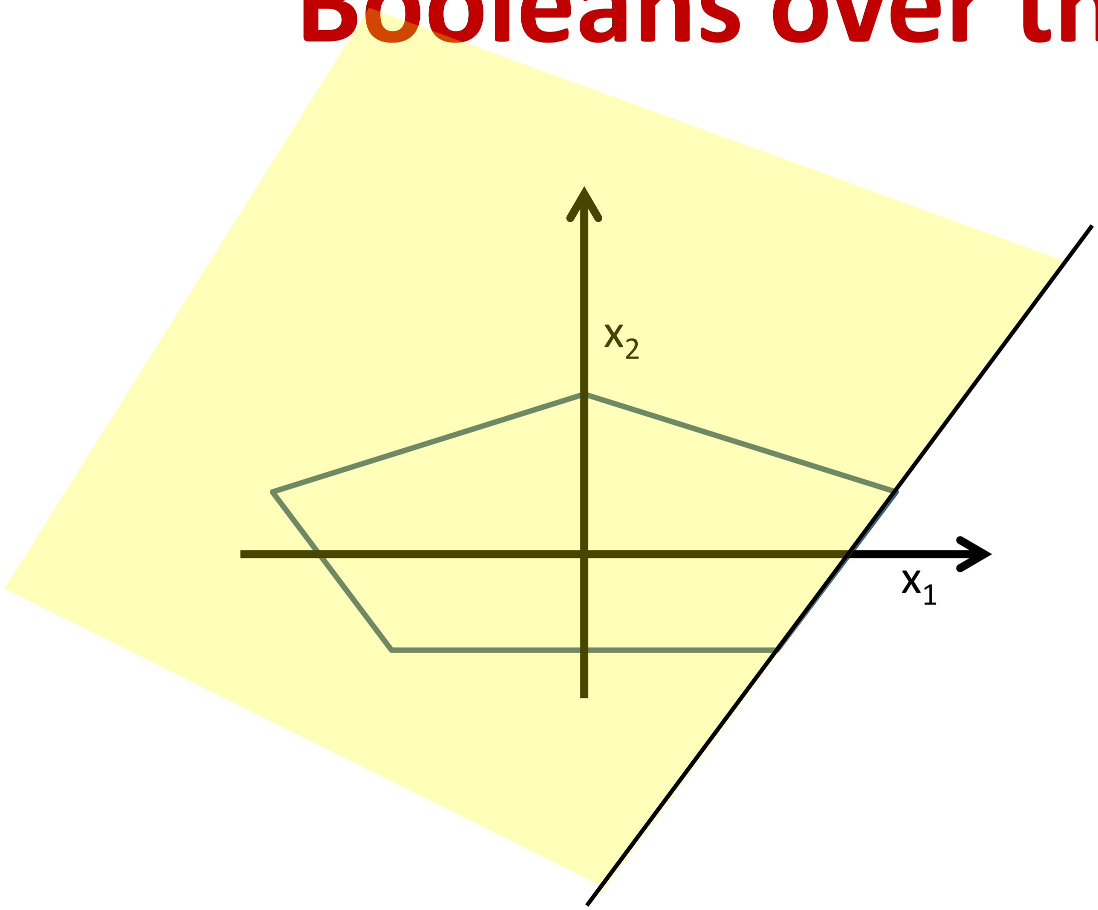
- Build a network of units with a single output that fires if the input is in the coloured area

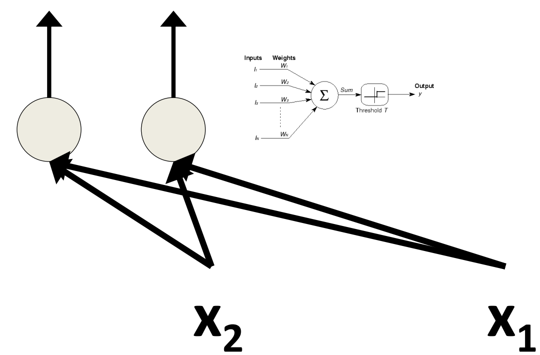
Booleans over the reals



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

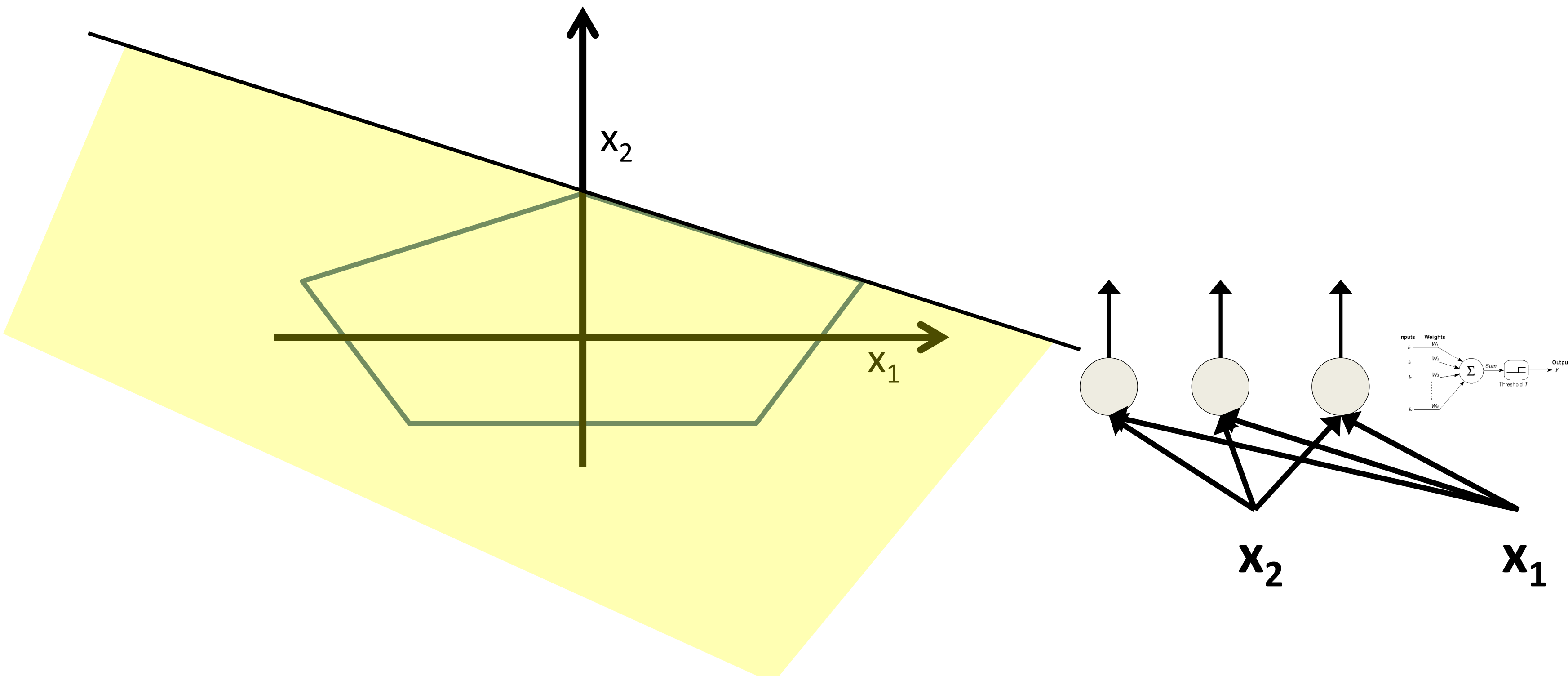
Booleans over the reals





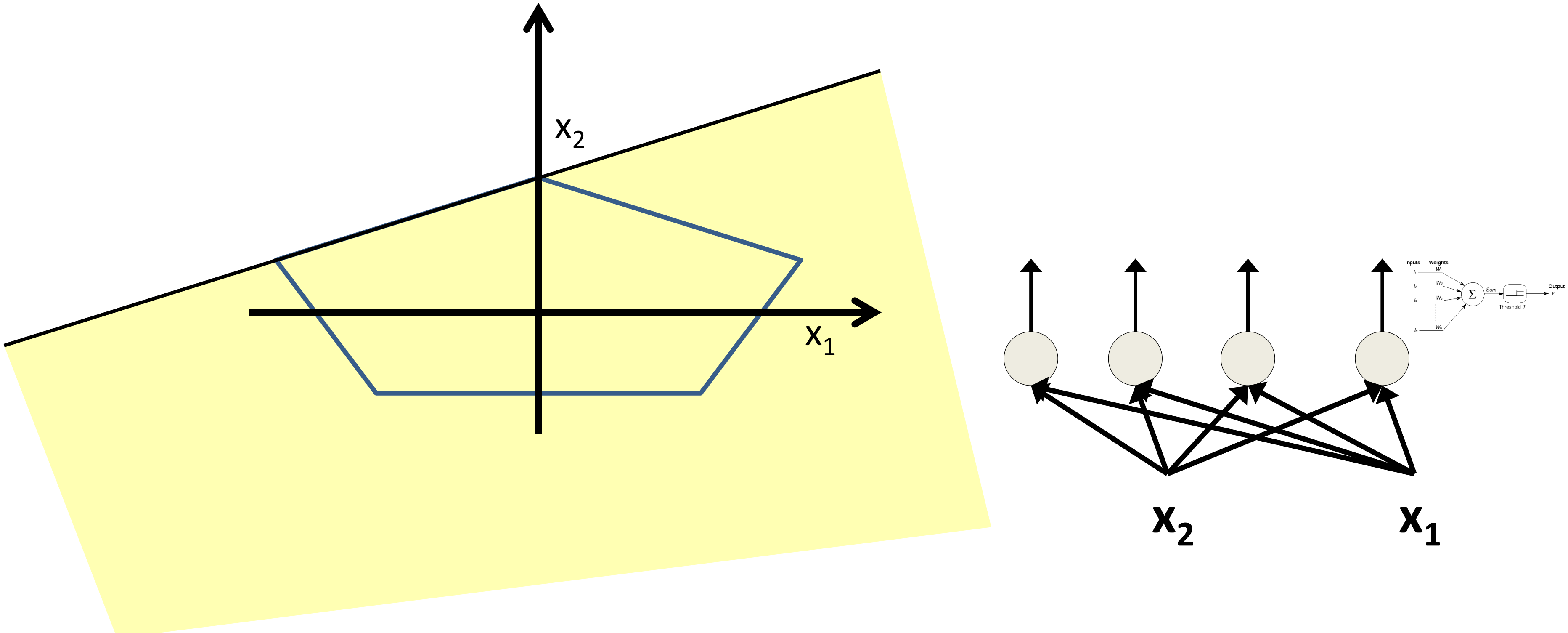
- The network must fire if the input is in the coloured area

Booleans over the reals



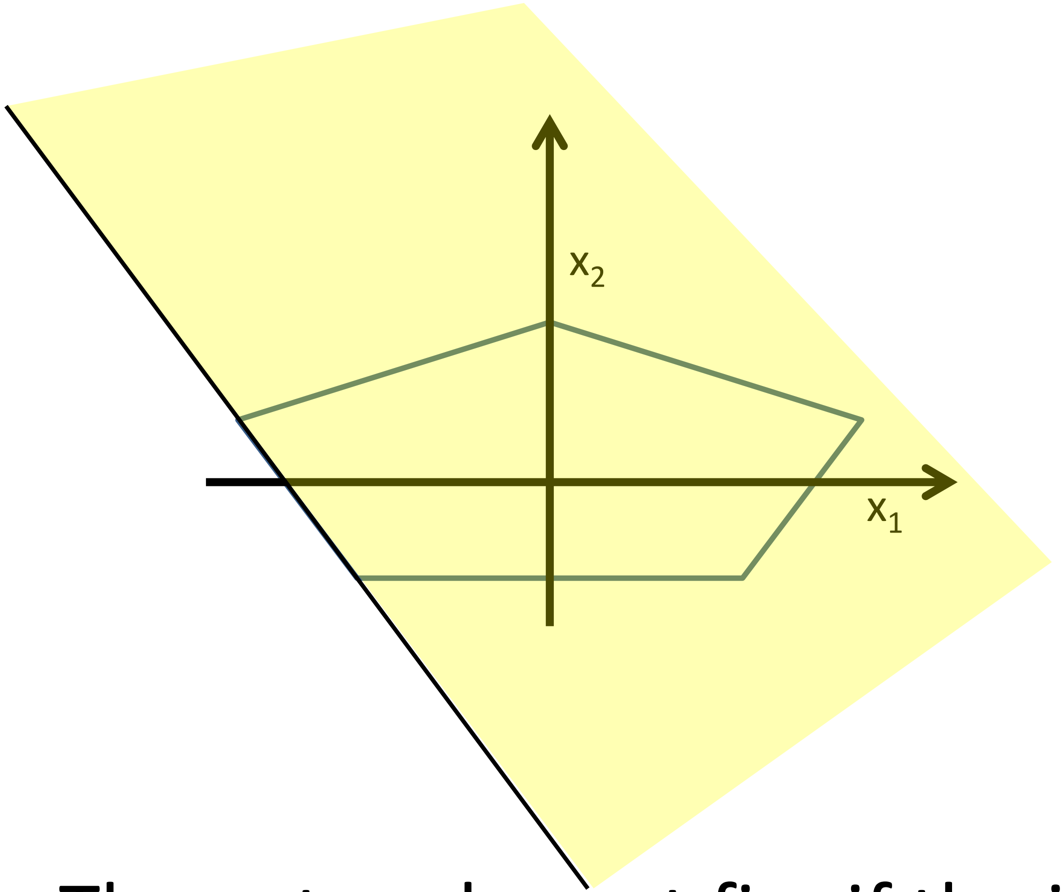
- The network must fire if the input is in the coloured area

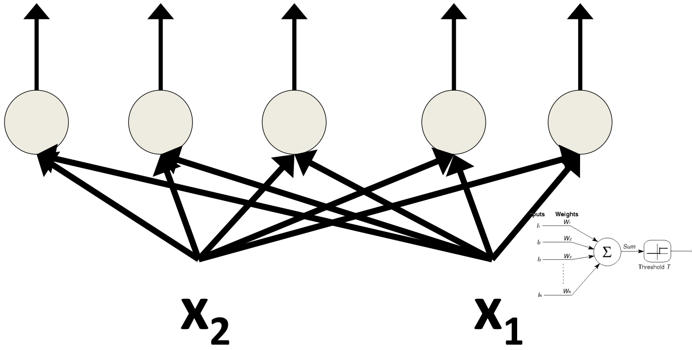
Booleans over the reals



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

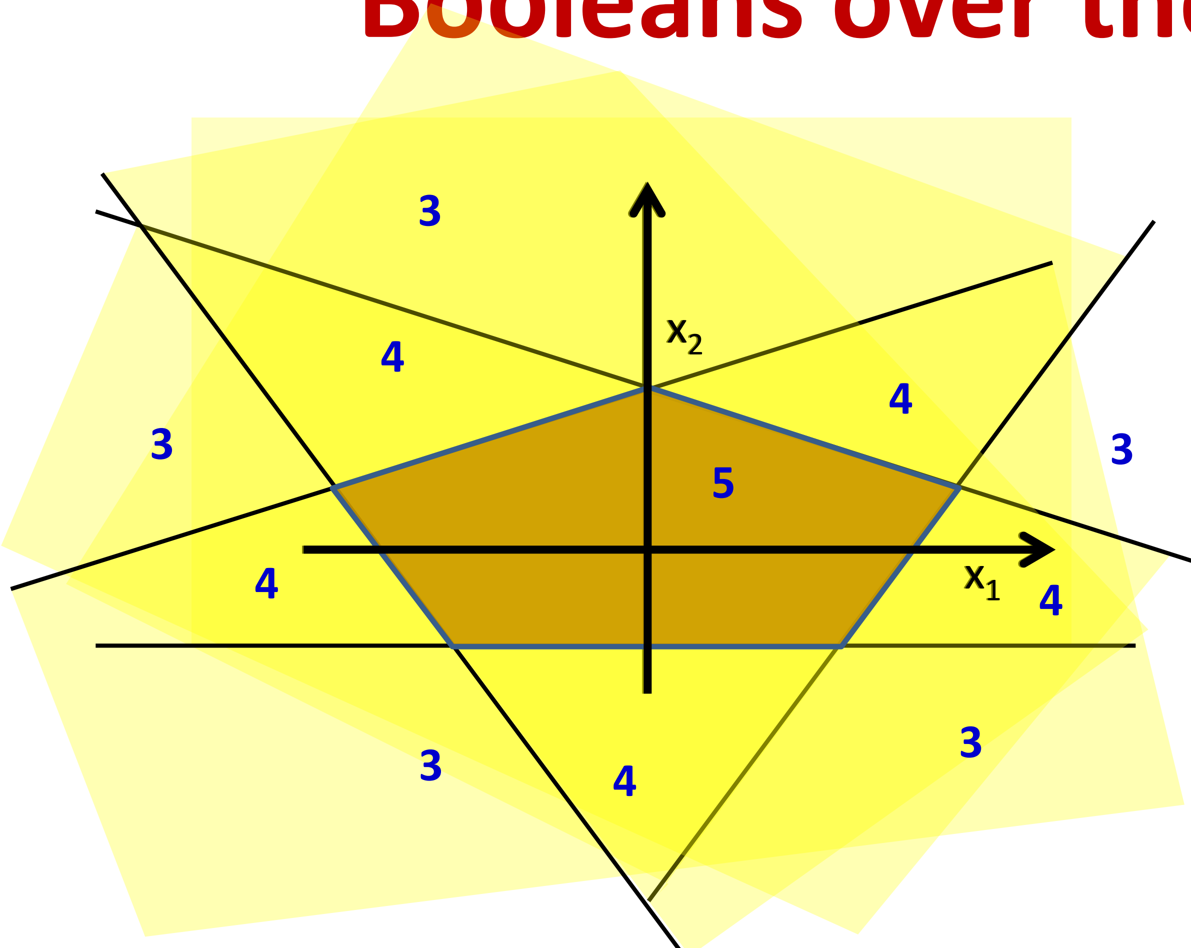
Booleans over the reals

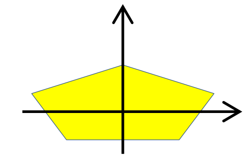


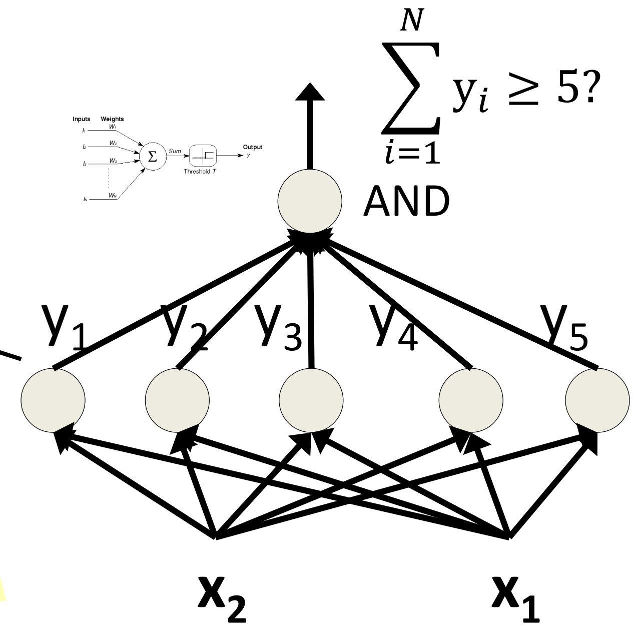


- The network must fire if the input is in the coloured area

Booleans over the reals

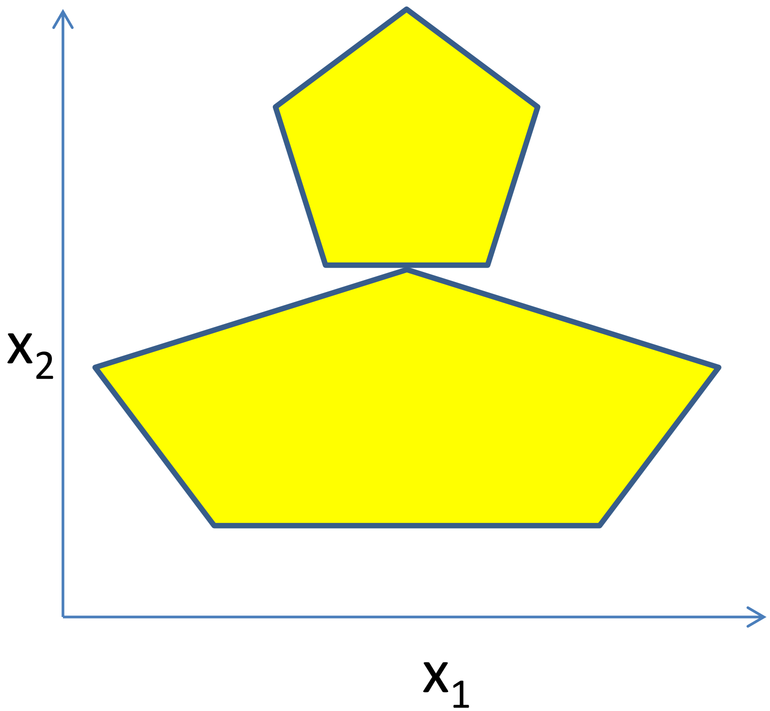


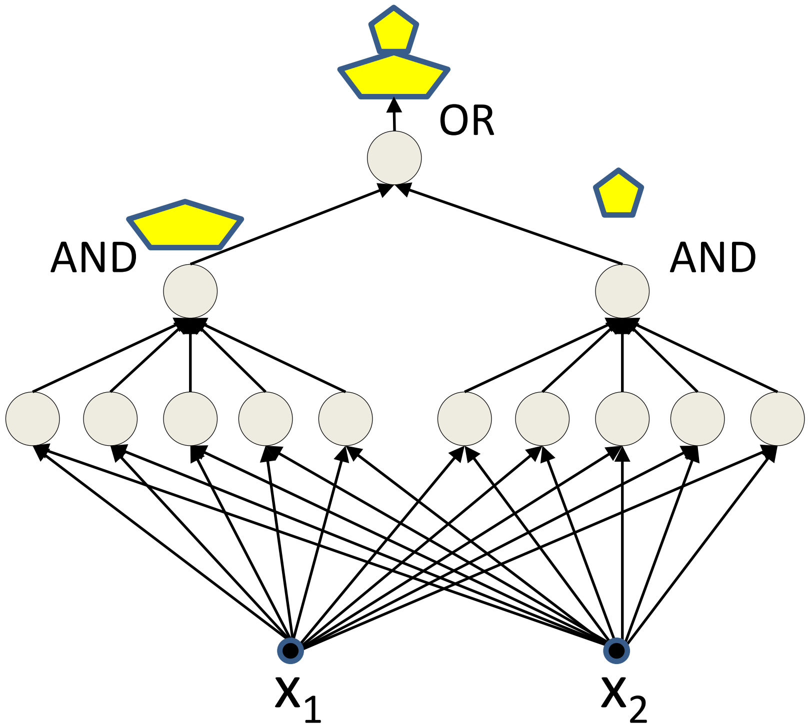




- The network must fire if the input is in the coloured area

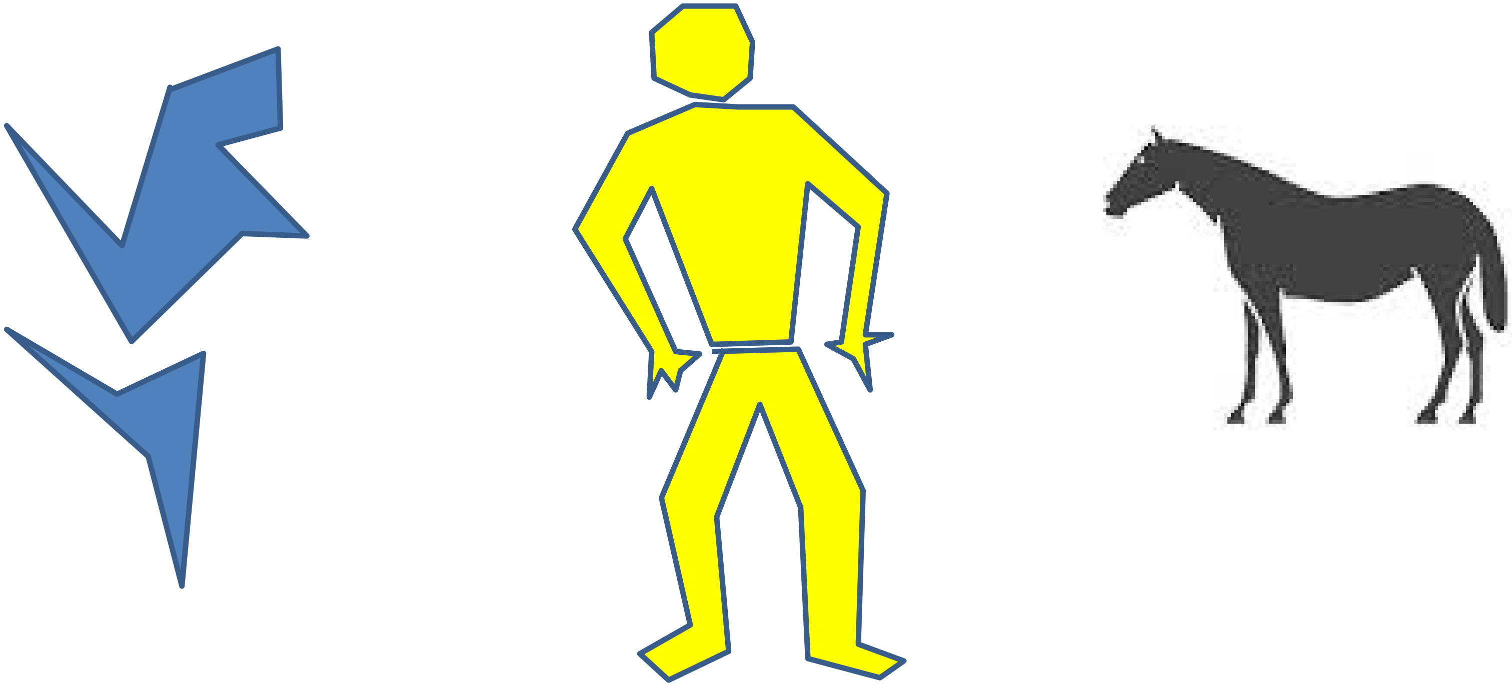
More complex decision boundaries





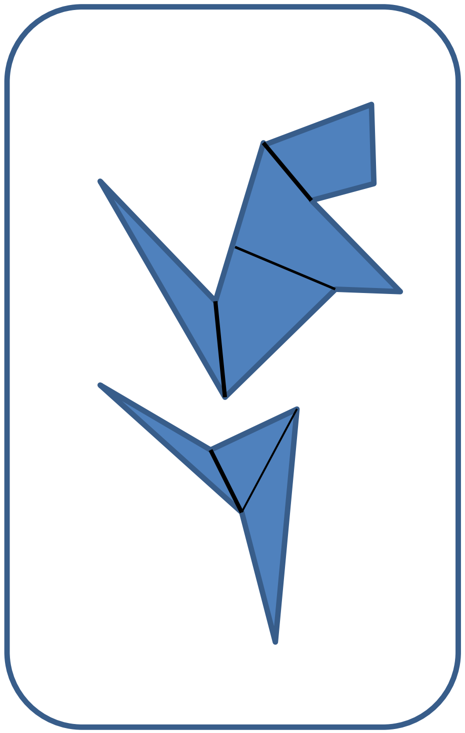
- Network to fire if the input is in the yellow area
  - "OR" two polygons
  - A third layer is required

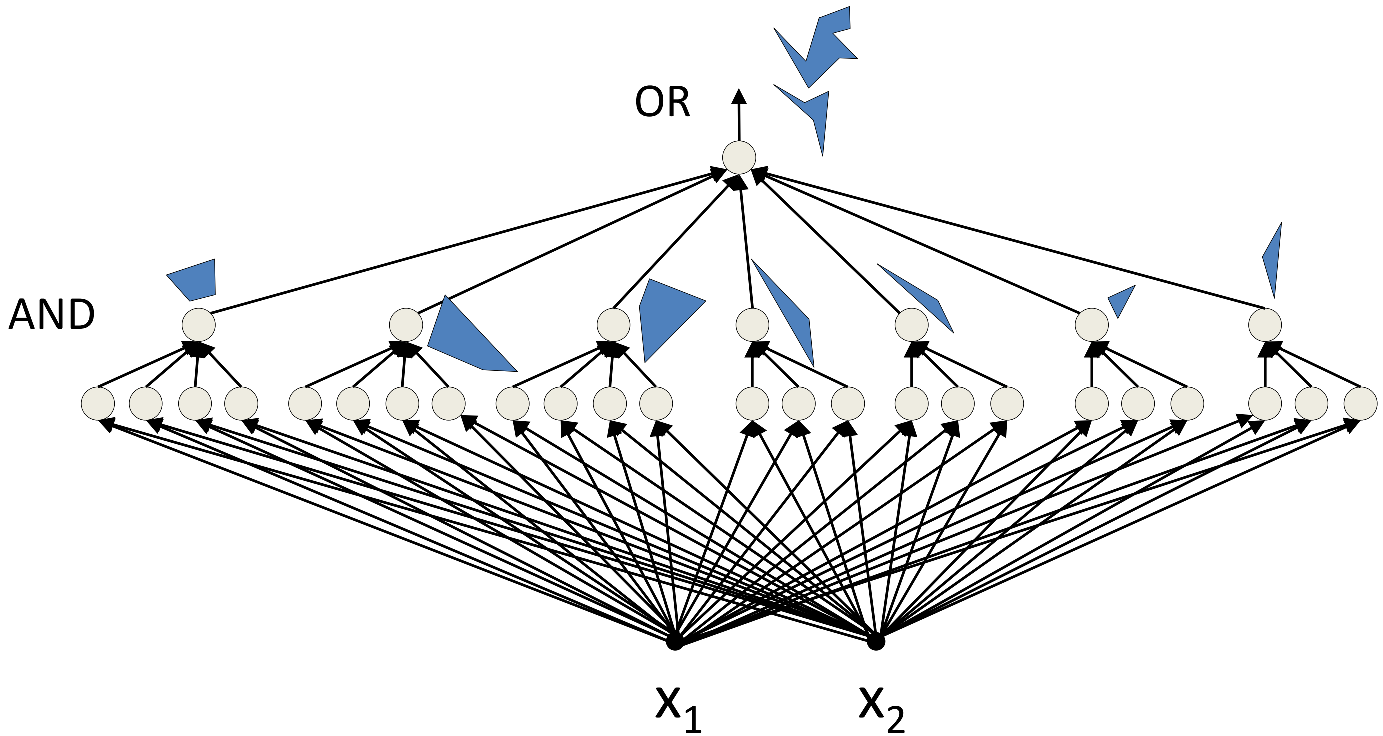
Complex decision boundaries



- Can compose *arbitrarily* complex decision boundaries

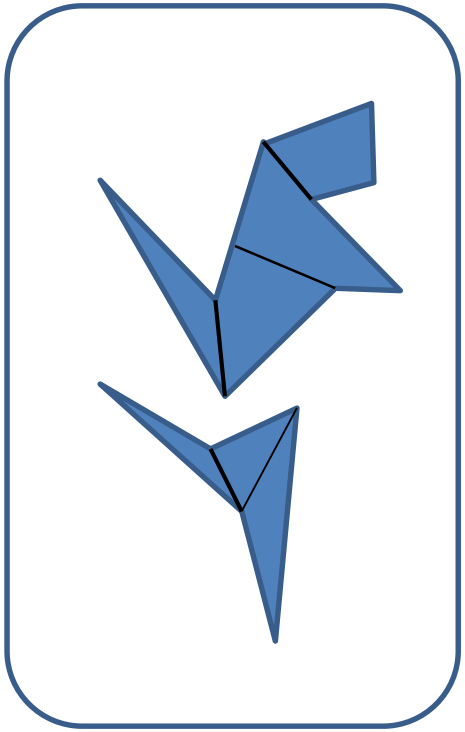
Complex decision boundaries

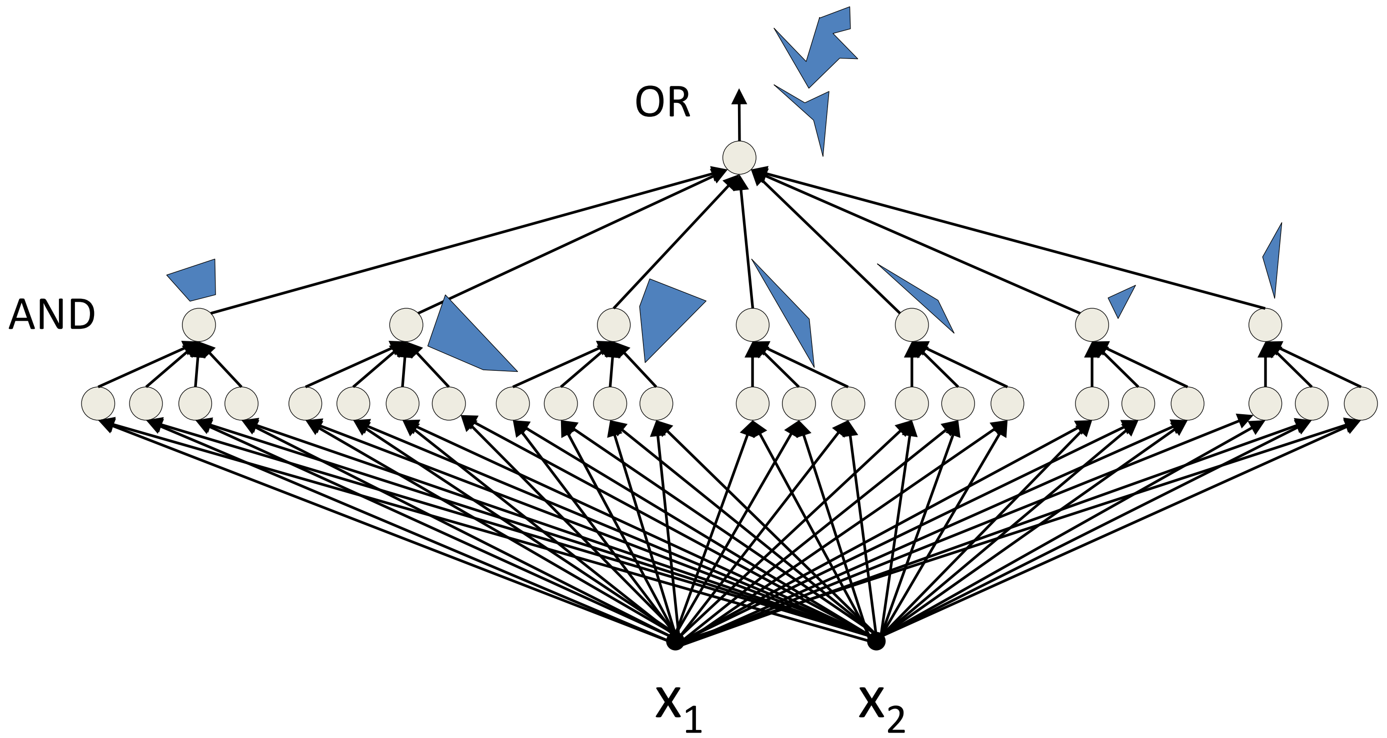




- Can compose *arbitrarily* complex decision boundaries

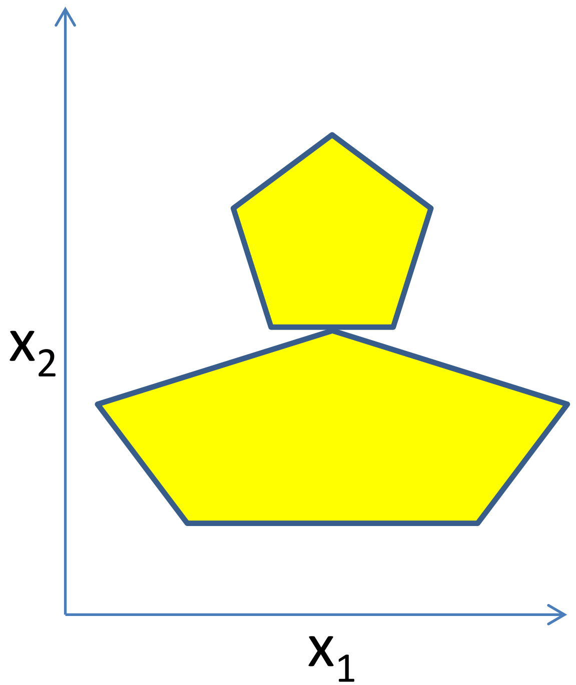
Complex decision boundaries

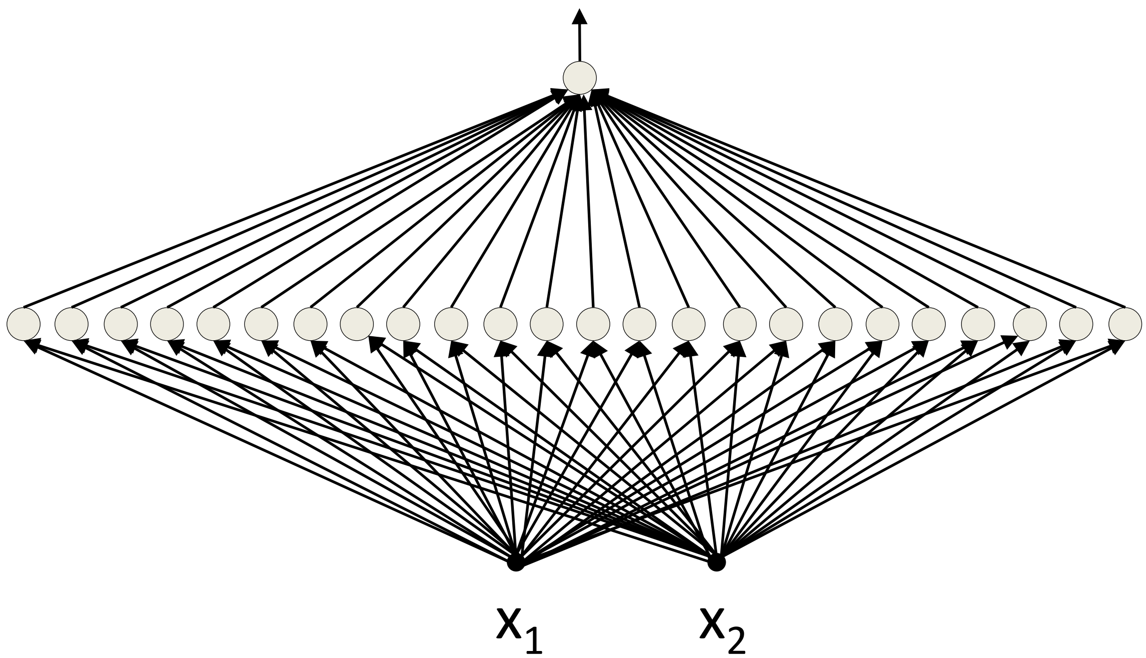




- Can compose *arbitrarily* complex decision boundaries
  - With *only one hidden layer!*
  - **How?**

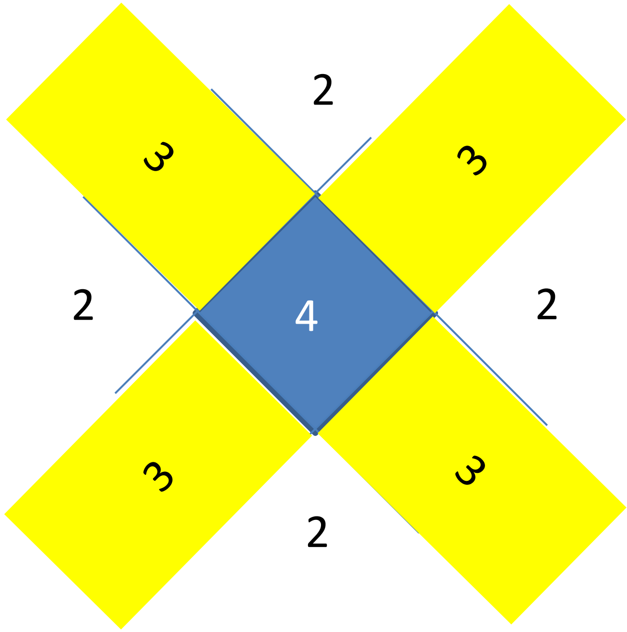
Exercise: compose this with one hidden layer

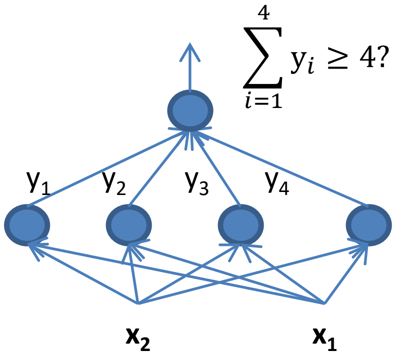




- How would you compose the decision boundary to the left with only *one* hidden layer?

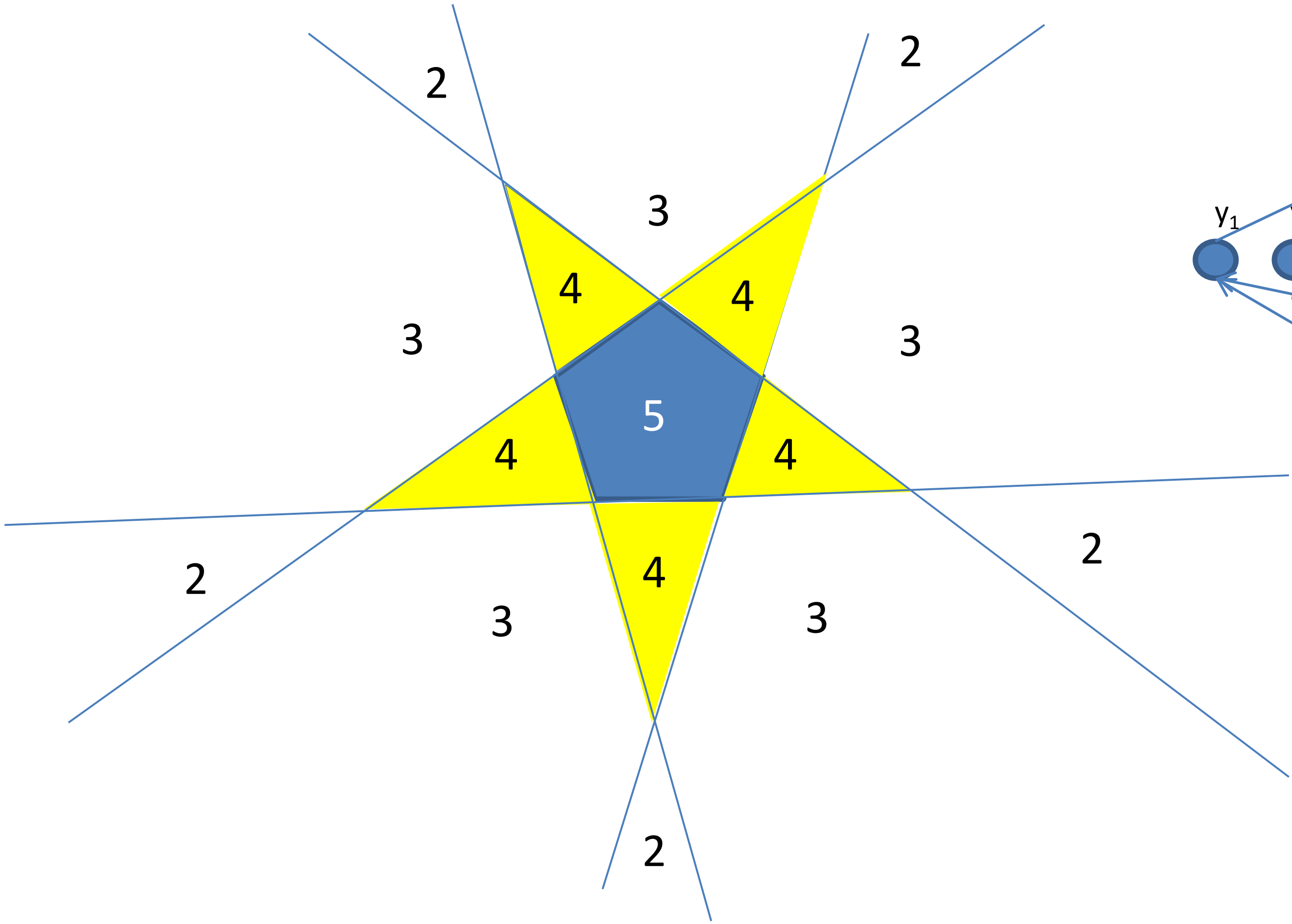
Composing a Square decision boundary

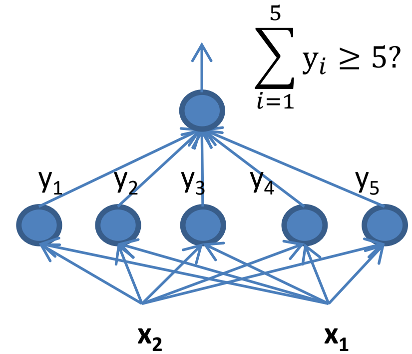




- The polygon net

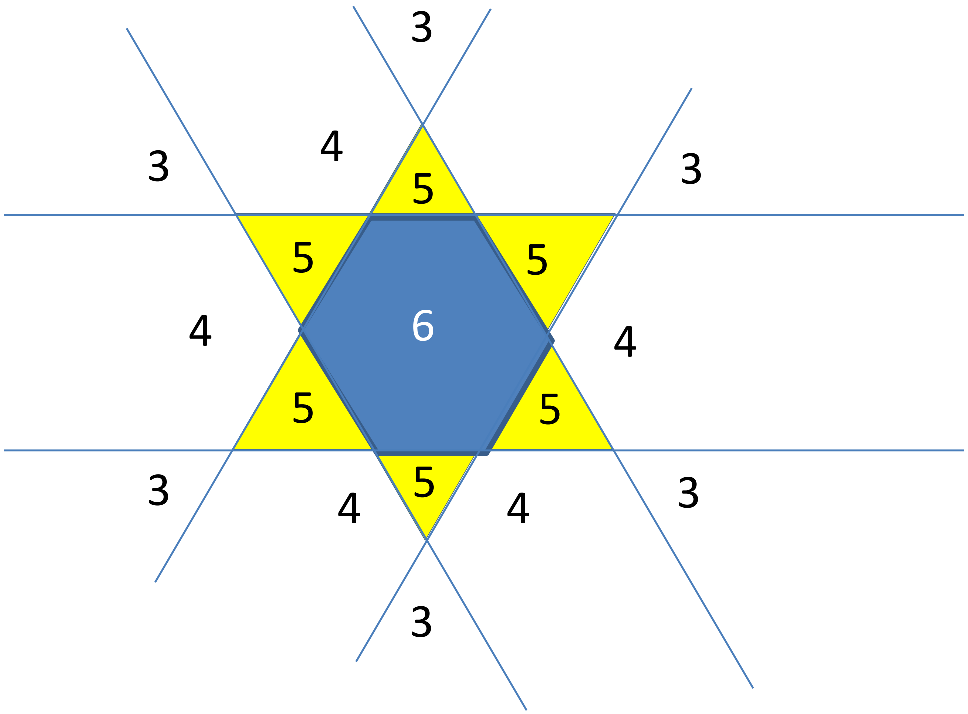
Composing a pentagon

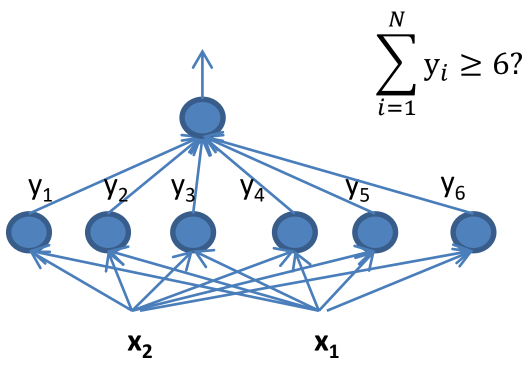




- The polygon net

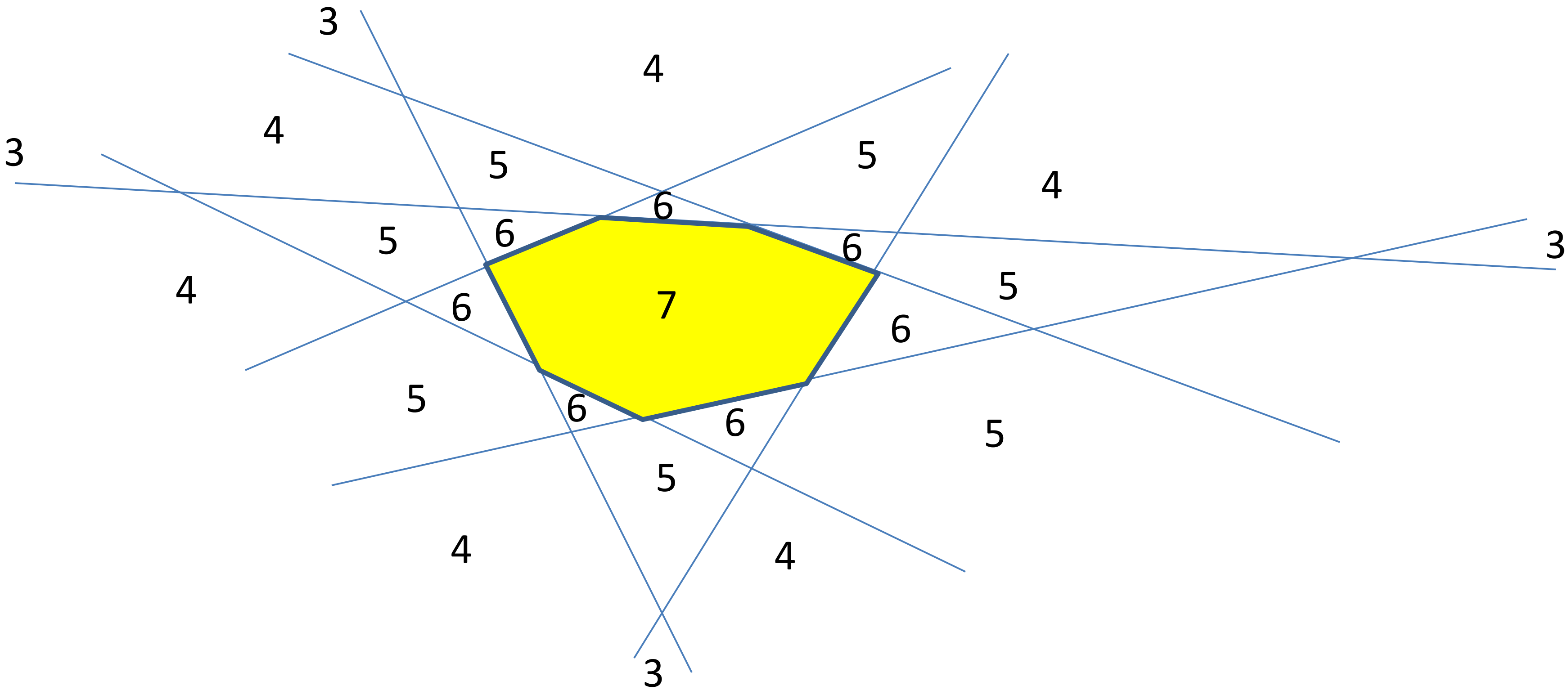
Composing a hexagon





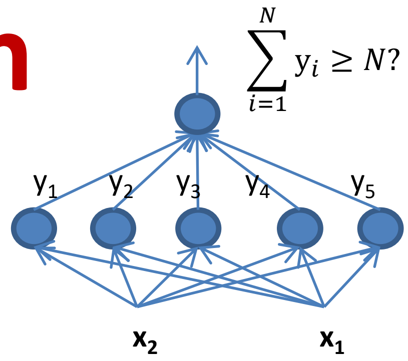
- The polygon net

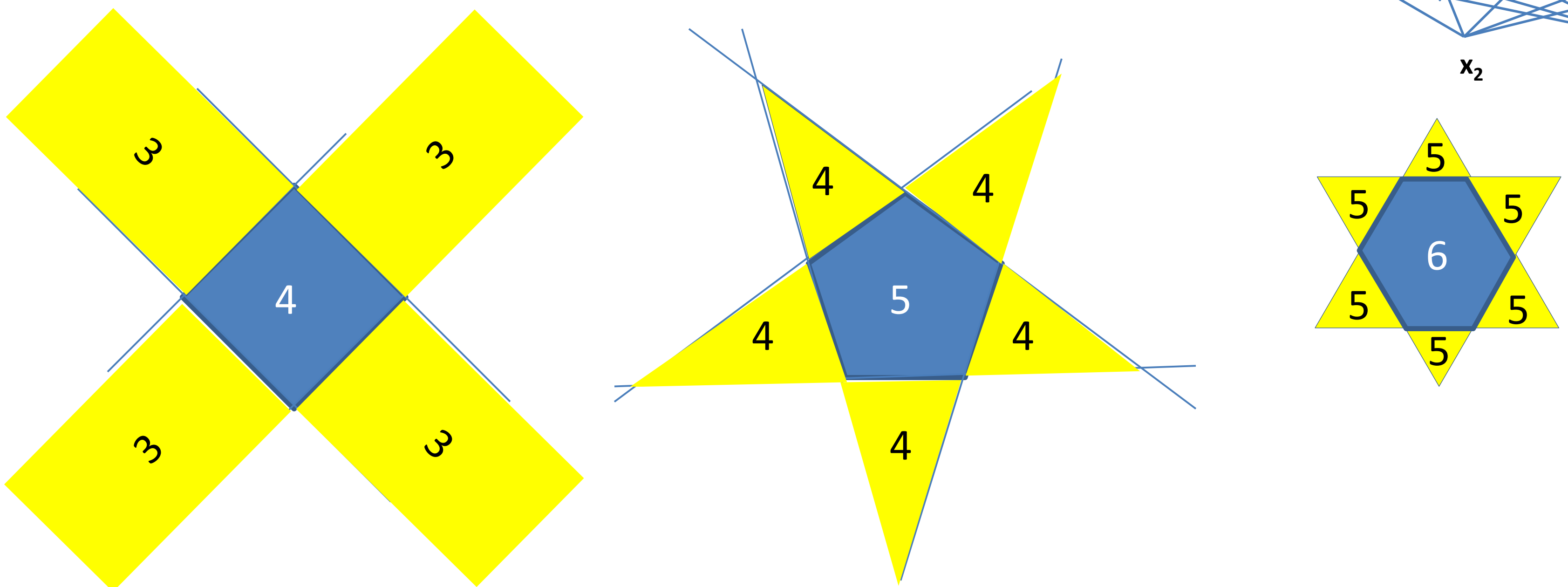
How about a heptagon



- What are the sums in the different regions?
  - A pattern emerges as we consider N > 6..

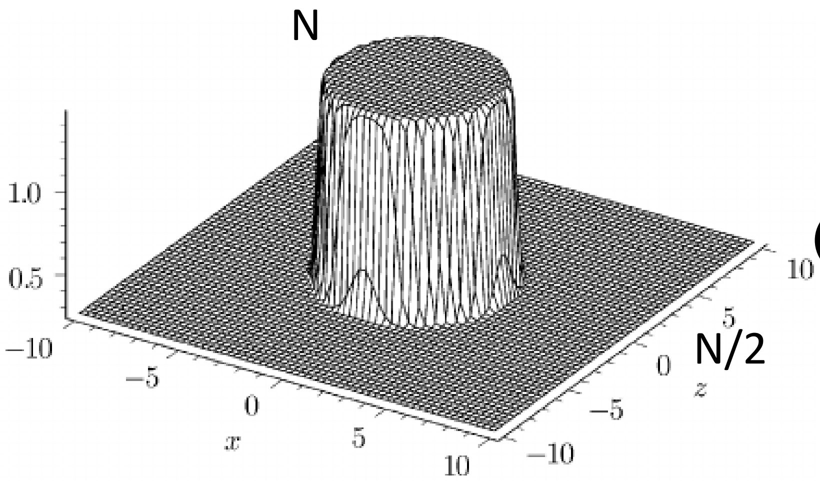
Composing a polygon

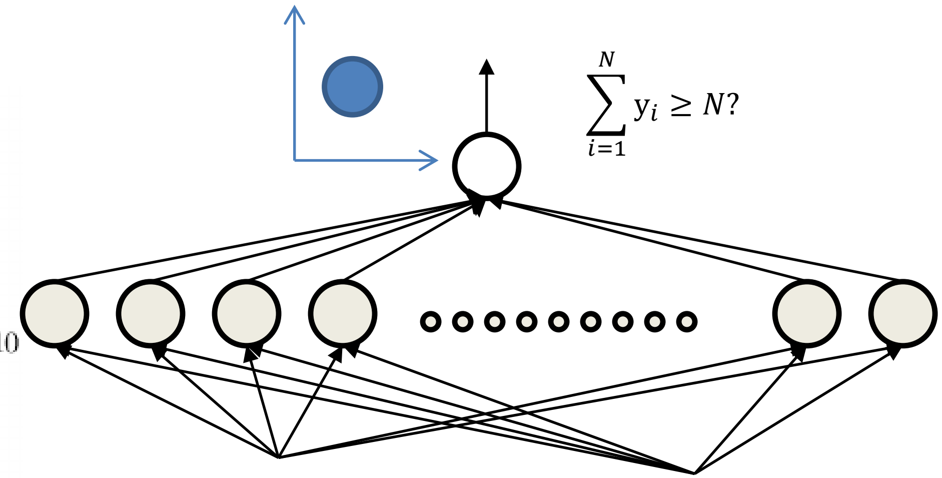




- The polygon net
- Increasing the number of sides reduces the area outside the polygon that have N/2 < Sum < N

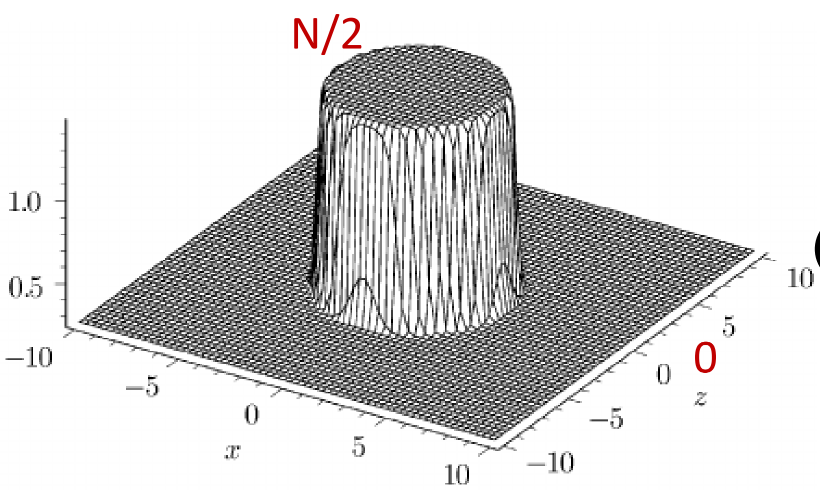
Composing a circle

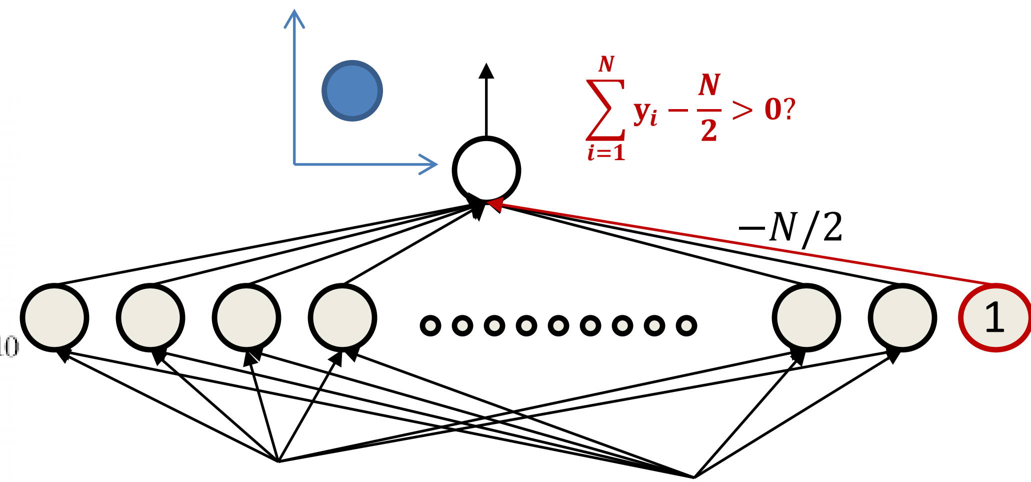




- The circle net
  - Very large number of neurons
  - *Sum is N inside the circle, N/2 outside everywhere*
  - Circle can be of arbitrary diameter, at any location

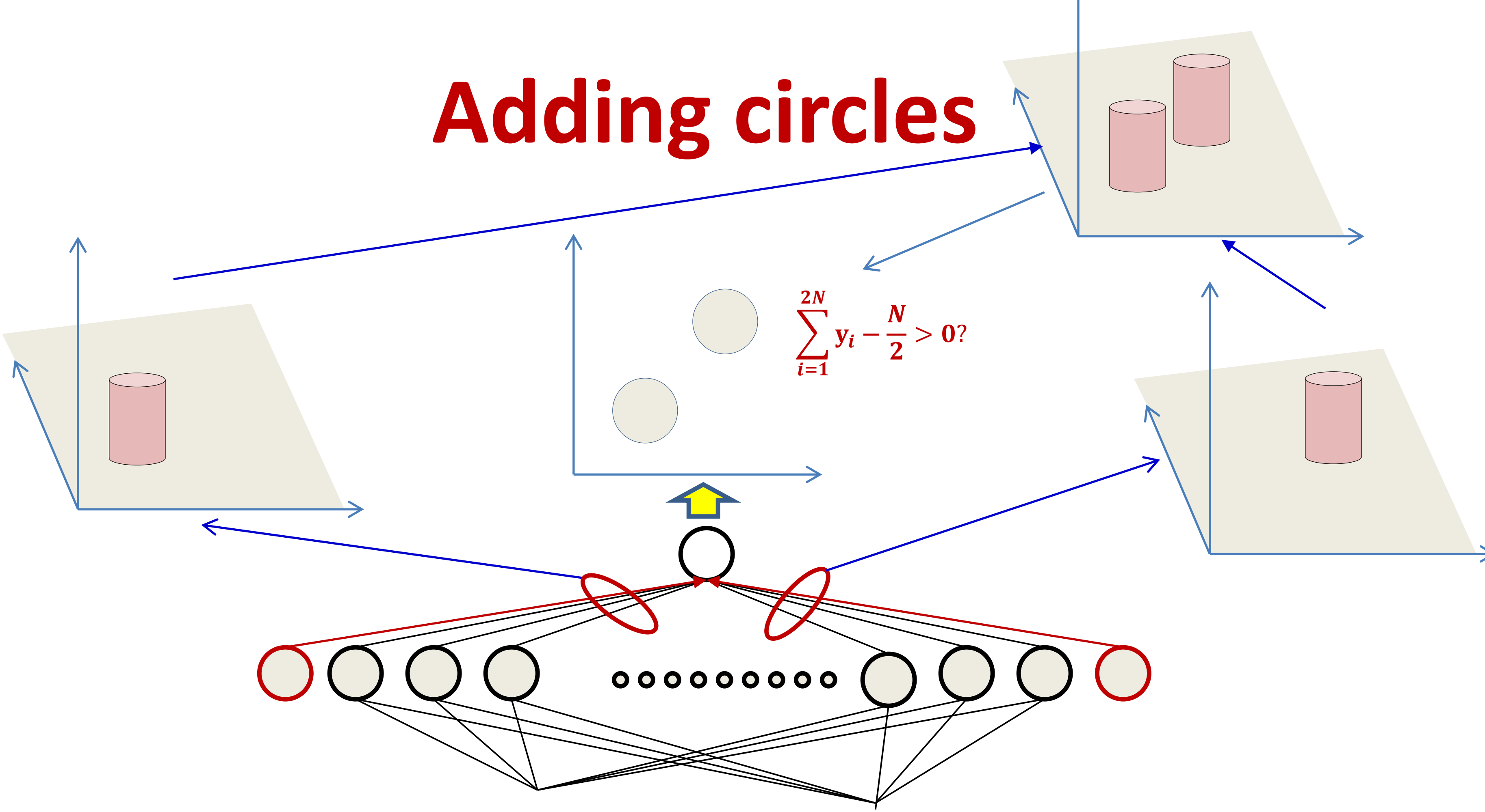
Composing a circle





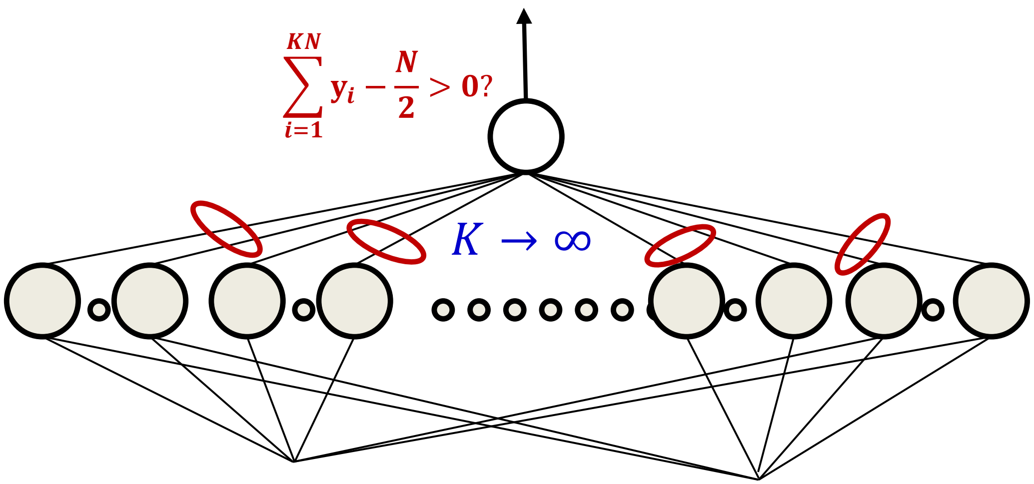
- The circle net
  - Very large number of neurons
  - *Sum is N/2 inside the circle, 0 outside everywhere*
  - Circle can be of arbitrary diameter, at any location

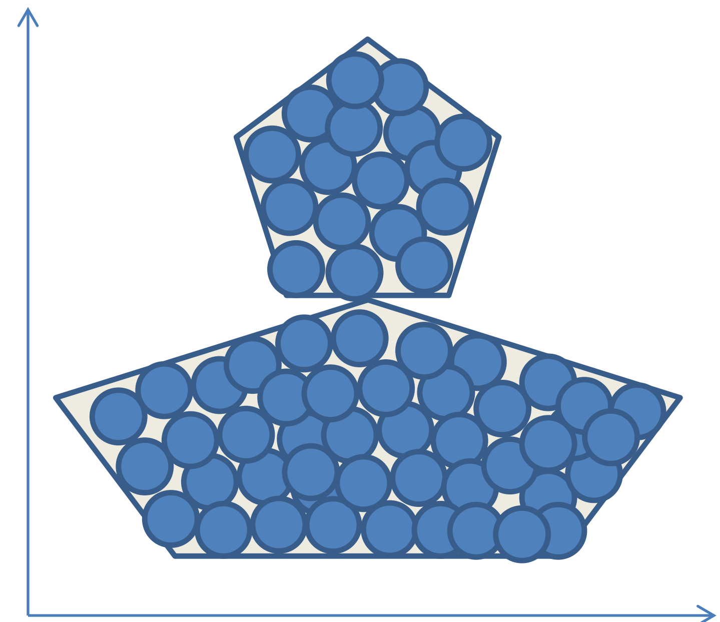
Adding circles



- The "sum" of two circles sub nets is exactly N/2 inside either circle, and 0 outside

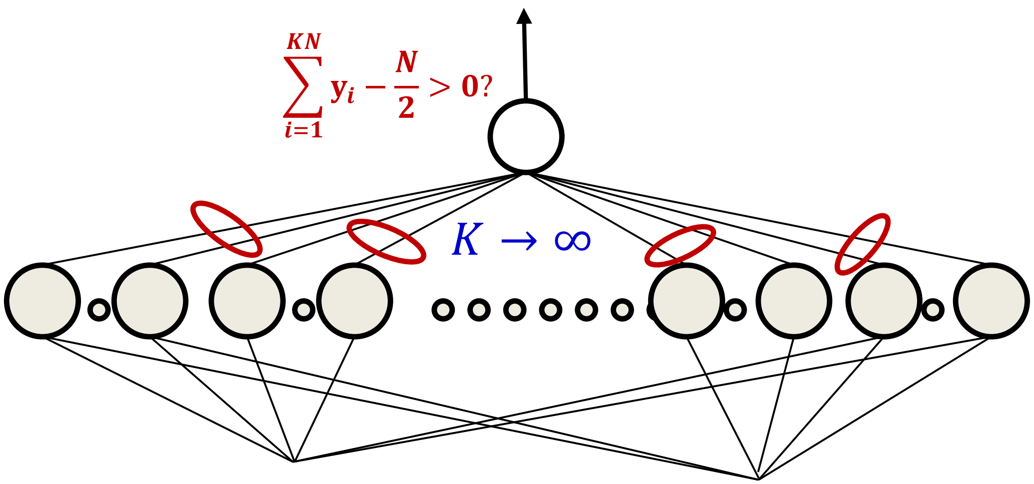
Composing an arbitrary figure

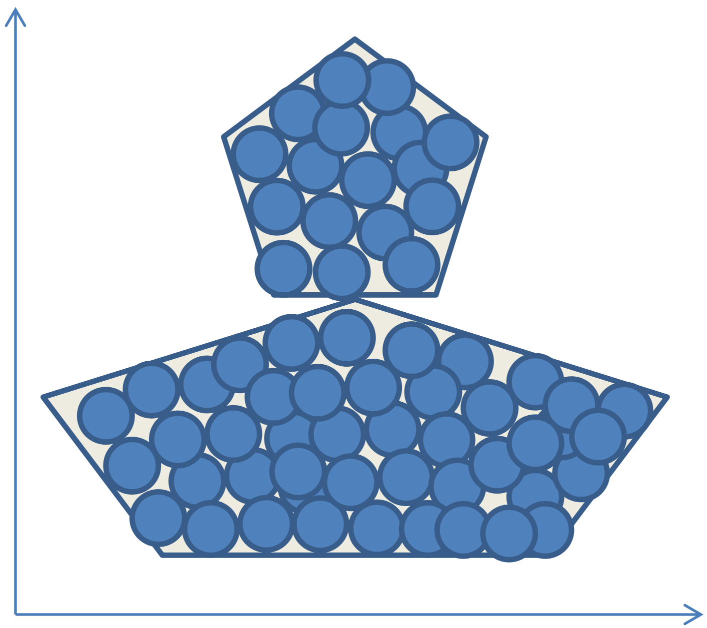




- Just fit in an arbitrary number of circles
  - More accurate approximation with greater number of smaller circles
  - Can achieve arbitrary precision

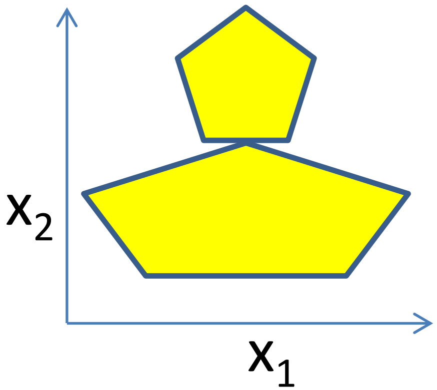
MLP: Universal classifier

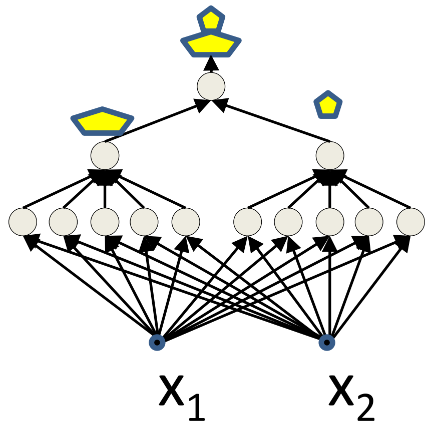


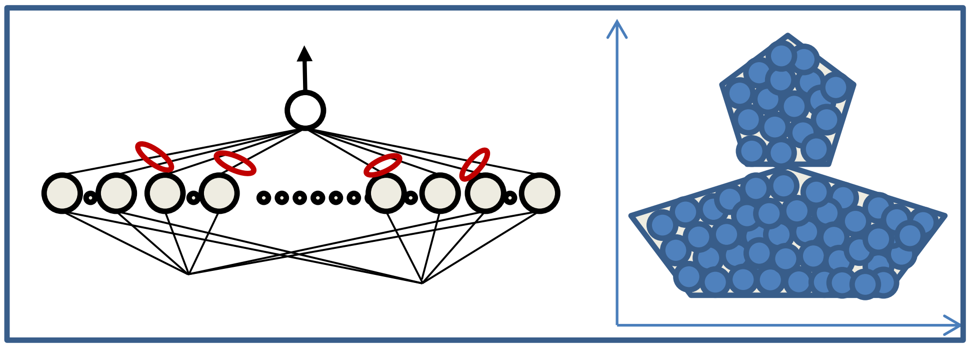


- MLPs can capture *any* classification boundary
- A *one-layer MLP* can model any classification boundary
- *MLPs are universal classifiers*

Depth and the universal classifier

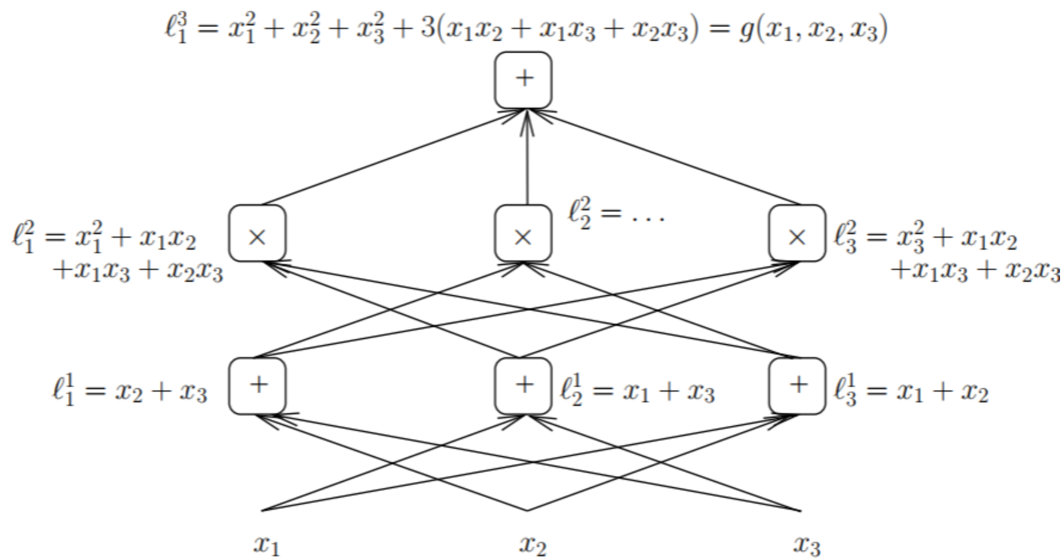






- Deeper networks can require far fewer neurons

Special case: Sum-product nets



- "Shallow vs deep sum-product networks," Oliver Dellaleau and Yoshua Bengio
  - For networks where layers alternately perform either sums or products, a deep network may require an exponentially fewer number of layers than a shallow one

Depth in sum-product networks

Theorem 5

A certain class of functions $\mathcal{F}$ of n inputs can be represented using a deep network with $\mathcal{O}(n)$ units, whereas it would require $\mathcal{O}(2^{\sqrt{n}})$ units for a shallow network.

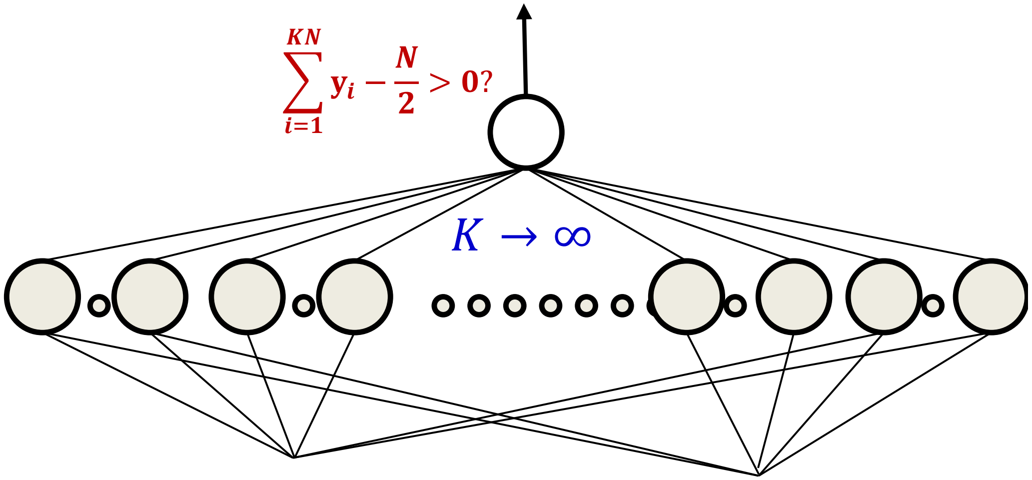
Theorem 6

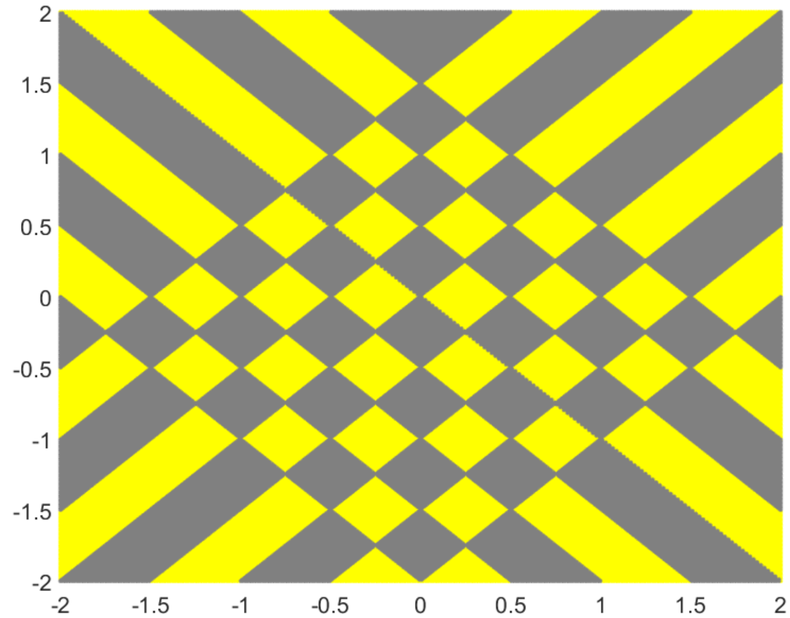
For a certain class of functions $\mathcal{G}$ of n inputs, the deep sum-product network with depth k can be represented with $\mathcal{O}(nk)$ units, whereas it would require $\mathcal{O}((n-1)^k)$ units for a shallow network.

Optimal depth in *generic* nets

- We look at a different pattern:
  - "worst case" decision boundaries
- For *threshold-activation* networks
  - Generalizes to other nets

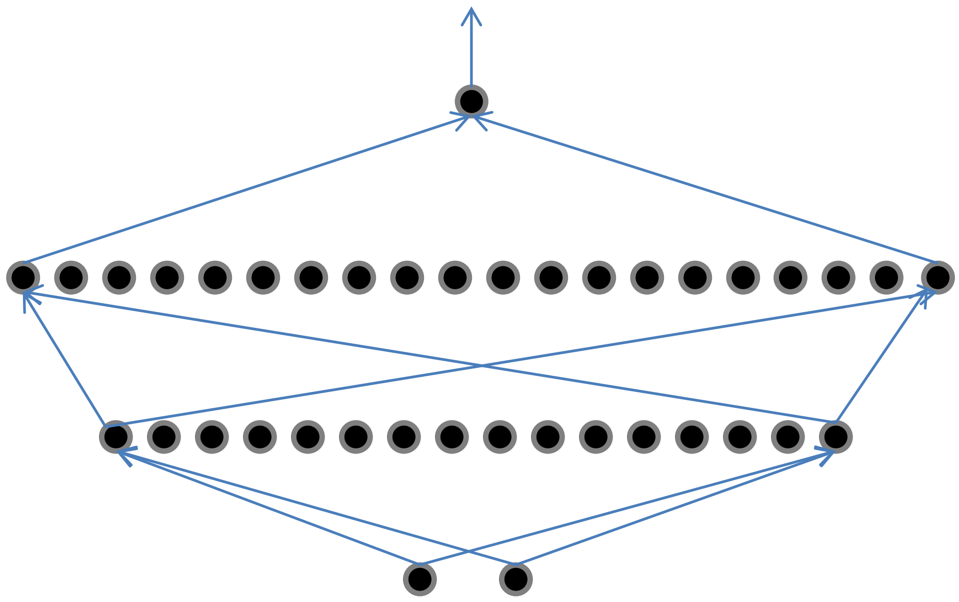
Optimal depth

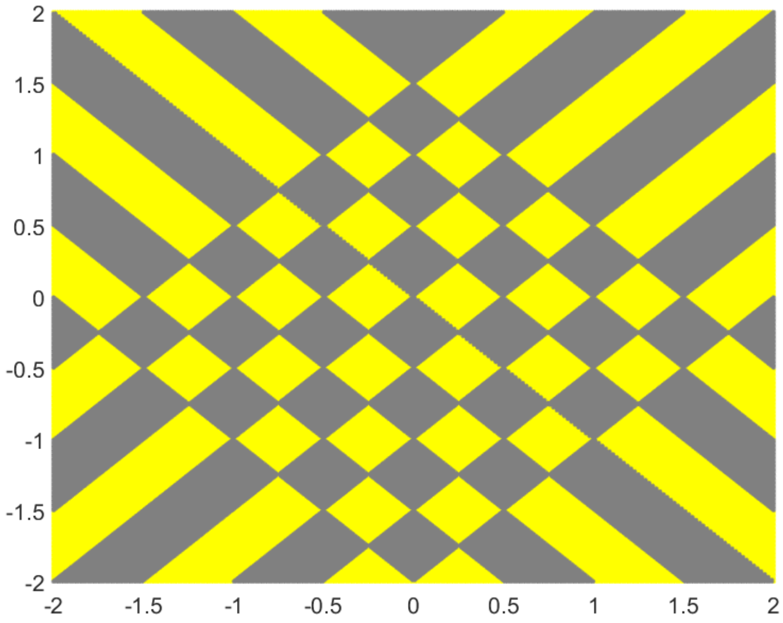




- A one-hidden-layer neural network will required infinite hidden neurons

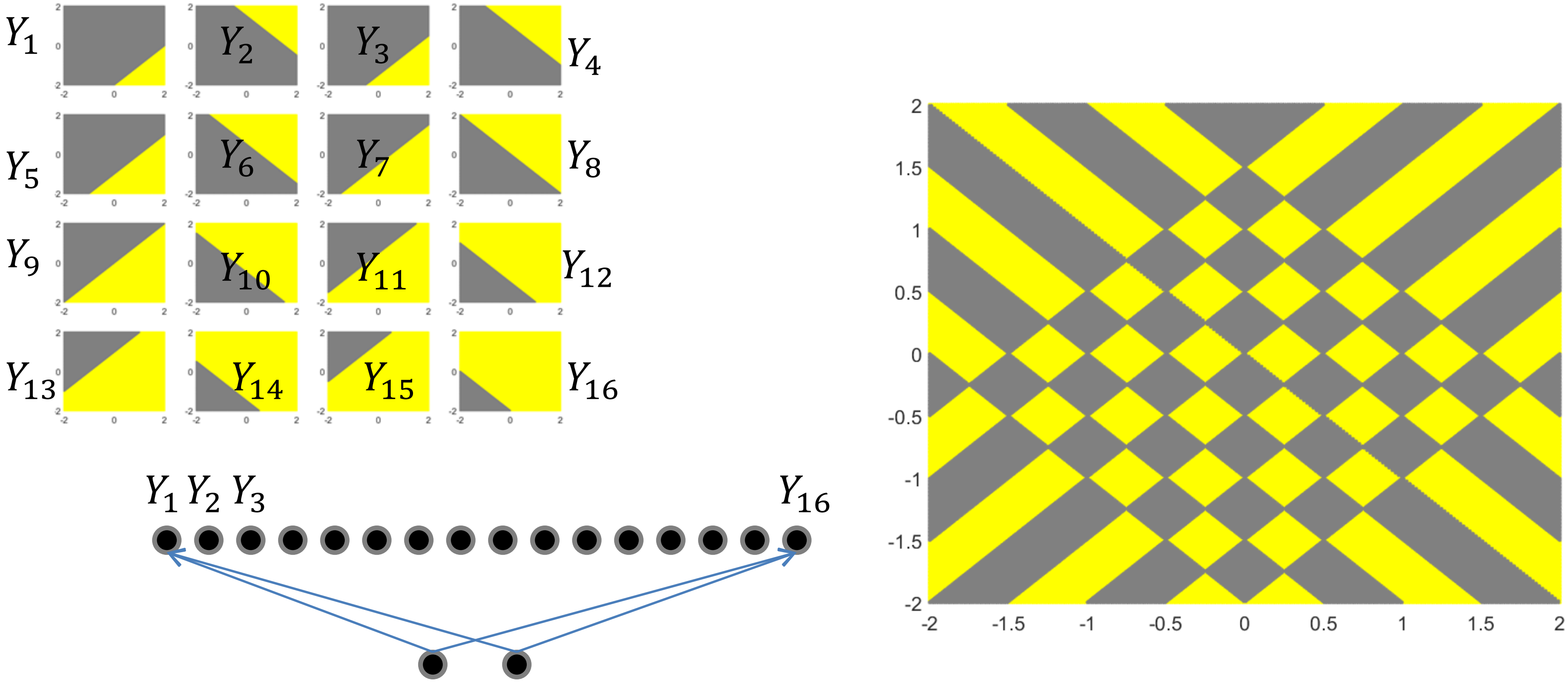
Optimal depth





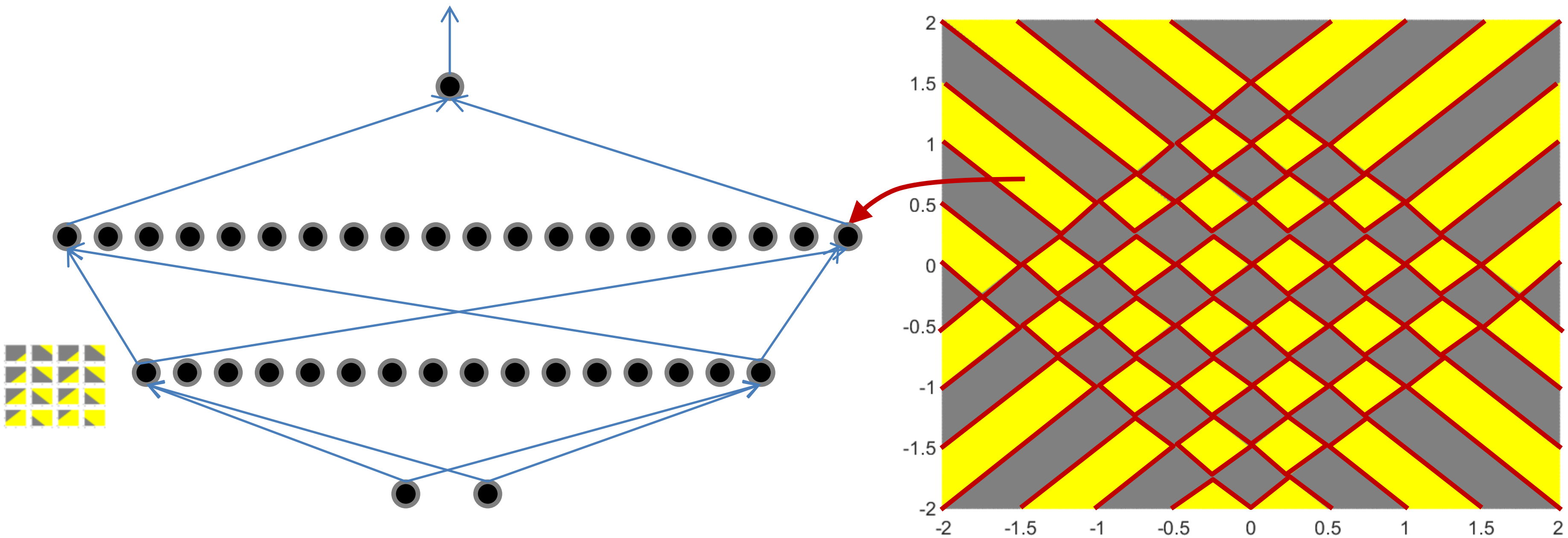
- Two layer network: 56 hidden neurons

Optimal depth



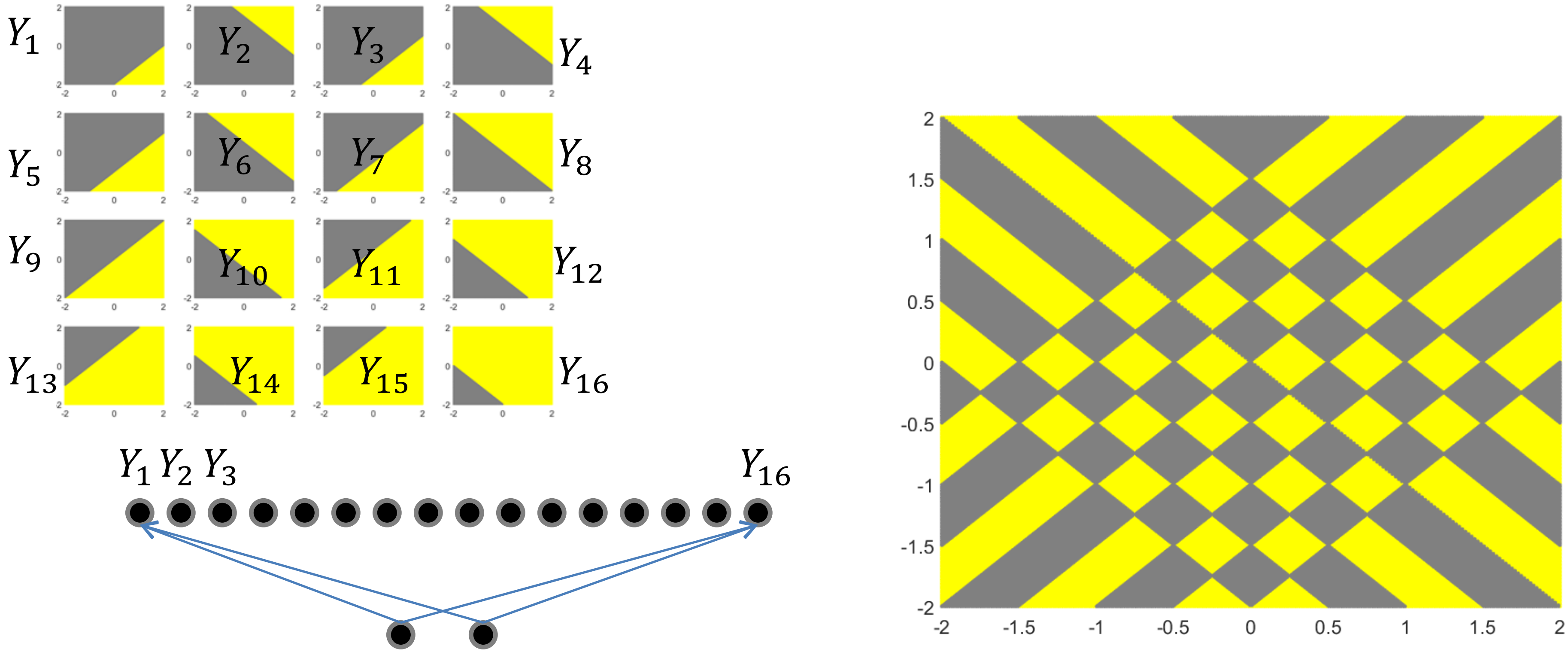
- Two layer network: 56 hidden neurons
  - 16 neurons in hidden layer 1

Optimal depth



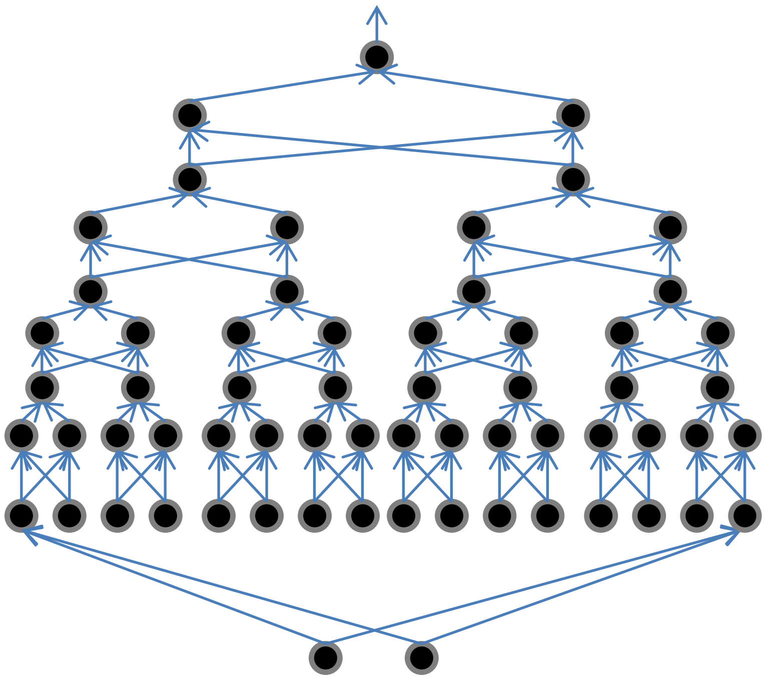
- Two-layer network: 56 hidden neurons
  - 16 in hidden layer 1
  - 40 in hidden layer 2
  - 57 total neurons, including output neuron

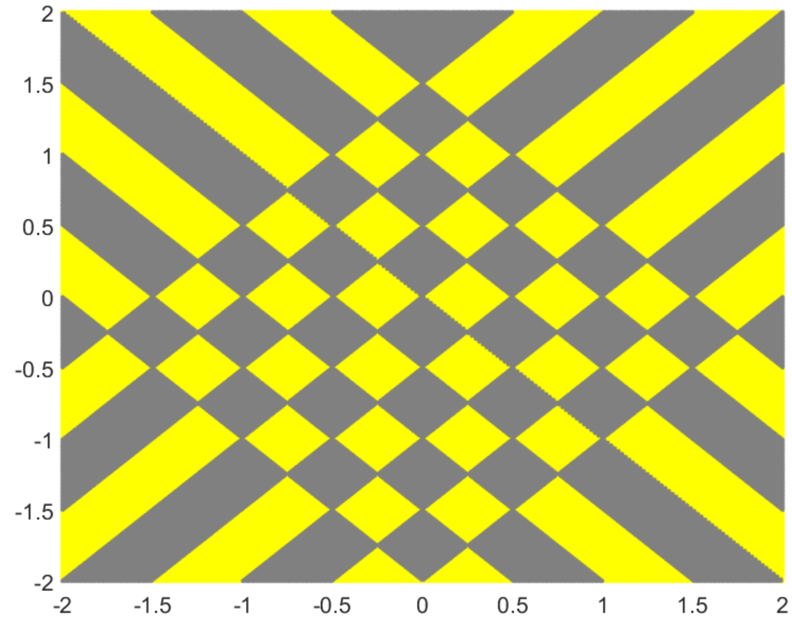
Optimal depth



- But this is just $Y_1 \oplus Y_2 \oplus \cdots \oplus Y_{16}$

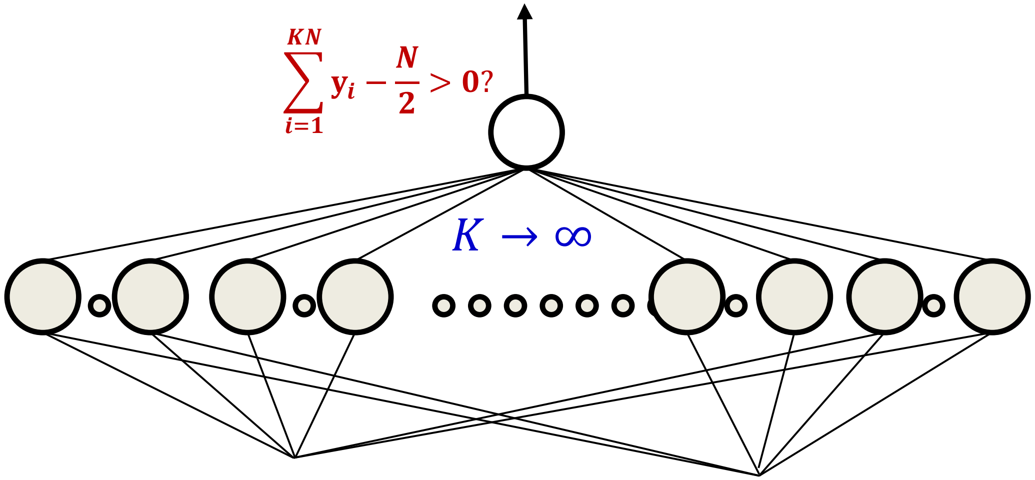
Optimal depth

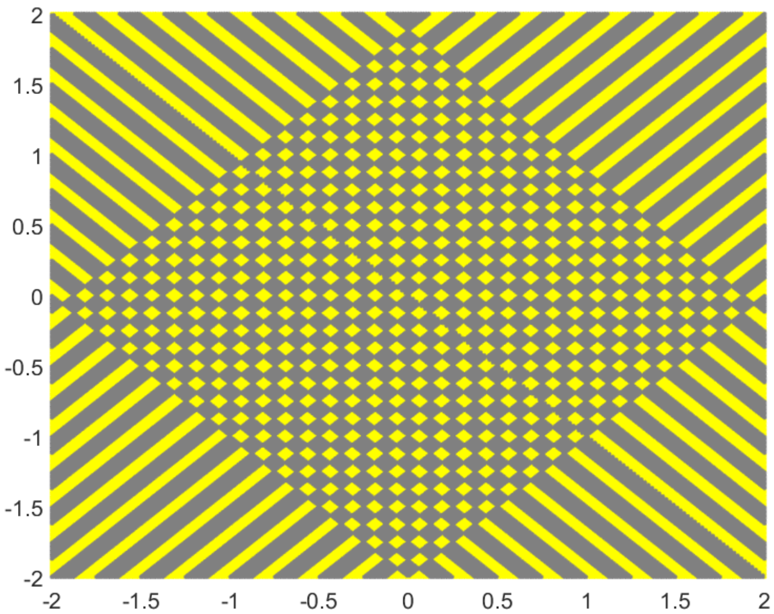




- But this is just $Y_1 \oplus Y_2 \oplus \cdots \oplus Y_{16}$
  - The XOR net will require 16 + 15x3 = 61 neurons
    - Greater than the 2-layer network with only 52 neurons

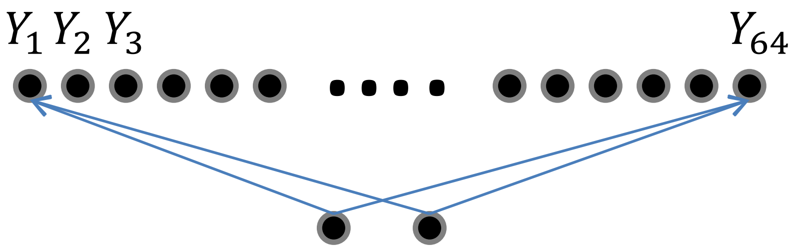
Optimal depth

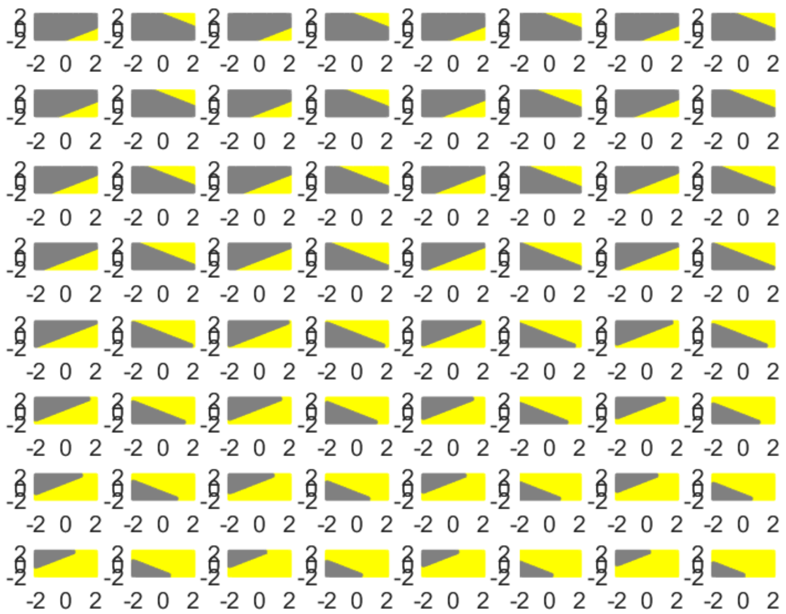




- A one-hidden-layer neural network will required infinite hidden neurons

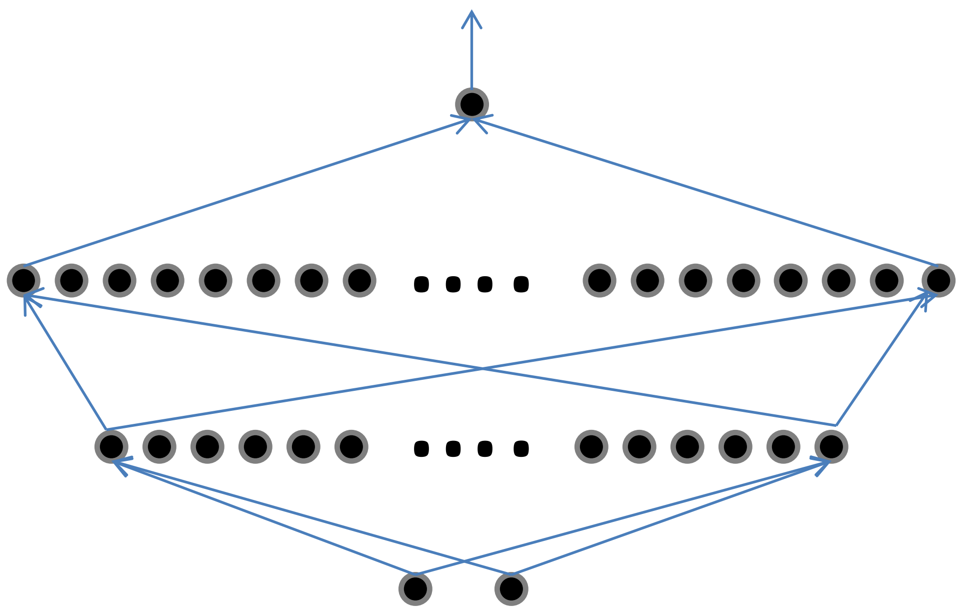
Actual linear units

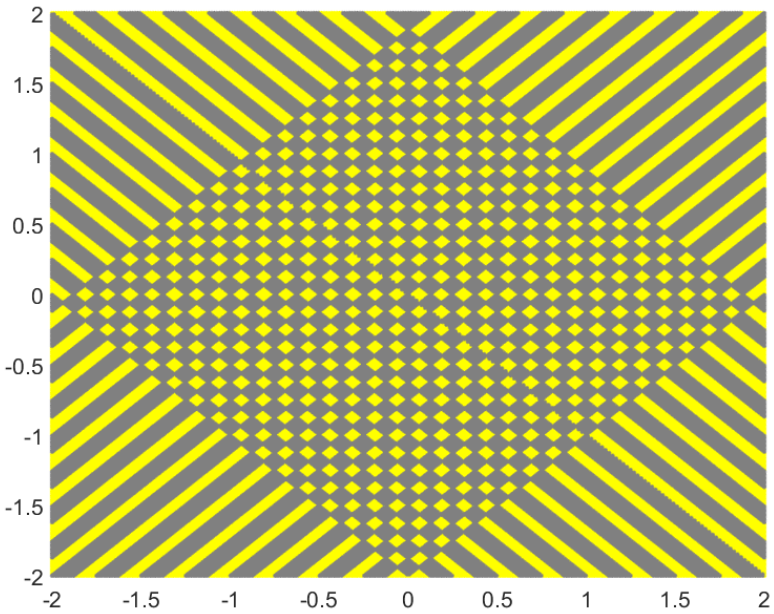




- 64 basic linear feature detectors

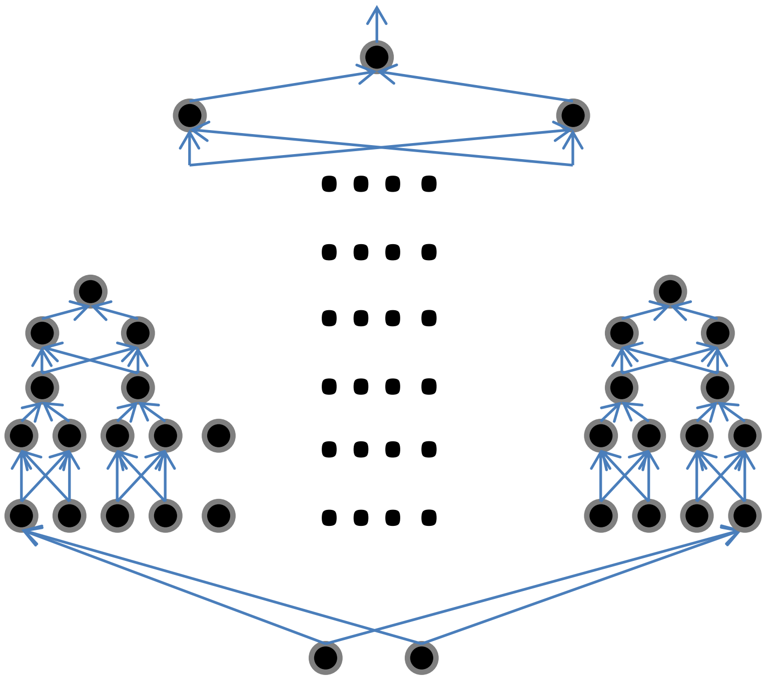
Optimal depth

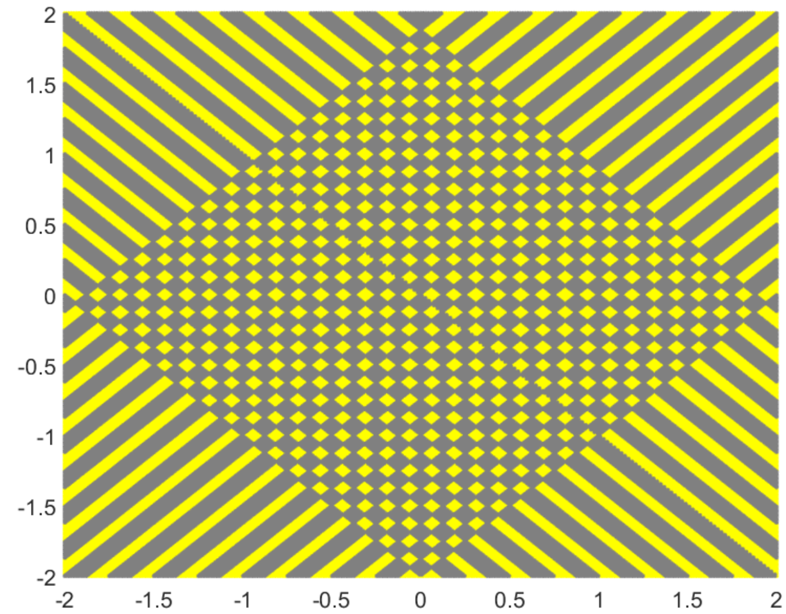




- Two hidden layers: 608 hidden neurons
  - 64 in layer 1
  - 544 in layer 2
- 609 total neurons (including output neuron)

Optimal depth

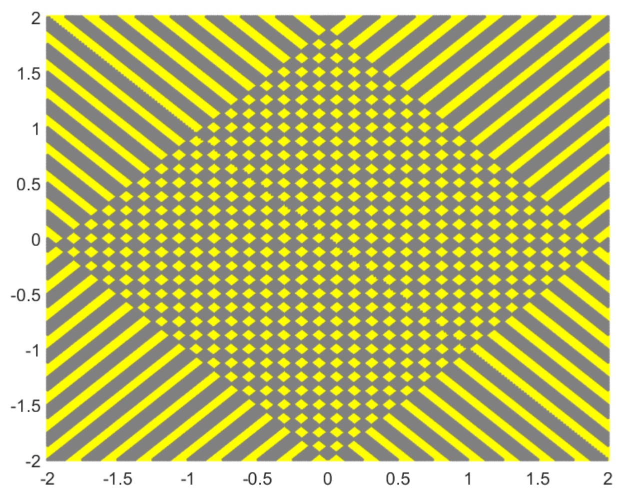




- XOR network (12 hidden layers): 253 neurons
- The difference in size between the deeper optimal (XOR) net and shallower nets increases with increasing pattern complexity

Network size?

- In this problem the 2-layer net was *quadratic* in the number of lines
  - $\lfloor (N+2)^2/8 \rfloor$ neurons in 2nd hidden layer
  - Not exponential
  - Even though the pattern is an XOR
  - Why?



- The data are two-dimensional!
  - Only two *fully independent* features
  - The pattern is exponential in the *dimension of the input (two)!*
- For general case of N lines distributed over D dimensions, we will need up to $\frac{1}{2}\left(\frac{N}{D}+1\right)^D$
  - 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 (N)

Depth: Summary

- The number of neurons required in a shallow network is
  - Polynomial in the number of basic patterns
  - Exponential in the dimensionality input
    - (this is the worst case)
    - Alternately, exponential in the number of statistically independent features

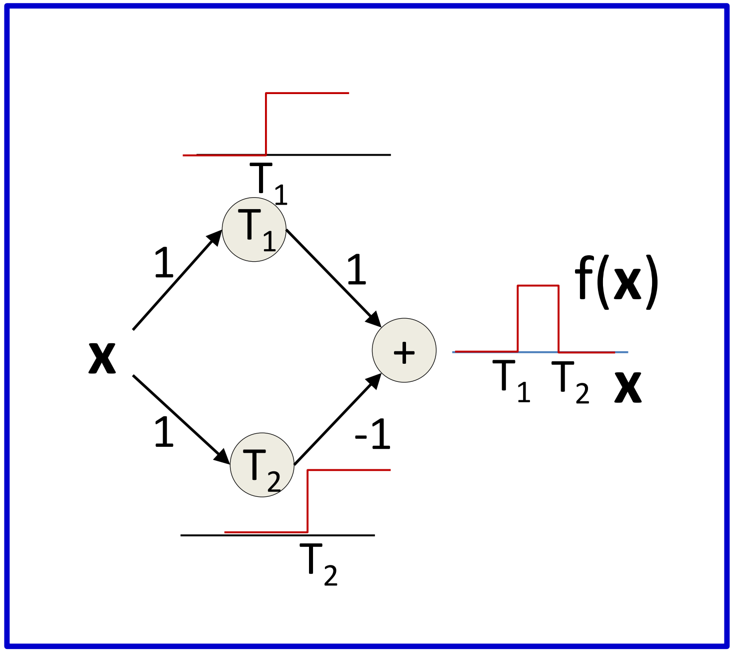
Story so far

- 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 exponentially fewer neurons than shallower networks to express the same function
  - Could be *exponentially* smaller
  - Deeper networks are more *expressive*

Today

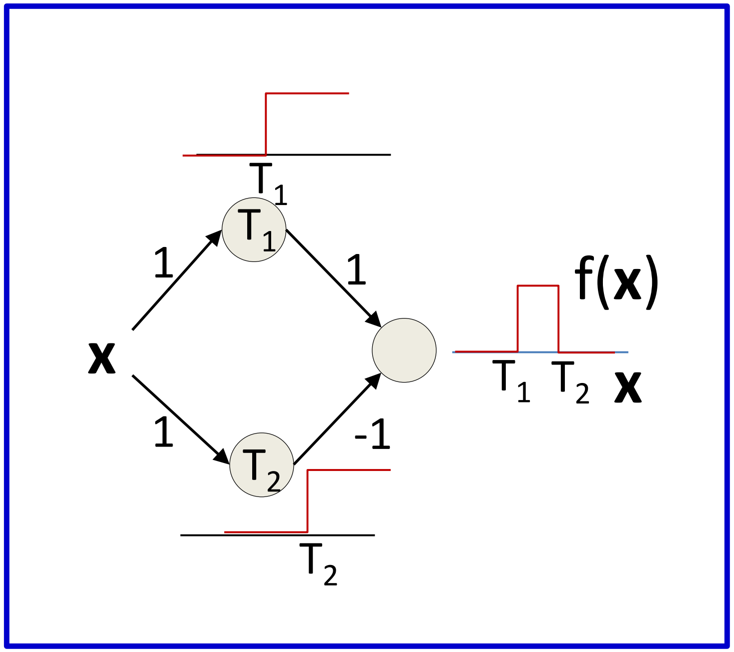
- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
- MLPs as universal classifiers
  - The need for depth
- MLPs as universal approximators
- A discussion of optimal depth and width
- Brief segue: RBF networks

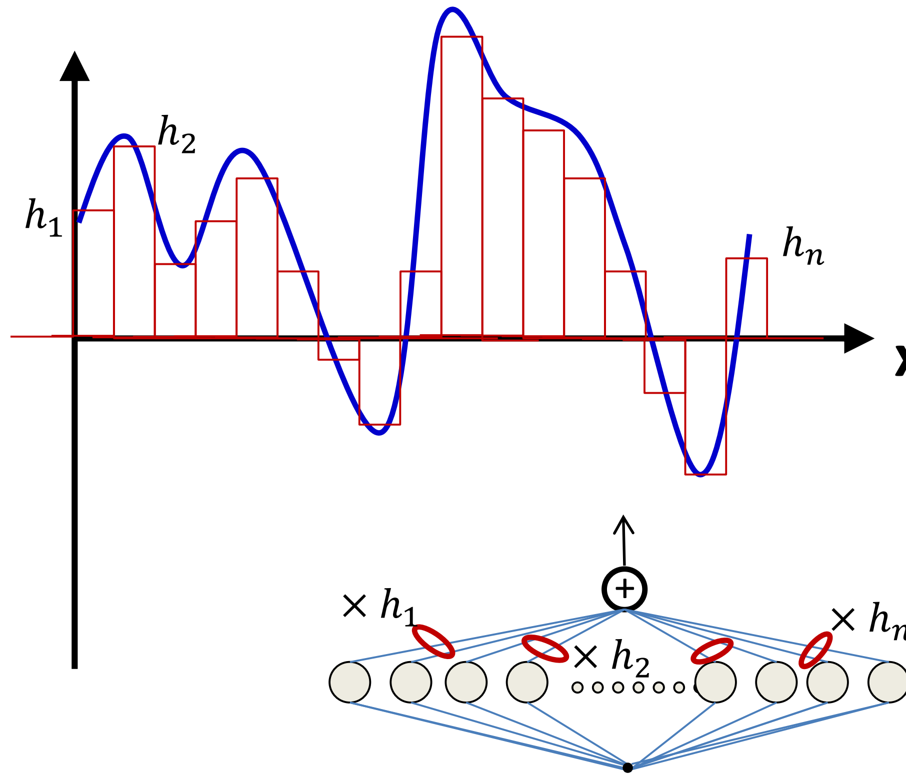
MLP as a continuous-valued regression



- 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

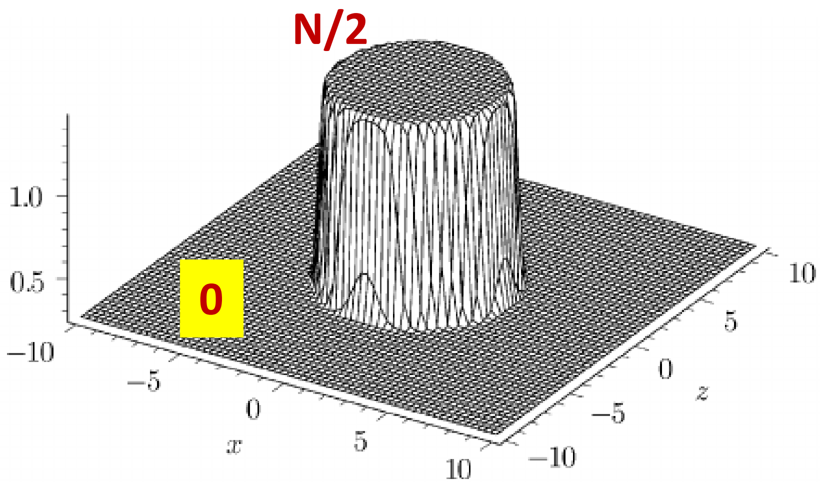
MLP as a continuous-valued regression

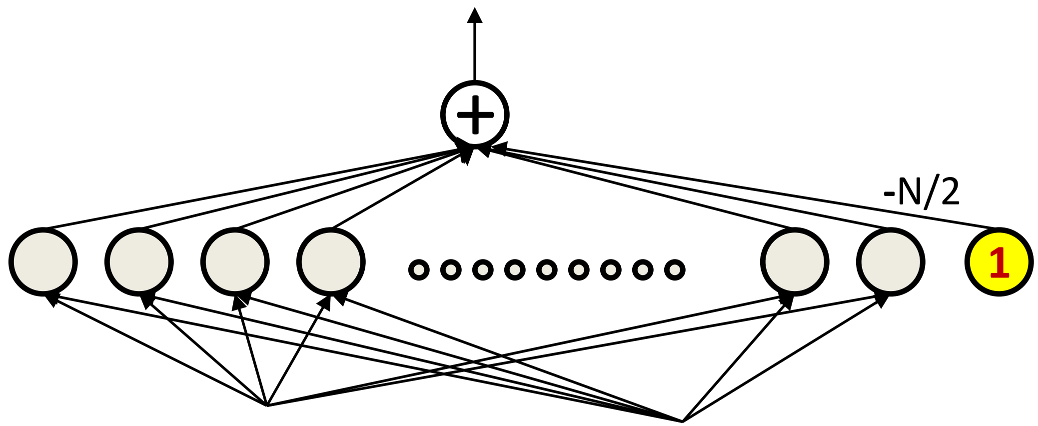




- A simple 3-unit MLP can generate a "square pulse" over an input
- **An MLP with many units can model an arbitrary function over an input**
  - To arbitrary precision
    - Simply make the individual pulses narrower
- ***A one-layer MLP can model an arbitrary function of a single input***

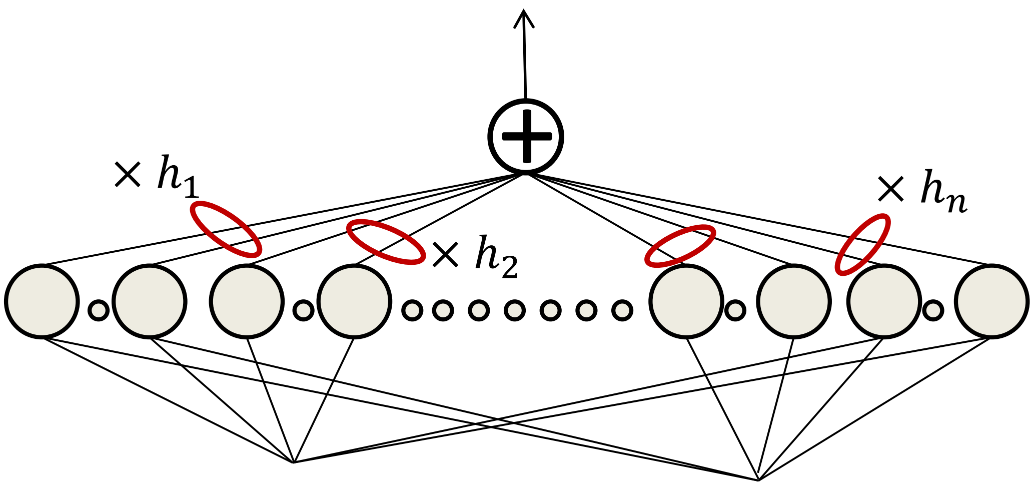
For higher dimensions

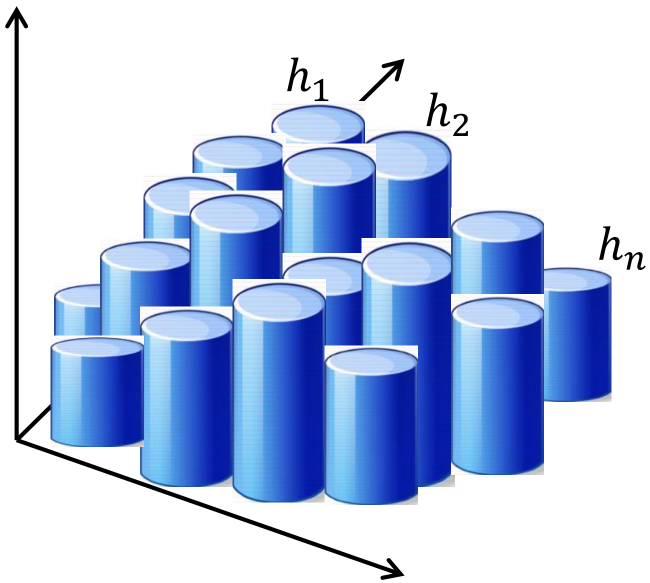




- An MLP can compose a cylinder
  - $N/2$ in the circle, 0 outside

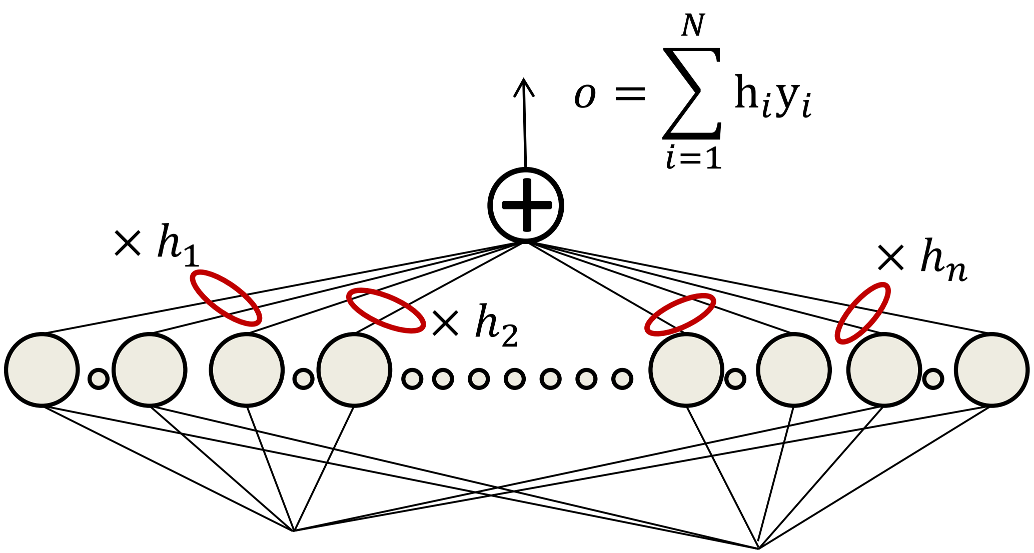
MLP as a continuous-valued function

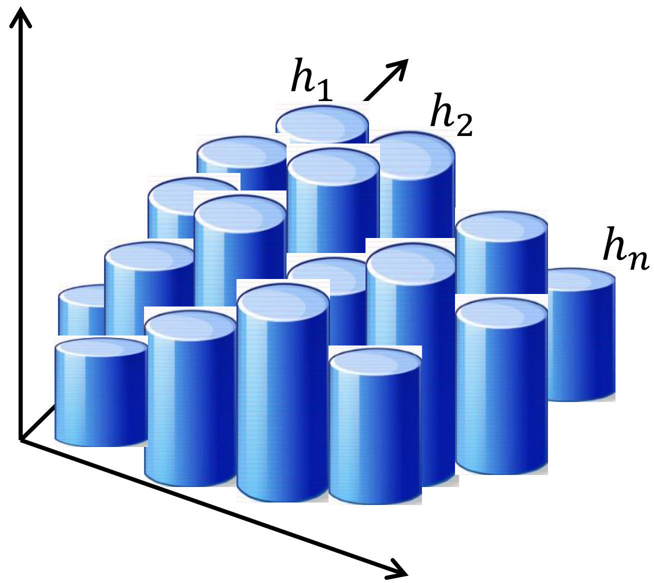




- MLPs can actually compose arbitrary functions in any number of dimensions!
  - Even with only one layer
    - As sums of scaled and shifted cylinders
  - To arbitrary precision
    - By making the cylinders thinner
  - **The MLP is a universal approximator!**

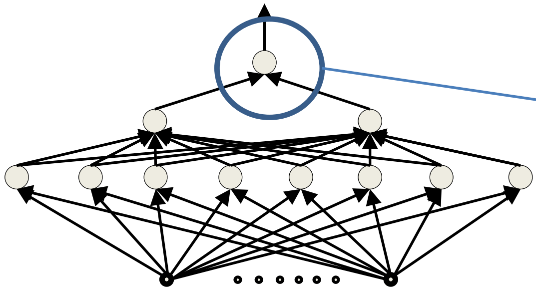
Caution: MLPs with additive output units are universal approximators

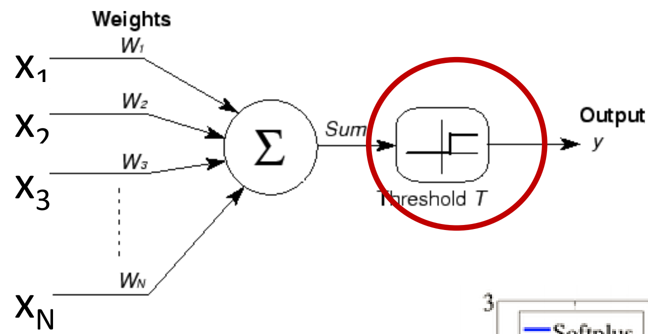




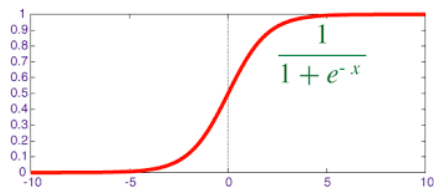
- MLPs can actually compose arbitrary functions
- But explanation so far only holds if the output unit only performs summation
  - i.e. does not have an additional "activation"

"Proper" networks: Outputs with activations

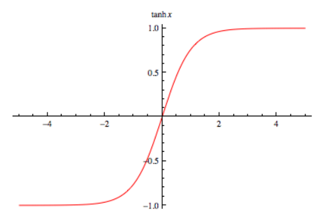


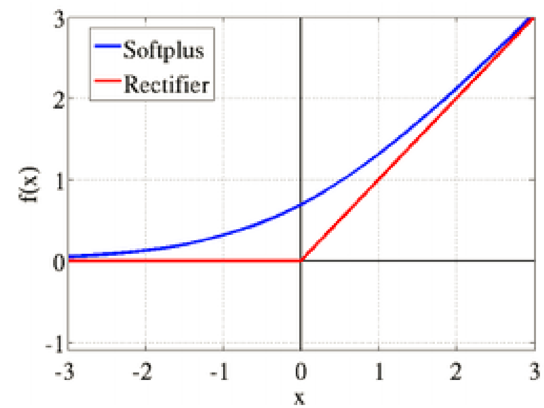


sigmoid



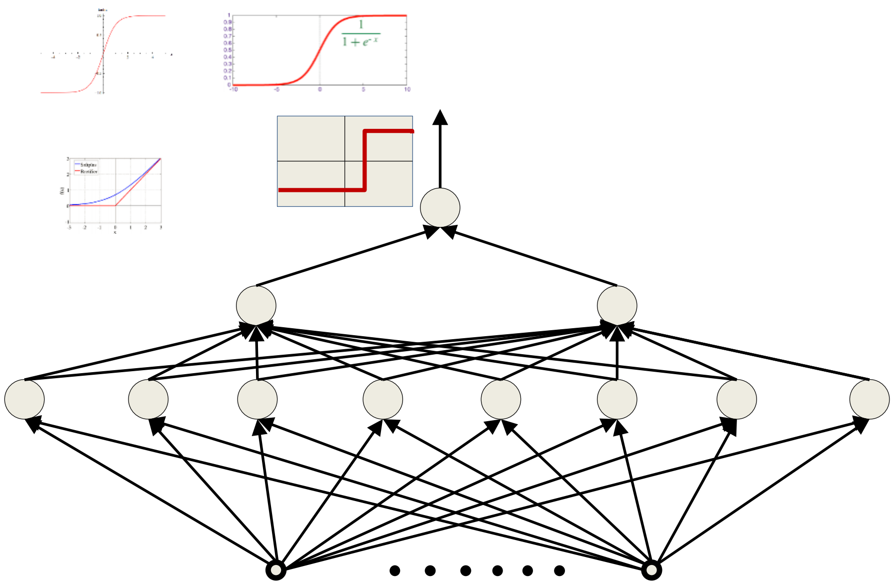
tanh





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

The network as a function



$f: \{0,1\}^N \rightarrow \{0,1\}$ *Boolean*

$f: R^N \rightarrow \{0,1\}$ *Threshold*

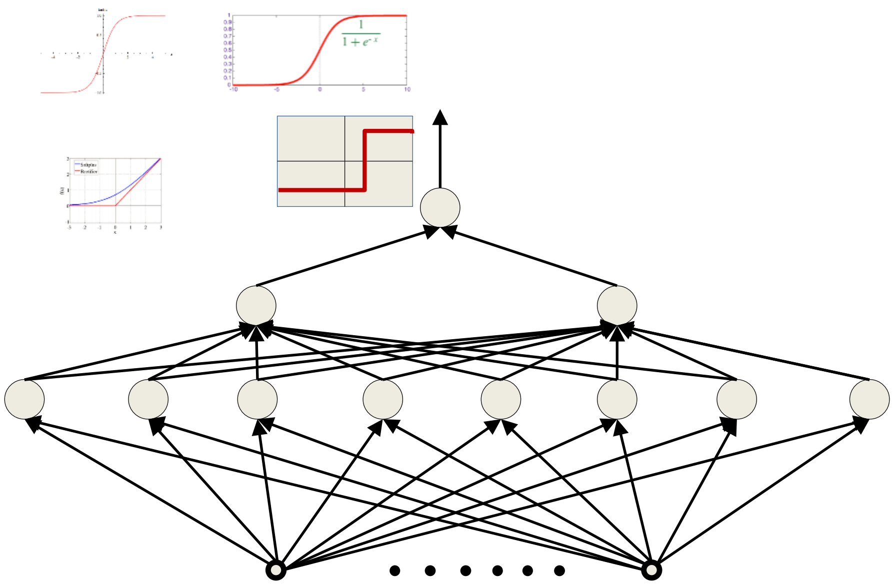
$f: R^N \rightarrow (0,1)$ *Sigmoid*

$f: R^N \rightarrow (-1,1)$ *Tanh*

$f: R^N \rightarrow (0,\infty)$ *Softrectifier, Rectifier*

- Output unit with *activation function*
  - Threshold or Sigmoid, or any other
- The network is actually a map from the set of all possible input values to all possible output values
  - All values the activation function of the output neuron

The network as a function



$f: \{0,1\}^N \rightarrow \{0,1\}$ *Boolean*

$f: R^N \rightarrow \{0,1\}$ *Threshold*

$f: R^N \rightarrow (0,1)$ *Sigmoid*

$f: R^N \rightarrow (-1,1)$ *Tanh*

$f: R^N \rightarrow (0,\infty)$ *Softmax, Rectifier*

The MLP is a *Universal Approximator* for the entire *class* of functions (maps) it represents!

  - Threshold or Sigmoid, or any other
- The network is actually a map from the set of all possible input values to all possible output values
  - All values the activation function of the output neuron

Today

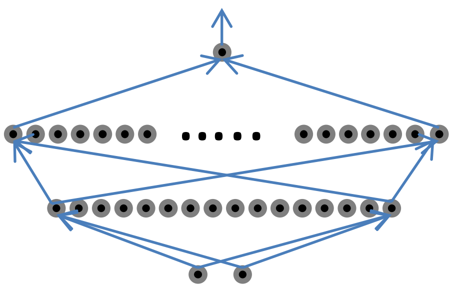
- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
- MLPs as universal classifiers
  - The need for depth
- MLPs as universal approximators
- A discussion of optimal depth and width
- Brief segue: RBF networks

The issue of depth

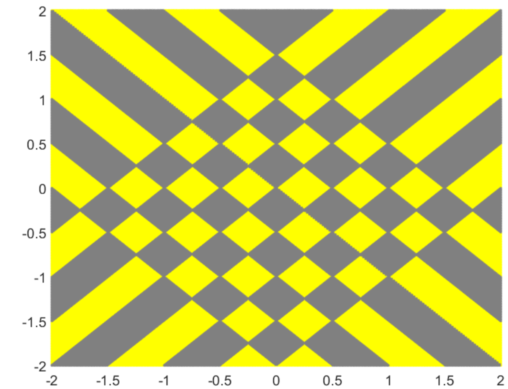
- Previous discussion showed that a *single-layer* MLP is a universal function approximator
  - Can approximate any function to arbitrary precision
  - But may require infinite neurons in the layer

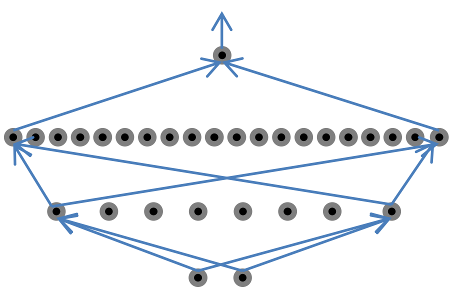
- More generally, deeper networks will require far fewer neurons for the same approximation error
  - The network is a generic map
    - The same principles that apply for Boolean networks apply here
  - Can be exponentially fewer than the 1-layer network

Sufficiency of architecture

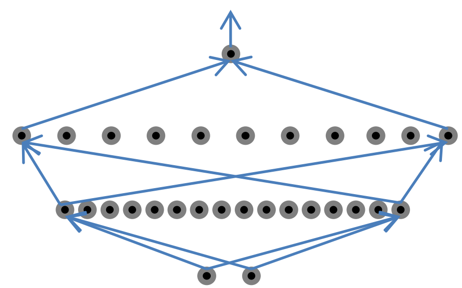


A network with 16 or more neurons in the first layer is capable of representing the figure to the right perfectly





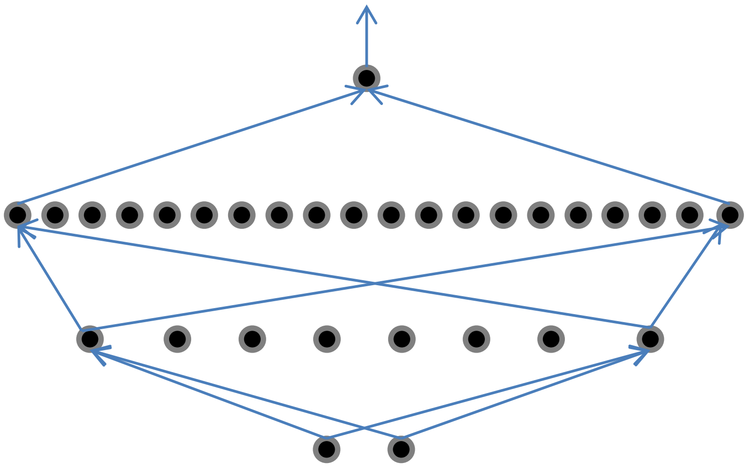
A network with less than 16 neurons in the first layer cannot represent this pattern exactly
- With caveats..

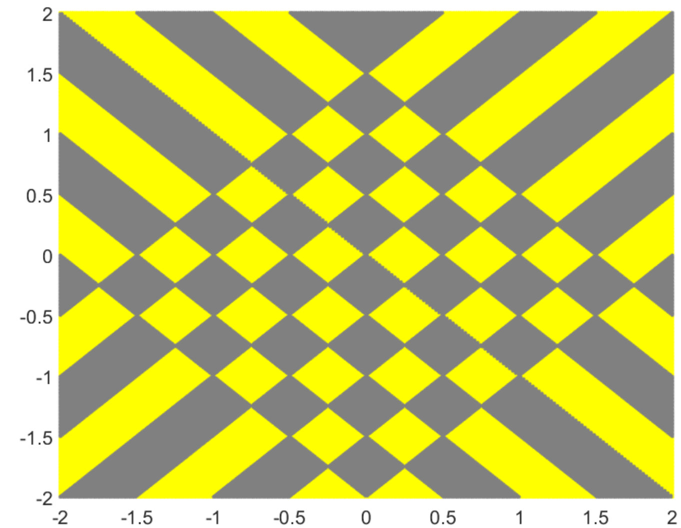


A 2-layer network with 16 neurons in the first layer cannot represent the pattern with less than 41 neurons in the second layer

- A neural network *can* represent any function provided it has sufficient *capacity*
  - I.e. sufficiently broad and deep to represent the function
- Not all architectures can represent any function

Sufficiency of architecture





- The *capacity* of a network has various definitions
  - *Information* or *Storage* capacity: how many patterns can it remember
  - VC dimension
    - bounded by the square of the number of weights in the network
  - From our perspective: largest number of disconnected convex regions it can represent

- A network with insufficient capacity *cannot* exactly model a function that requires a greater minimal number of convex hulls than the capacity of the network
  - But can approximate it with error

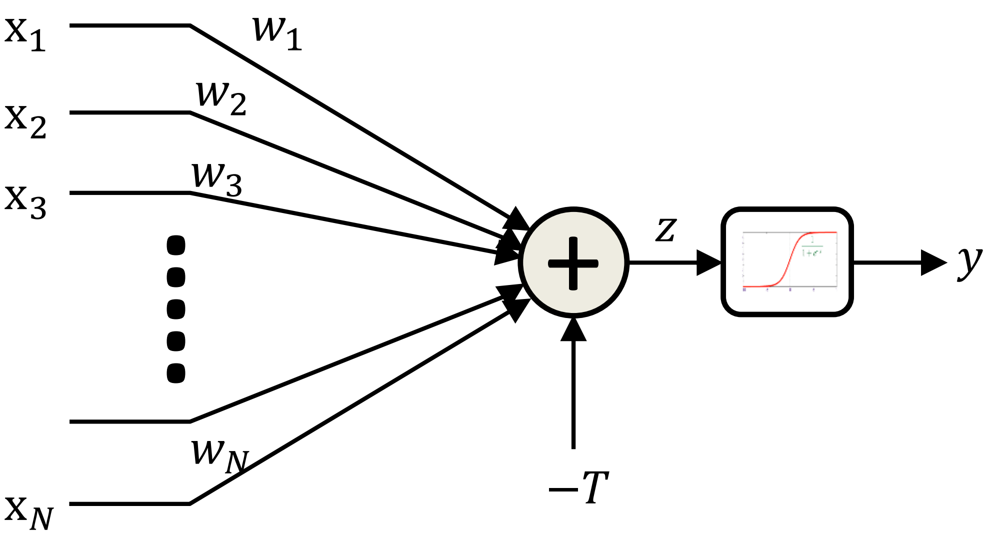
The "capacity" of a network

- VC dimension
- A separate lecture
  - Koiran and Sontag (1998): For "linear" or threshold units, VC dimension is proportional to the number of weights
    - For units with piecewise linear activation it is proportional to the square of the number of weights
  - Harvey, Liaw, Mehrabian "Nearly-tight VC-dimension bounds for piecewise linear neural networks" (2017):
    - For any W, L s.t. $W > CL > C^2$, there exisits a RELU network with $\leq L$ layers, $\leq W$ weights with VC dimension $\geq \frac{WL}{C}\log_2(\frac{W}{L})$
  - Friedland, Krell, "A Capacity Scaling Law for Artificial Neural Networks" (2017):
    - VC dimension of a linear/threshold net is $\mathcal{O}(MK)$, M is the overall number of hidden neurons, K is the weights per neuron

Today

- Multi-layer Perceptrons as universal Boolean functions
  - The need for depth
- MLPs as universal classifiers
  - The need for depth
- MLPs as universal approximators
- A discussion of optimal depth and width
- Brief segue: RBF networks

Perceptrons so far

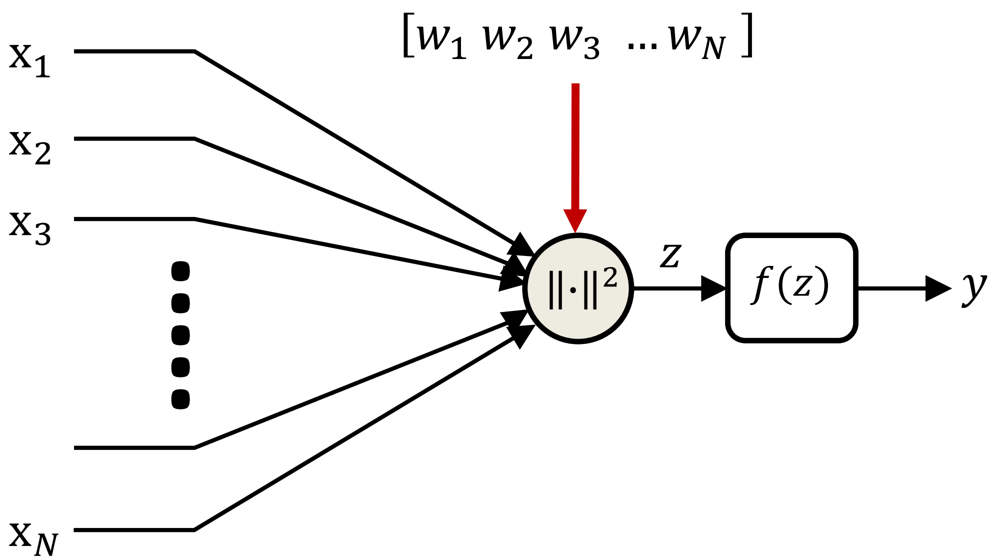


$$z = \sum_i w_i x_i - T$$

$$y = f(z)$$

- The output of the neuron is a function of a linear combination of the inputs and a bias

An alternate type of neural unit:
Radial Basis Functions



$$z = \|\mathbf{x} - \mathbf{w}\|^2$$

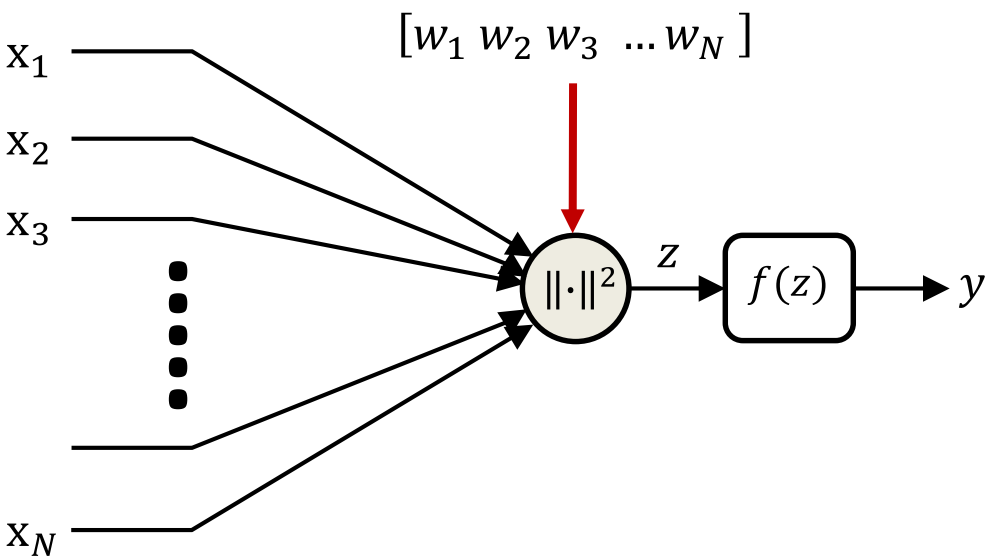
$$y = f(z)$$

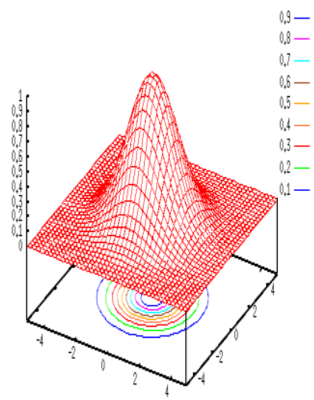
Typical activation

$$f(z) = \exp(-\beta z)$$

- The output is a function of the distance of the input from a "center"
  - The "center" $\mathbf{w}$ is the parameter specifying the unit
  - The most common activation is the exponent
    - β is a "bandwidth" parameter
  - But other similar activations may also be used
    - Key aspect is radial symmetry, instead of linear symmetry

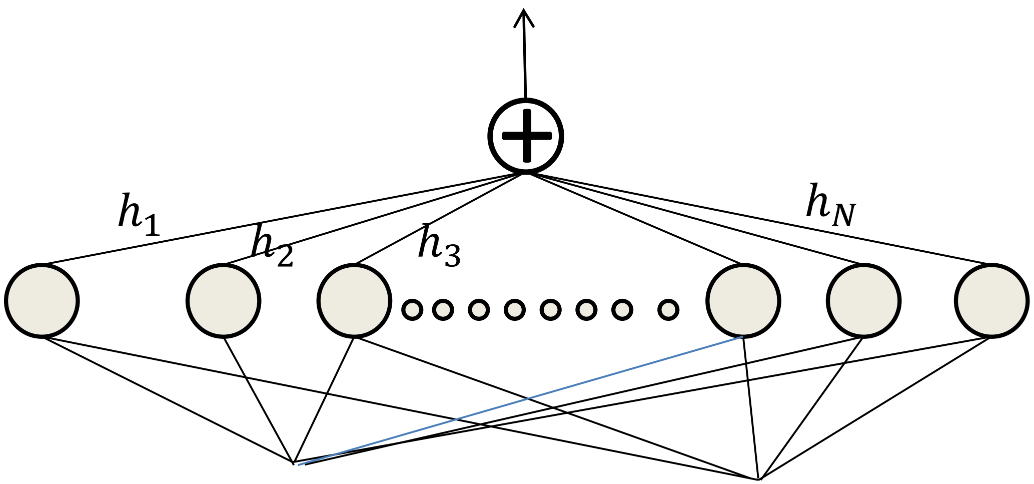
An alternate type of neural unit: Radial Basis Functions

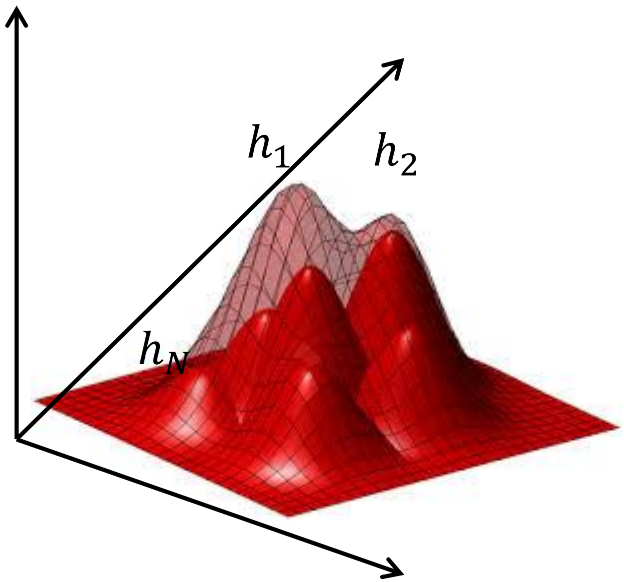




- Radial basis functions can compose cylinder-like outputs with just a single unit with appropriate choice of bandwidth (or activation function)
  – As opposed to $N \rightarrow \infty$ units for the linear perceptron

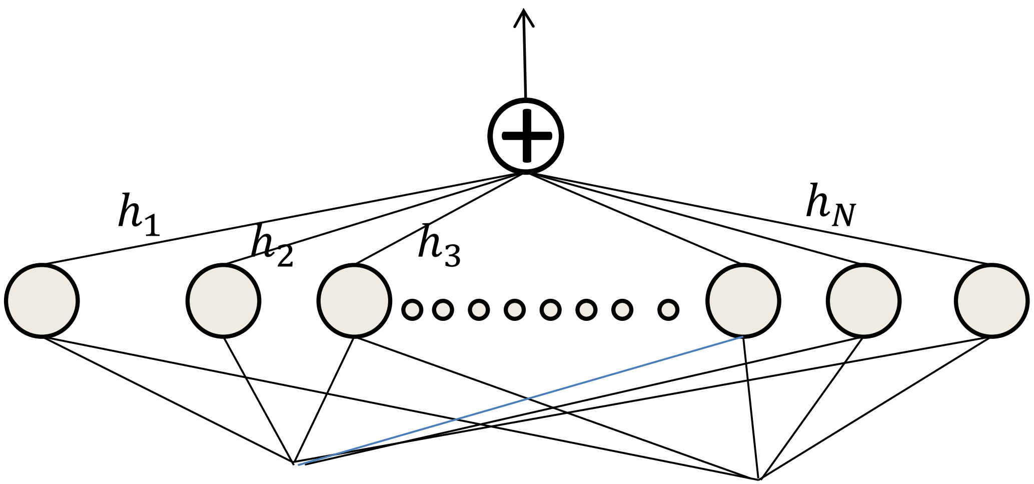
RBF networks as universal approximators

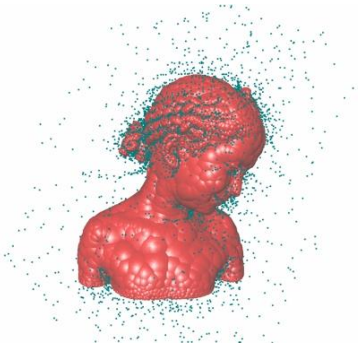




- RBF networks are more effective approximators of continuous-valued functions
  - A one-hidden-layer net only requires *one* unit per "cylinder"

RBF networks as universal approximators





- RBF networks are more effective approximators of continuous-valued functions
  - A one-hidden-layer net only requires *one* unit per "cylinder"

RBF networks

- More effective than conventional linear perceptron networks in some problems

- We will revisit this topic, time permitting

Lessons today

- 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

- RBFs are good, now lets get back to linear perceptrons… ☺

Next up

- We *know* MLPs can emulate any function
- But how do we *make* them emulate a specific desired function
  - E.g. a function that takes an image as input and outputs the labels of all objects in it
  - E.g. a function that takes speech input and outputs the labels of all phonemes in it
  - Etc…
- *Training an MLP*