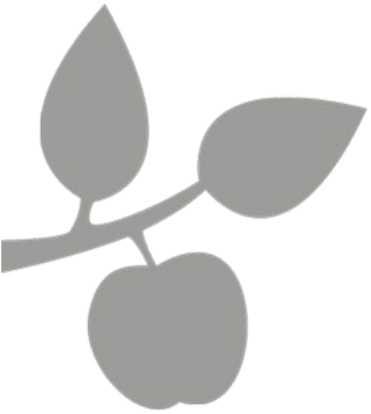
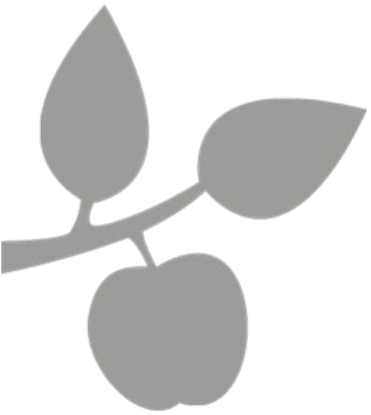


SDU Summer School

Deep Learning

Summer 2022

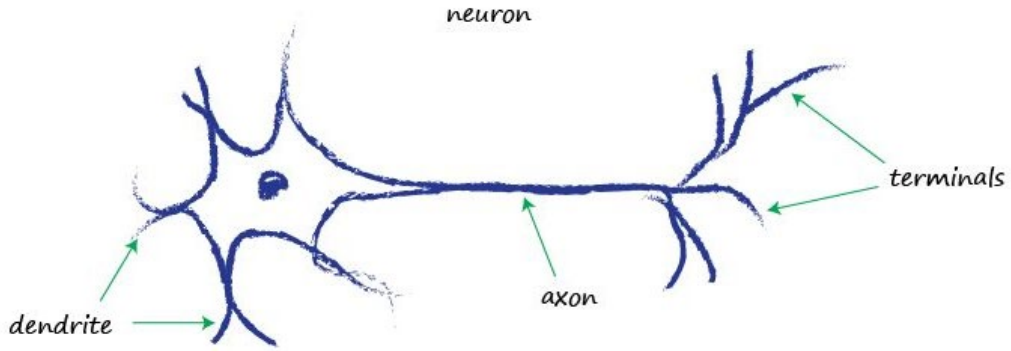
Welcome to the Summer School

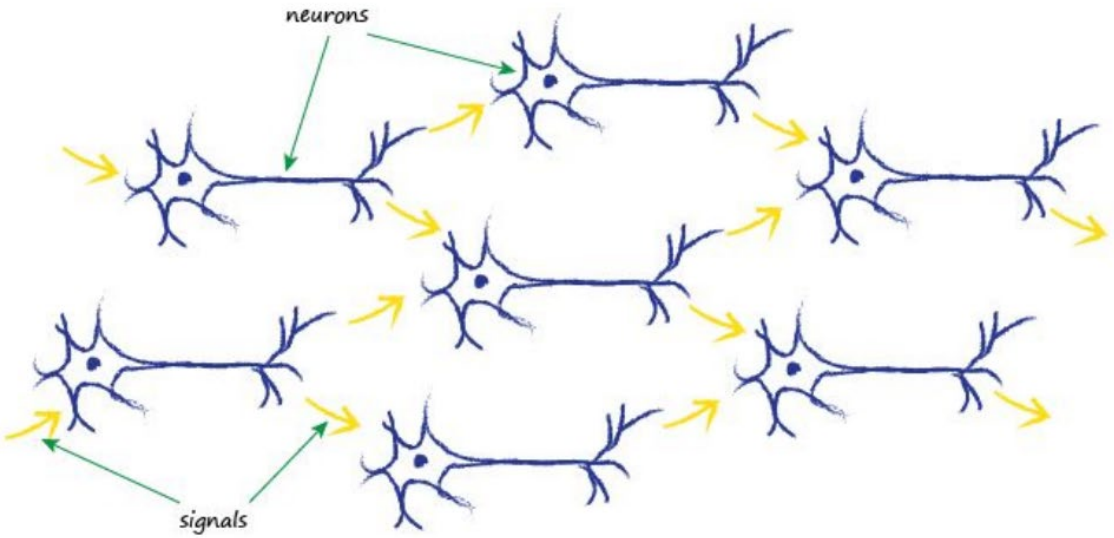


Deep Feedforward Networks Part II

- **PART I**
  - What is a Neuron?
  - How to build a Network
- **Intermezzo: Some Math**
- **PART II**
  - **Networks**
  - Output Units
  - Hidden Units
  - Architecture Design

From Neuron to "Brain"

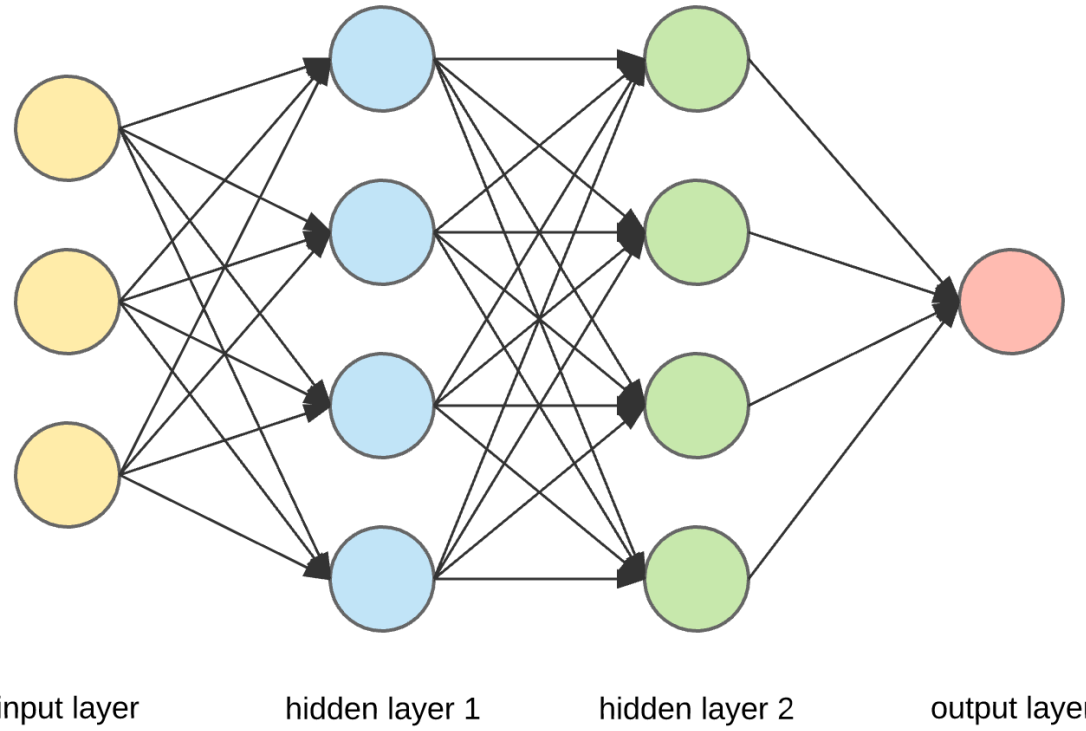




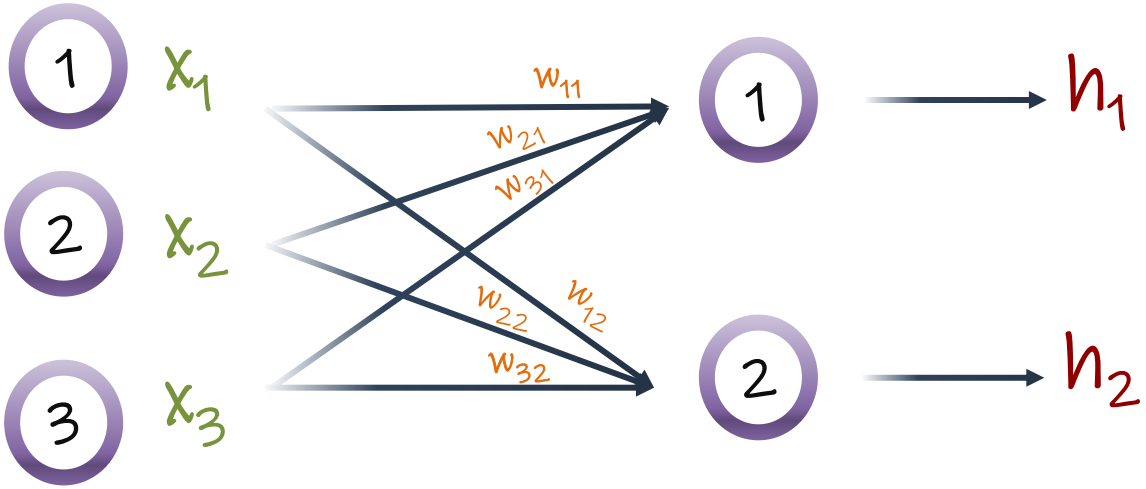
- We now can connect neurons
- The output of one neuron becomes the input of other neurons

In a more structured way

- We normally have more than one node
- Multiple Nodes are arranged in layers
- Each layer receives the generated output from the previous layer

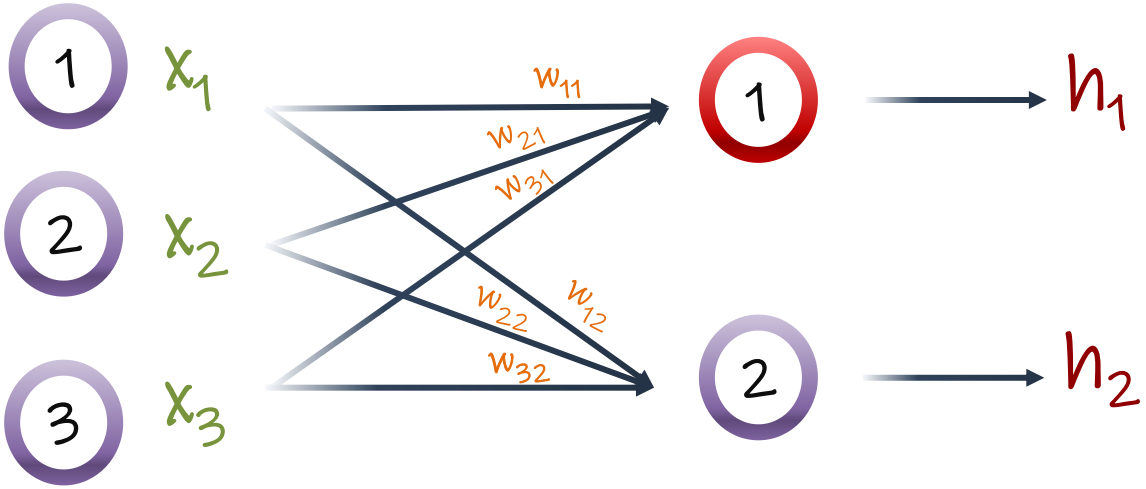


What does such a Network do?



- Remember from before:
  - We have a weighted sum
  - Then we have an "activation function" (which we ignore for now)

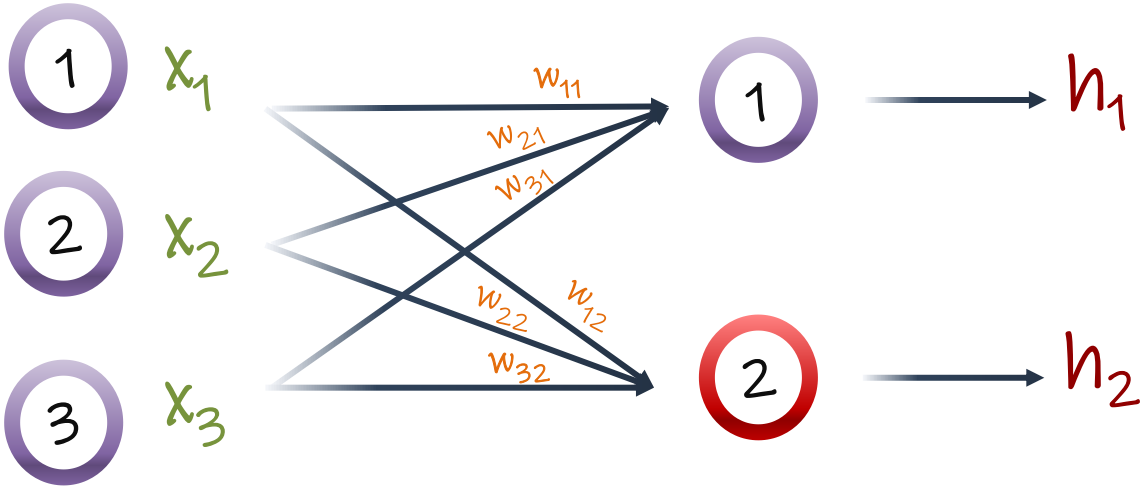
What does such a Network do?



- Remember from before:
  - We have a weighted sum
  - Then we have an "activation function" (which we ignore for now)
- For **Node 1**, we get:

$$h_1 = w_{11} \cdot x_1 + w_{21} \cdot x_2 + w_{31} \cdot x_3$$

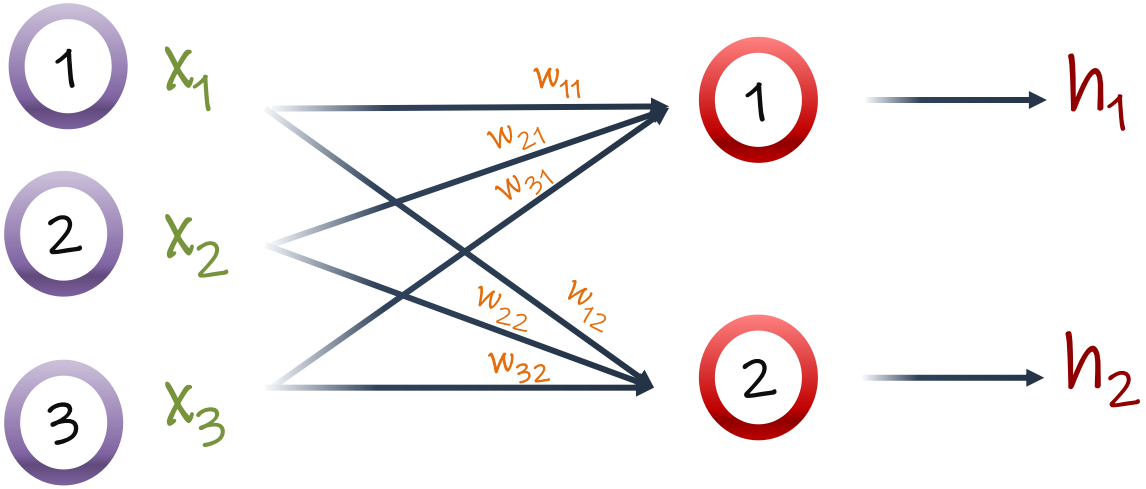
What does such a Network do?



- Remember from before:
  - We have a weighted sum
  - Then we have an "activation function" (which we ignore for now)
- For **Node 2**, we get:

$$h_2 = w_{12} \cdot x_1 + w_{22} \cdot x_2 + w_{32} \cdot x_3$$

What does such a Network do?

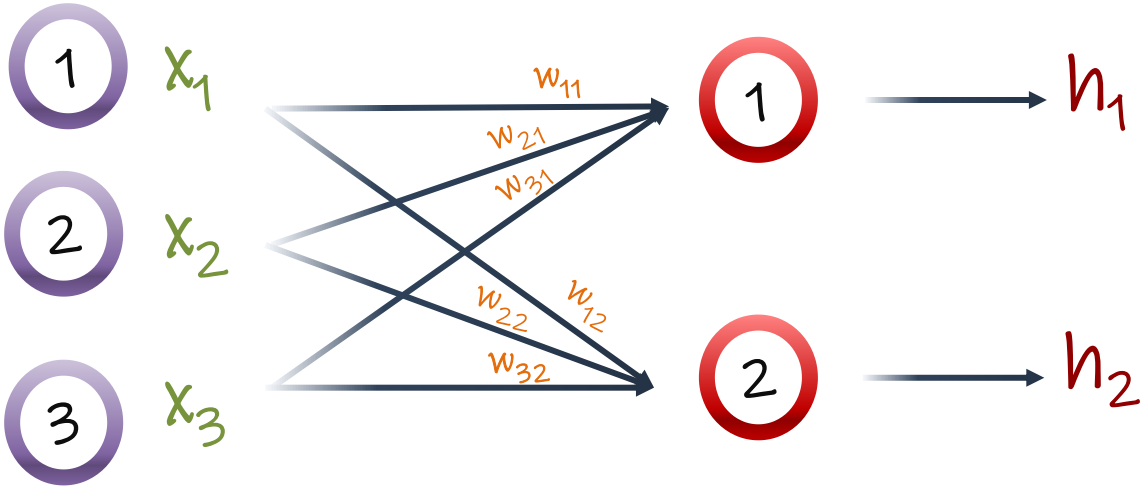


- **Together**:

$$h_1 = w_{11} \cdot x_1 + w_{21} \cdot x_2 + w_{31} \cdot x_3$$
$$h_2 = w_{12} \cdot x_1 + w_{22} \cdot x_2 + w_{32} \cdot x_3$$

- Looks familiar, doesn't it?

What does such a Network do?

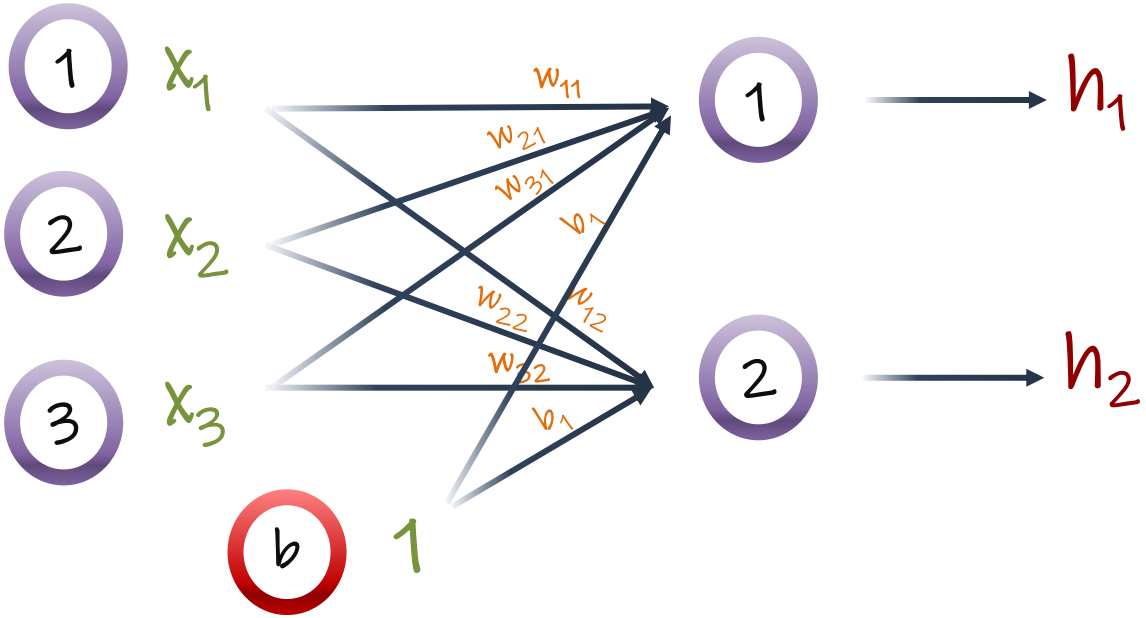


- Rewrite:

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$h = \boldsymbol{W}\boldsymbol{x}$$

What does such a Network do?

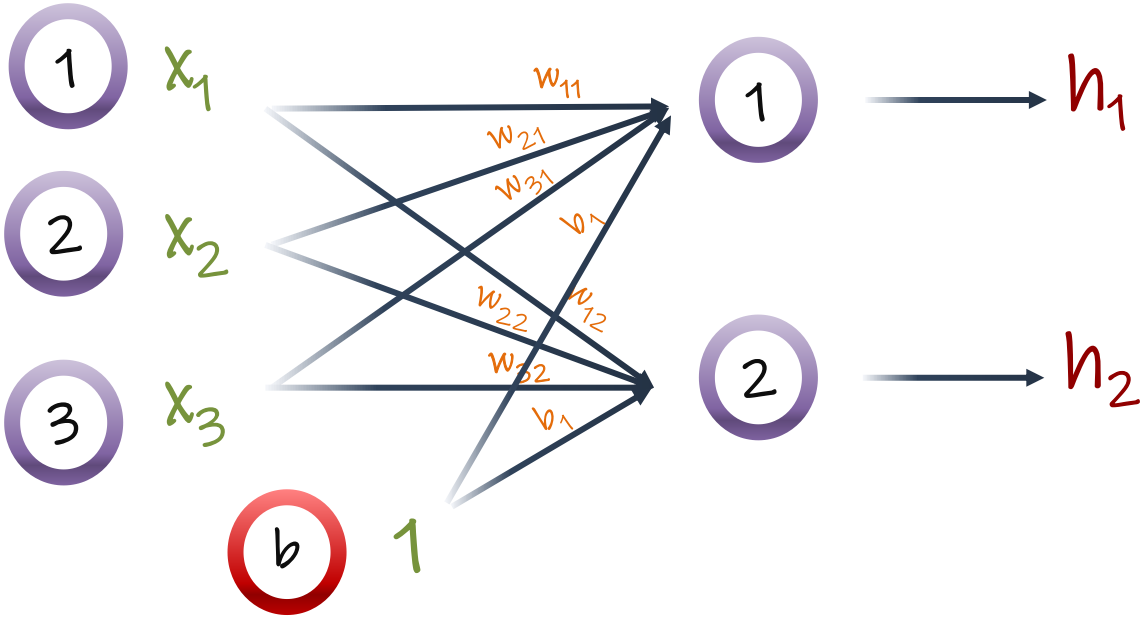


- Adding a **Bias**:

$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

$$\boldsymbol{h} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

What does such a Network do?



- Adding a **Bias** (rewritten):

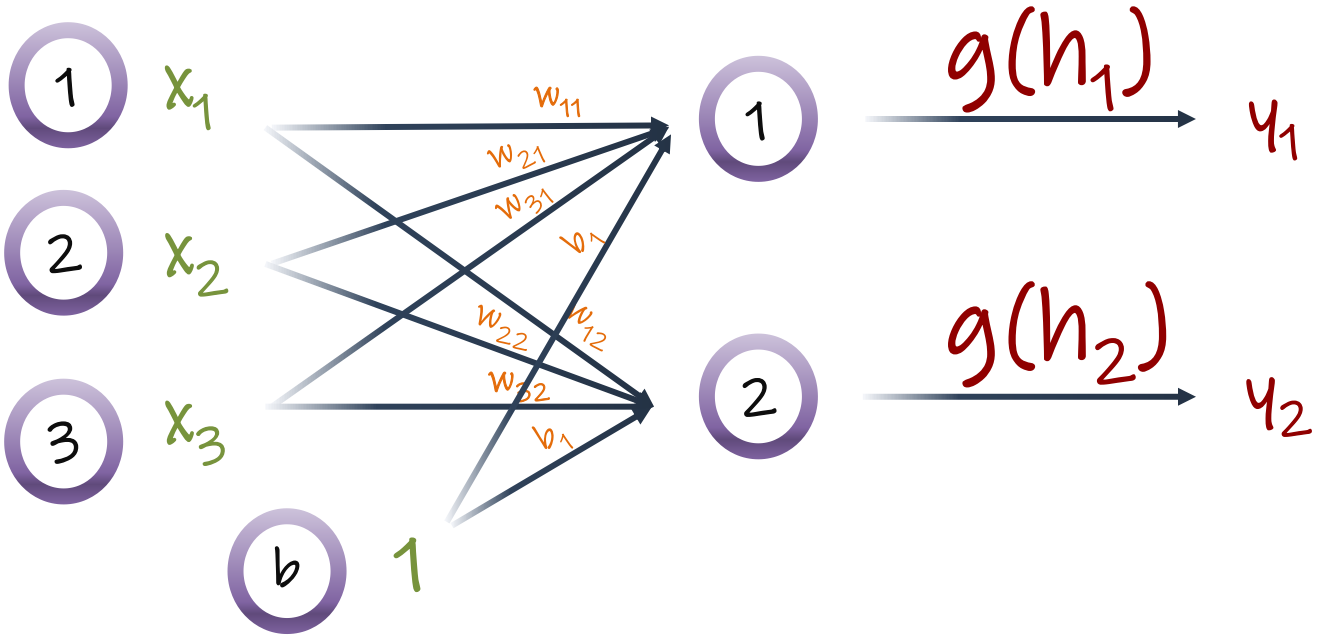
$$\begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} w_{11} & w_{21} & w_{31} & b_1 \\ w_{12} & w_{22} & w_{32} & b_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 1 \end{pmatrix}$$

$$\boldsymbol{h} = \boldsymbol{W}\boldsymbol{x}$$

Adding the Activation Function

What do you think, how important is the activation function?

What does such a Network do?



- Adding the **activation function**:

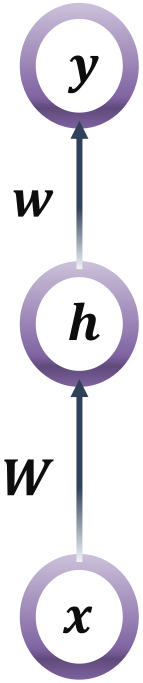
$$\boldsymbol{y} = \boldsymbol{g}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

More Compact Representation

- We can summarize these networks to their essential parts:
  - We receive the vector $\boldsymbol{x}$ and perform an affine transformation according to the weight matrix

$$\boldsymbol{h}' = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

  - Afterward, the internal representation is component wise feed through an activation function $h_i = g(h_i')$ to generate the input vector $\boldsymbol{h}$ for the next layer
- Please note the slight shift in notation. From now on:
  - $\boldsymbol{x}$ denotes the input
  - $\boldsymbol{W}$ denotes weight matrices, w denotes weight vectors
  - $\boldsymbol{h}$ denotes hidden layer "outputs"
  - $\boldsymbol{y}$ is the final output of the network

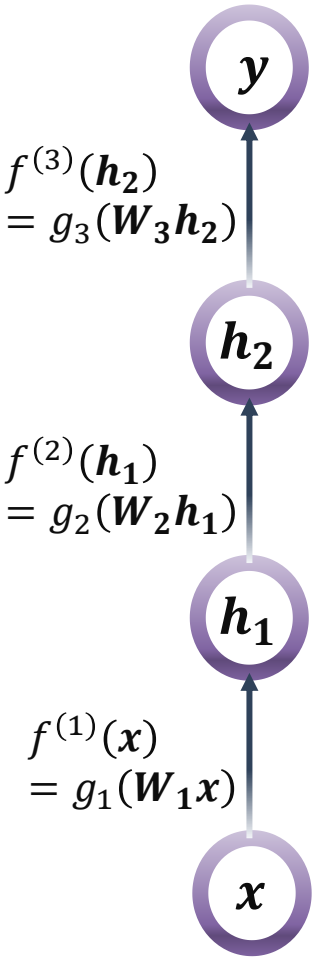


Composition of Complicated Functions

- Now let's look at a deeper Network:
  - E.g., functions $f^{(1)}$, $f^{(2)}$, $f^{(3)}$ connected in a chain to form

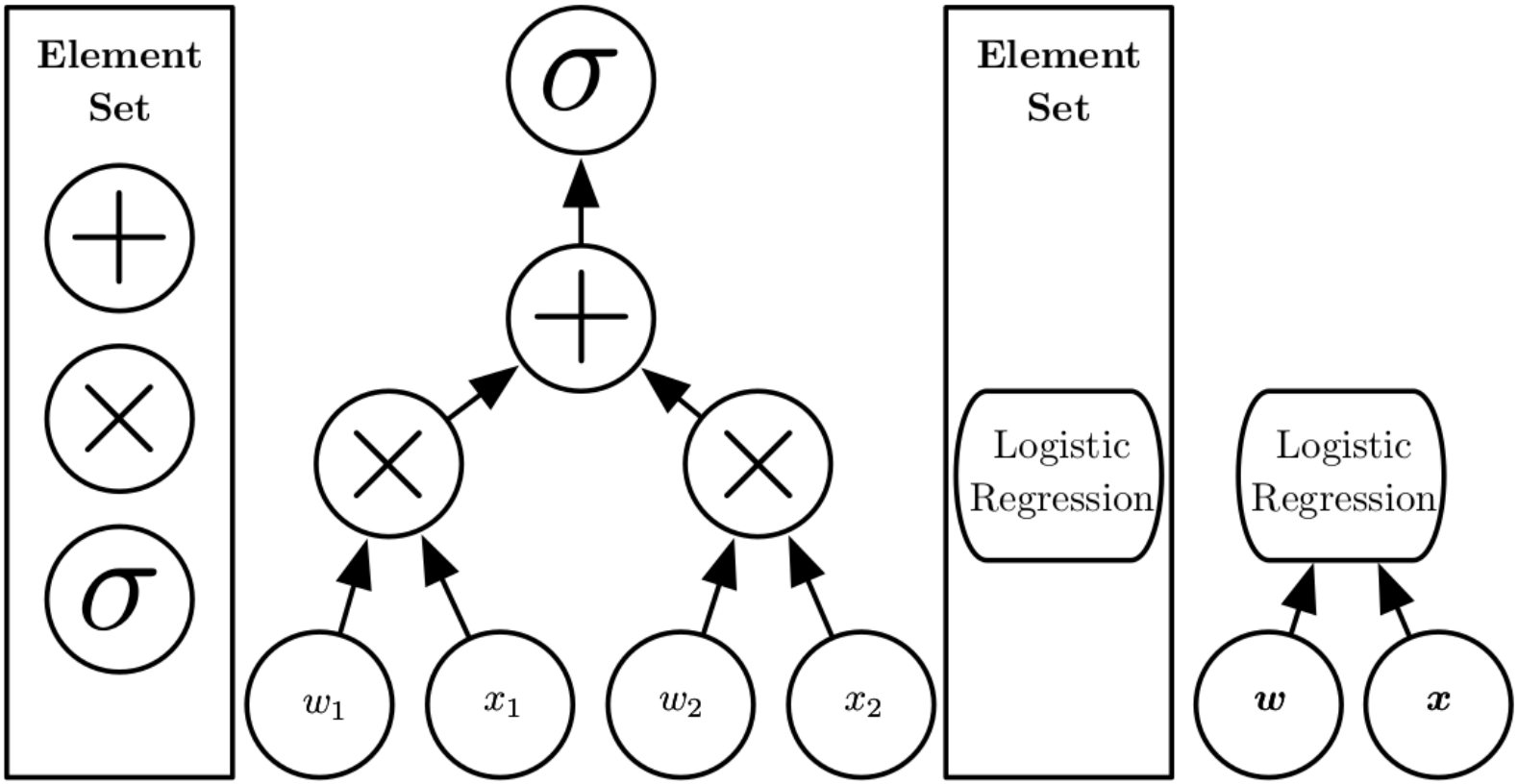
$$f(\boldsymbol{x}) = f^{(3)}\left(f^{(2)}\left(f^{(1)}(\boldsymbol{x})\right)\right)$$

  - $f^{(1)}$ is the first layer, $f^{(2)}$ the second, etc.
  - The length of the chain is the depth of the model



- The name deep learning arises from this terminology
- Final layer of a feedforward network, (here $f^{(3)}$) is the output layer

Regarding the Depth of a Model



$$p(y = 1|\boldsymbol{x}; \boldsymbol{w}) = \sigma\left([w_1, w_2]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right)$$

What are Hidden Layers

- Behavior of other layers is not directly specified by the data
- Learning algorithm must decide how to use those layers to produce a final value that is close to y
- Training data does not say what individual layers should do
  - This is one of the main tasks: Define the appropriate structure of the network and the hidden layers
- Since the desired output for these layers is not shown, they are called hidden layers

Extending Linear Models

To represent non-linear functions of $\boldsymbol{x}$

- Apply linear model to transformed input $\phi(\boldsymbol{x})$ with non-linear ϕ
  - Equivalently kernel trick of SVM obtains nonlinearity

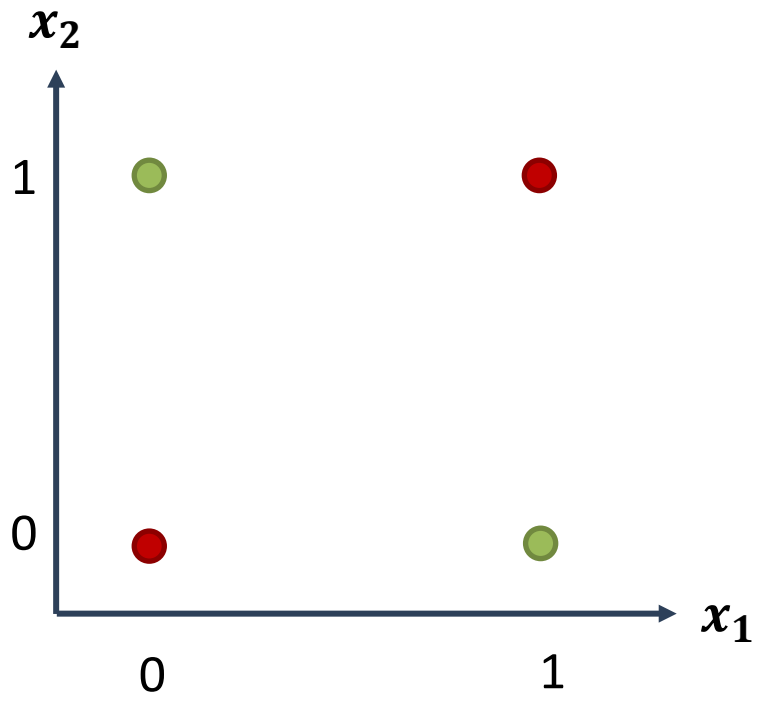
- Function is nonlinear wrt x but linear wrt $\phi(x)$
- We can think of ϕ as providing a set of features resulting in a new representation for x

- Get ϕ
  - Generic functions: There exists a set of useful kernel functions
  - Manually engineer ϕ: Laborious and not transformable
  - **Deep Learning**: Learn ϕ

On the importance of Activation Functions

- The XOR Problem:
  - XOR is a logical function
  - It takes two inputs, x_1 and x_2

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0



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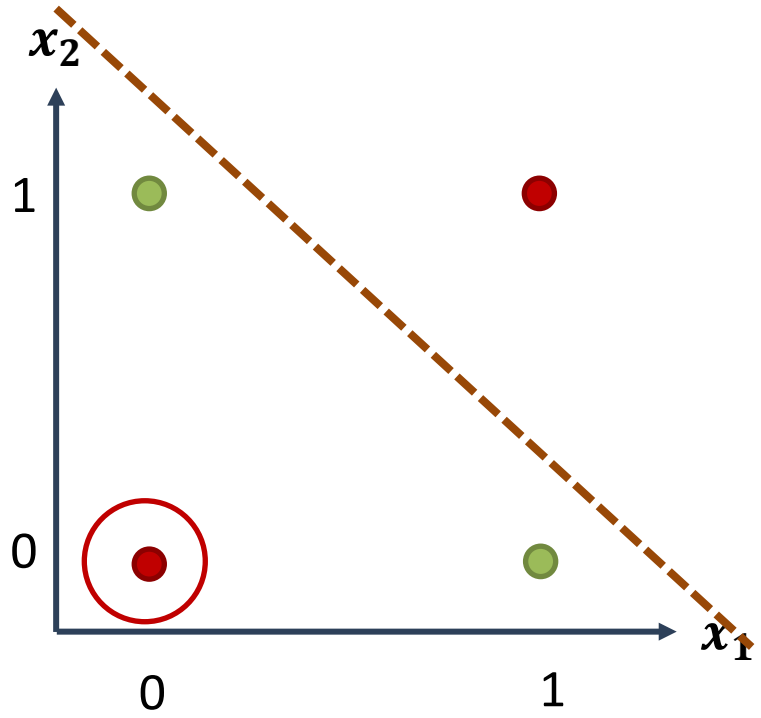

- **The problem is not linearly separable**

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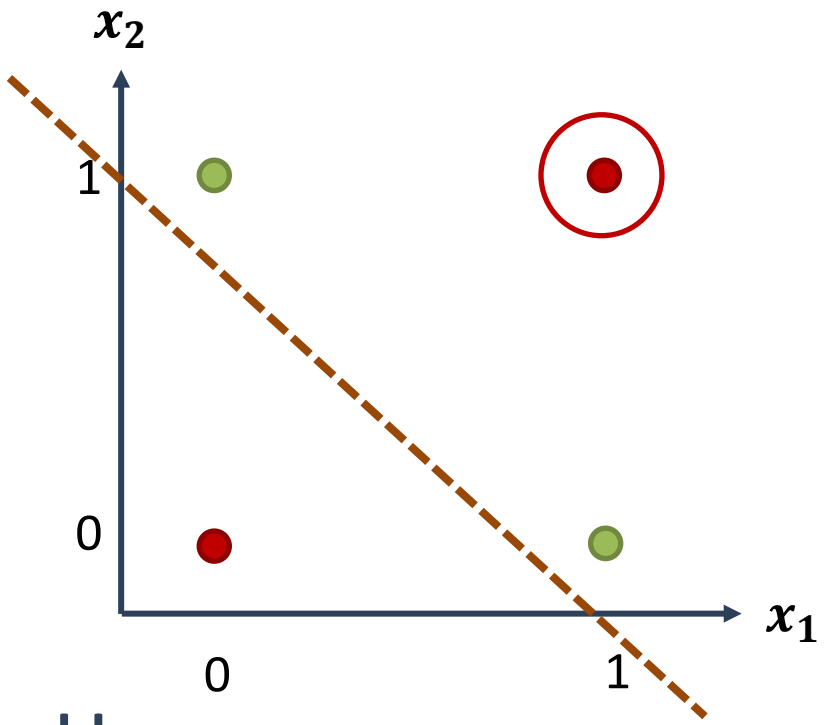


- **The problem is not linearly separable**

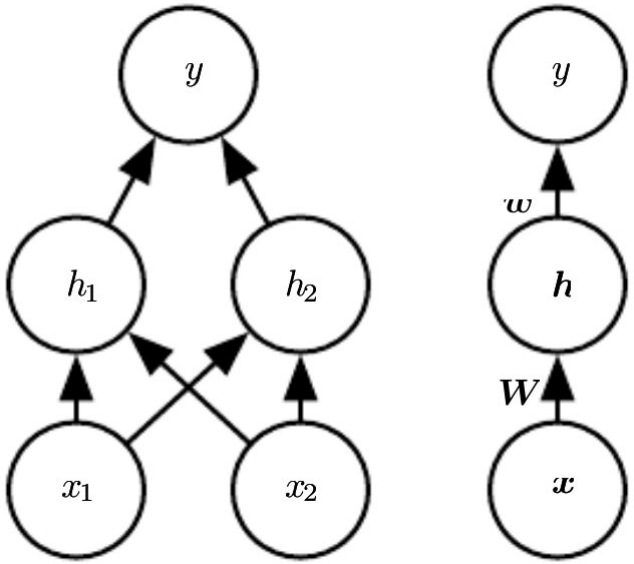
The XOR Problem

- We are trying to approximate the XOR function
  - Our training points: $X = \{[0,0]^T, [1,0]^T, [0,1]^T, [1,1]^T\}$
  - Using linear regression: $y = f([x_1, x_2]; \boldsymbol{w}, b) = \boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{w} + b$ to learn XOR
  - When using "mean squared error" as loss function, the result would be $\boldsymbol{w} = 0$ and $b = \frac{1}{2}$ … horizontal line outputting 0.5 everywhere

The XOR Problem

- We are trying to approximate the XOR function
  - Our training points: $X = \{[0,0]^T, [1,0]^T, [0,1]^T, [1,1]^T\}$
  - A we have seen, linear separation is not possible!

- Now lets use a FFN
  - One hidden layer, containing two units
  - Both representations are equivalent
    - Matrix $\boldsymbol{W}$ describes mapping $\boldsymbol{x}$ to $\boldsymbol{h}$
    - Vector $\boldsymbol{w}$ describes mapping $\boldsymbol{h}$ to y
    - (biases omitted)



What is gonna be computed

- Layer 1 (hidden layer): vector of hidden units $\boldsymbol{h}$ computed by function

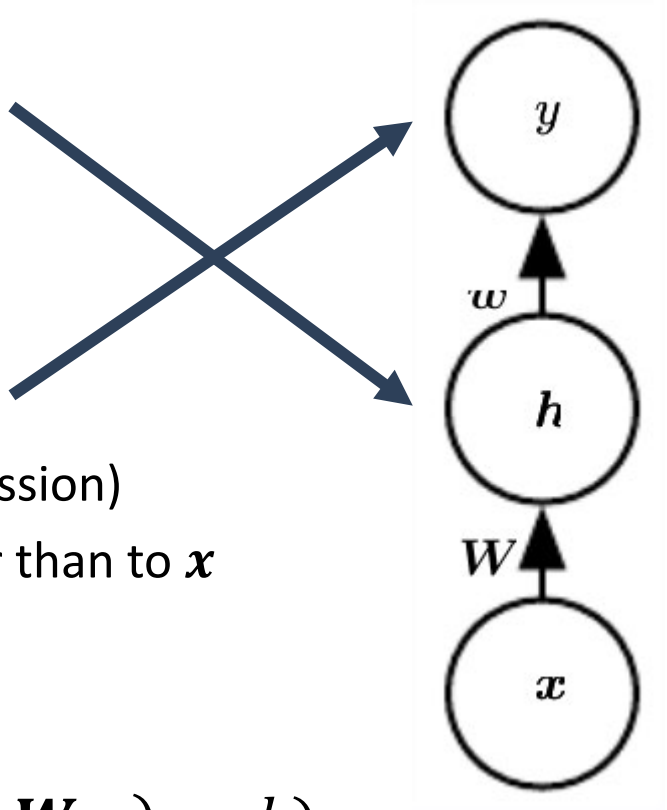
$$\boldsymbol{h} = f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, c)$$

  - c are bias variables

- Layer 2 (output layer) computes

$$y = f^{(2)}(\boldsymbol{h}; \boldsymbol{w}, b)$$

  - $\boldsymbol{w}$ are the weights (it is basically a linear regression)
  - Output is linear regression applied to $\boldsymbol{h}$ rather than to $\boldsymbol{x}$



- Complete model is

$$f(\boldsymbol{x}; \boldsymbol{W}, c, \boldsymbol{w}, b) = f^{(2)}(f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, c), \boldsymbol{w}, b)$$

Activation Function

- If we choose both $f^{(1)}$ and $f^{(2)}$ to be linear, the total function will still be linear; which is insufficient (as already seen)

- Therefore, we need an **Activation Function**:
- Remember, our function looks as follows:

$$y = \boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{w} + b$$

- Activation function g is typically chosen to be applied element-wise:

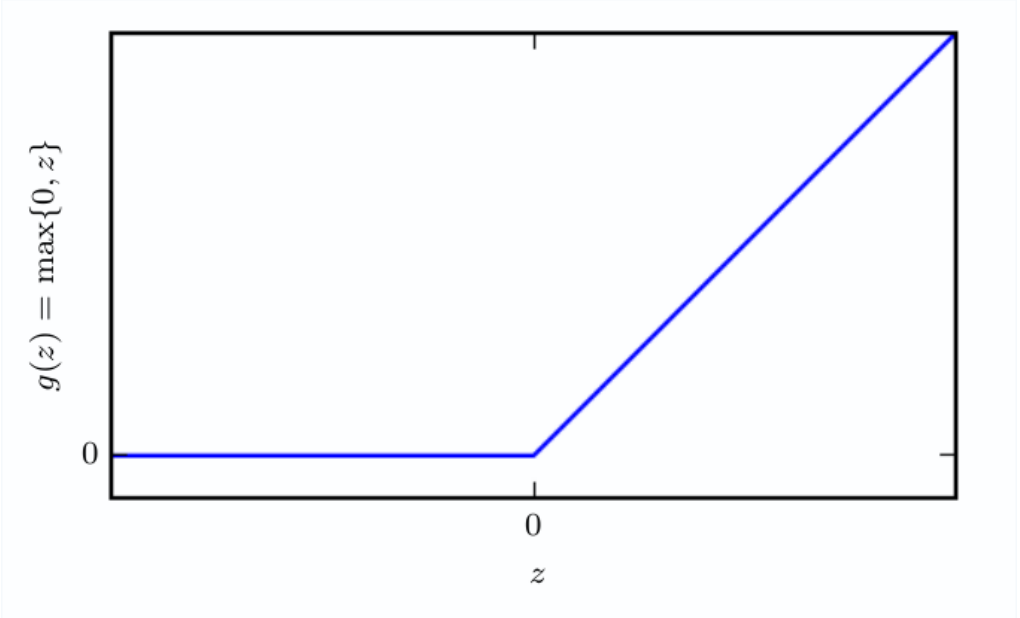
$$h_i = g(x^T W_{:i} + c_i)$$

Default Activation Function: ReLU

- Activation:

$$g(z) = \max\{0, z\}$$

- This already yields to a non-linear transformation
  - But still piecewise linear
  - Preserves couple of nice properties making gradient-based learning easy
  - Generalizes well



Back to our XOR Problem

- The complete equation is now:

$$f(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}, \boldsymbol{w}, b) = \boldsymbol{w}^T \max\{0, \boldsymbol{W}^T \boldsymbol{x} + \boldsymbol{c}\} + b$$

Lets use the following weights:

$$\boldsymbol{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \boldsymbol{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0 \; and \; \boldsymbol{X} = \begin{bmatrix} 0101 \\ 0011 \end{bmatrix}^T$$

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$$\boldsymbol{XW} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{bmatrix}$$

Back to our XOR Problem

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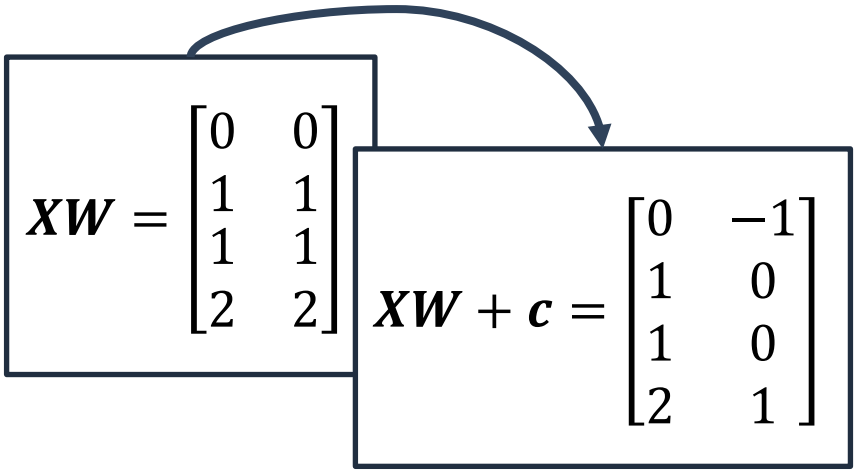

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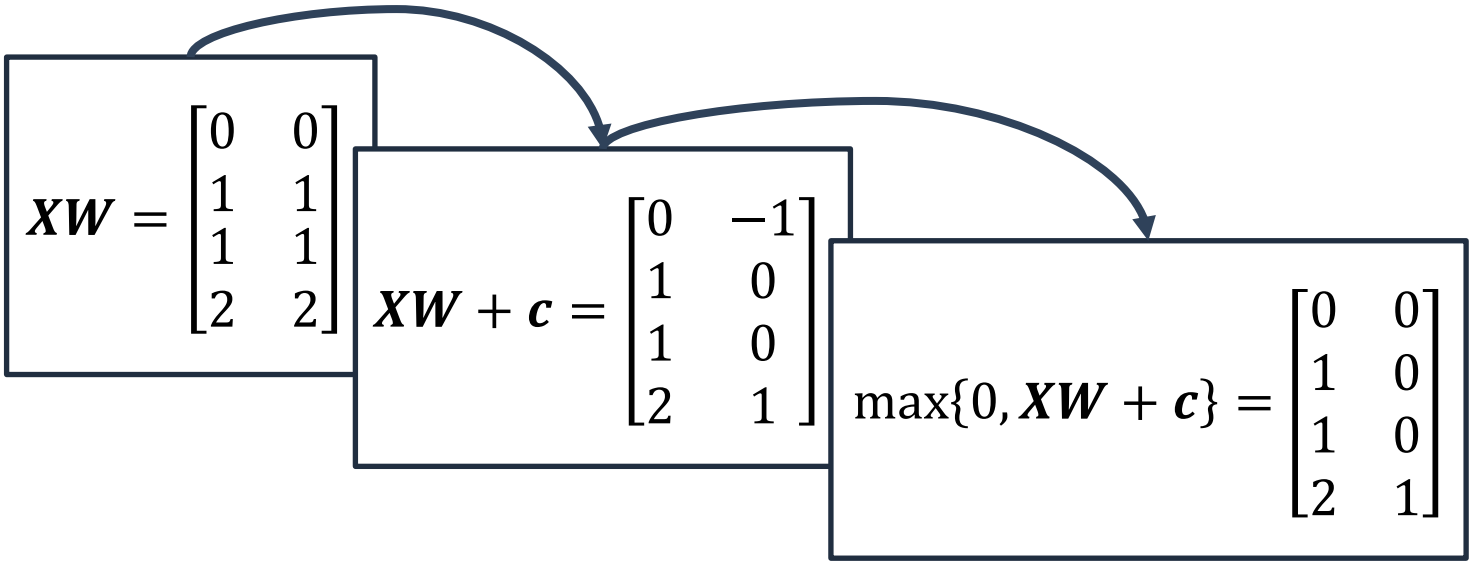

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$$\boldsymbol{XW} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{bmatrix}$$

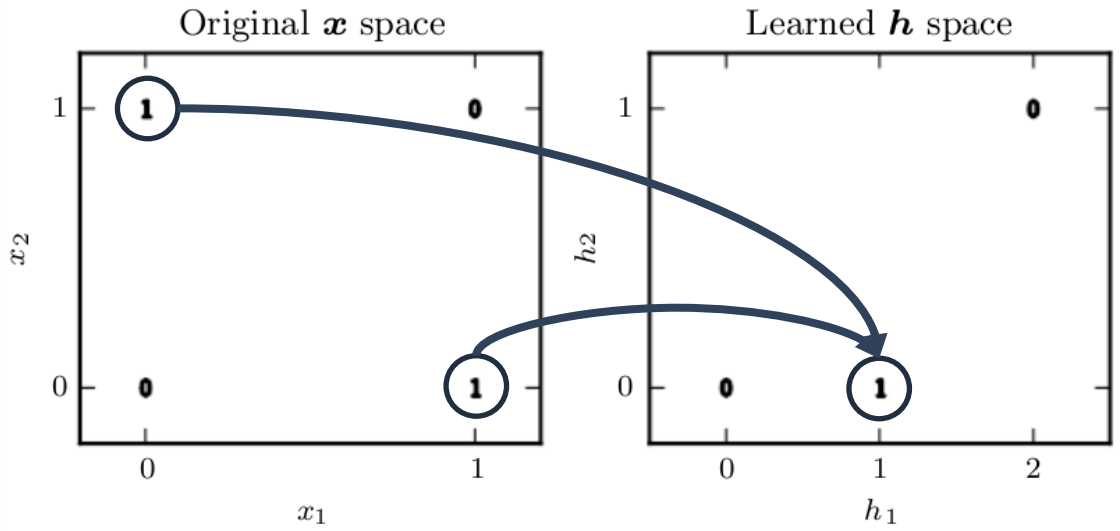
$$\boldsymbol{XW} + \boldsymbol{c} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

$$\max\{0, \boldsymbol{XW} + \boldsymbol{c}\} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \boldsymbol{w} = \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \\ \mathbf{1} \\ \mathbf{0} \end{bmatrix}$$

“Learned XOR”

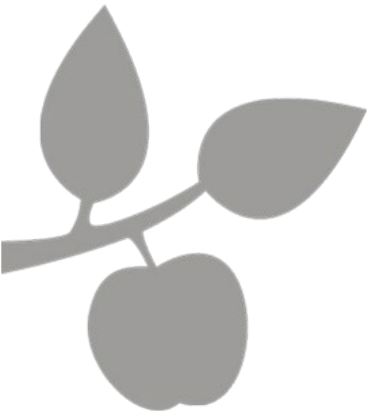
- Two points that must have output 1 have been collapsed into one



- Can be separated in a linear model:
  - For fixed h_2 output has to increase in h_1

- Of course, we “cheated”: We have “guessed” the parameters correctly which lead to the desired result

- In reality: Millions of parameters which we have to actually learn



Deep Feedforward Networks Part II

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  - What is a Neuron?
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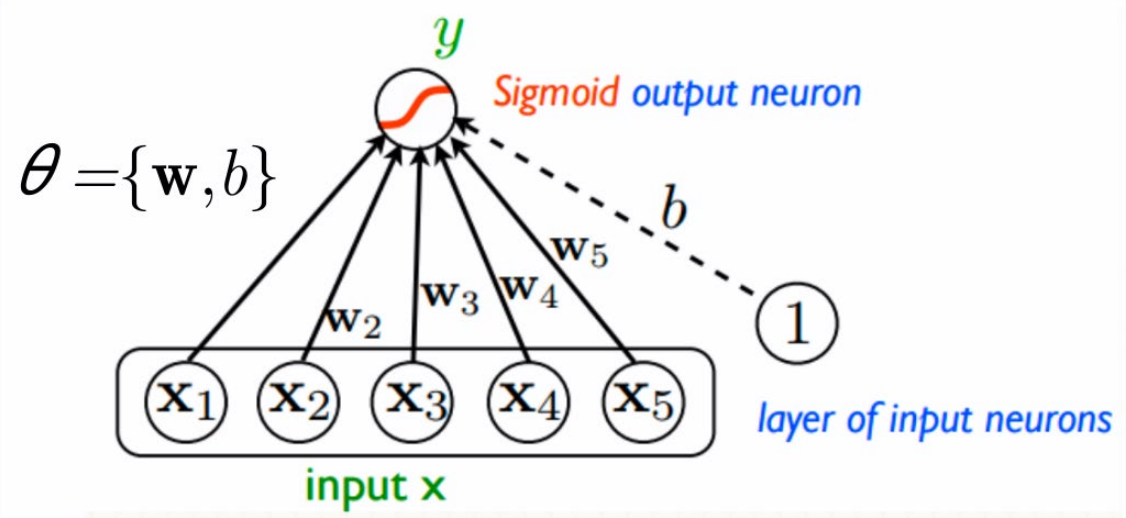
- **Intermezzo: Some Math**
- **PART II**
  - Networks
  - **Output Units**
  - Hidden Units
  - Architecture Design

Output Units

- The choice of cost function is **tightly** coupled with the choice of output unit (later…)
- Most of the time we use cross-entropy between data distribution and model distribution (later …)
- Choice of how to represent the output then determines the form of the cross-entropy function



Role of a Output Unit

- Any output unit is in principal also usable as a hidden unit
- A feedforward network provides a hidden set of features

$$\boldsymbol{h} = f(\boldsymbol{x}; \boldsymbol{\theta})$$

- Role of output layer is to provide some additional transformation from the features to the task that network must perform
- Common Output Units
  - **Linear units**: no non-linearity (used for Regressions)
  - **Sigmoid units** (used for binary classification)
  - **Softmax units** (used for general classification)

Linear Units for Regressions

- Linear unit: simple output based on affine transformation with no nonlinearity

- Given features h, a layer of linear output units produces a vector

$$\hat{\boldsymbol{y}} = \boldsymbol{W}^T \boldsymbol{h} + \boldsymbol{b}$$

- Linear units are often used to produce mean $\hat{\boldsymbol{y}}$ of a conditional Gaussian distribution

$$P(\boldsymbol{y}|\boldsymbol{x}) = N(\boldsymbol{y}; \hat{\boldsymbol{y}}, \sigma^2)$$

  - We will see later why this is interesting

➢ You will understand these slides later on.

Sigmoid Units for Binary Classification

- Task of predicting value of binary variable y
  - Classification problem with two classes

- Maximum likelihood approach is to define a Bernoulli distribution over y conditioned on $\boldsymbol{x}$

- Neural net needs to predict $p(y = 1|\boldsymbol{x}) \in [0,1]$:

$$P(y = 1|\boldsymbol{x}) = \max\{0, \min\{1, \boldsymbol{w}^T \boldsymbol{h} + \boldsymbol{b}\}\}$$

  - We would define a valid conditional distribution, but cannot train it effectively with gradient descent
  - A gradient of 0: learning algorithm cannot be guided

➢ You will understand these slides later on.

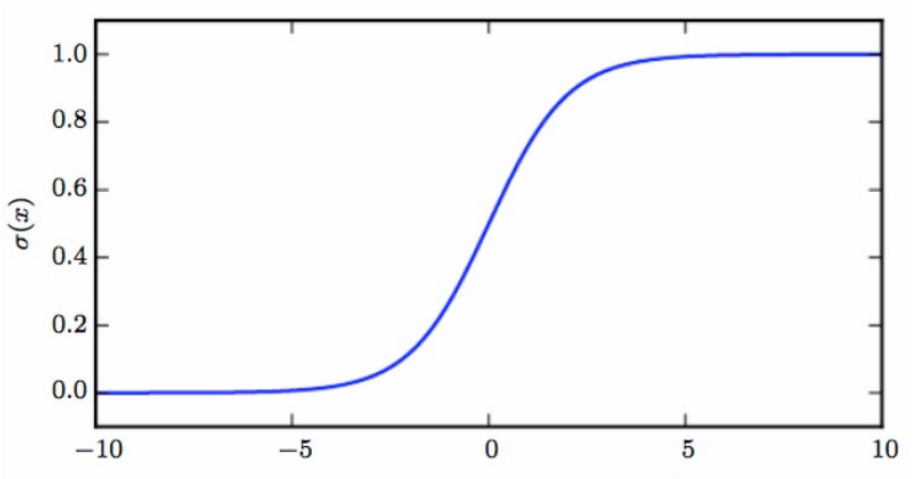
Sigmoid Units

- Sigmoid always gives a gradient

$$\hat{y} = \sigma(\boldsymbol{w}^T \boldsymbol{h} + b)$$

with

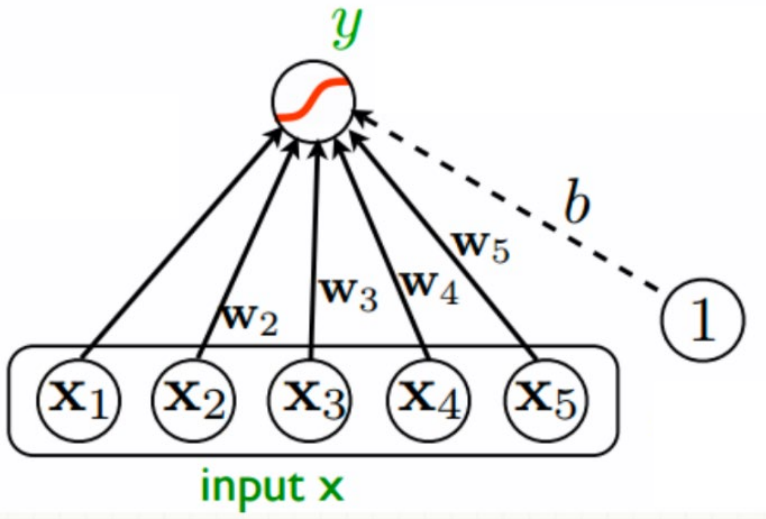
$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$



- Sigmoid Unit has two components:
  - A linear layer to compute

$$z = \boldsymbol{w}^T \boldsymbol{h} + b$$

  - A sigmoid activation function to convert z into a probability



➢ You will understand these slides later on.

Softmax units for general Classification

- Any time we want a probability distribution over a discrete variable with n values we may use the softmax function

- Softmax most often used for output of classifiers to represent distribution over n classes
  - Also inside the model itself when we wish to choose between one of n options

- For the Binary case we have produced a single number

$$\hat{y} = P(y = 1|\boldsymbol{x})$$

- Now, we have to produce a vector $\hat{\boldsymbol{y}}$

$$\hat{y}_i = P(y = i|\boldsymbol{x})$$

➢ You will understand these slides later on.

Softmax Defintion

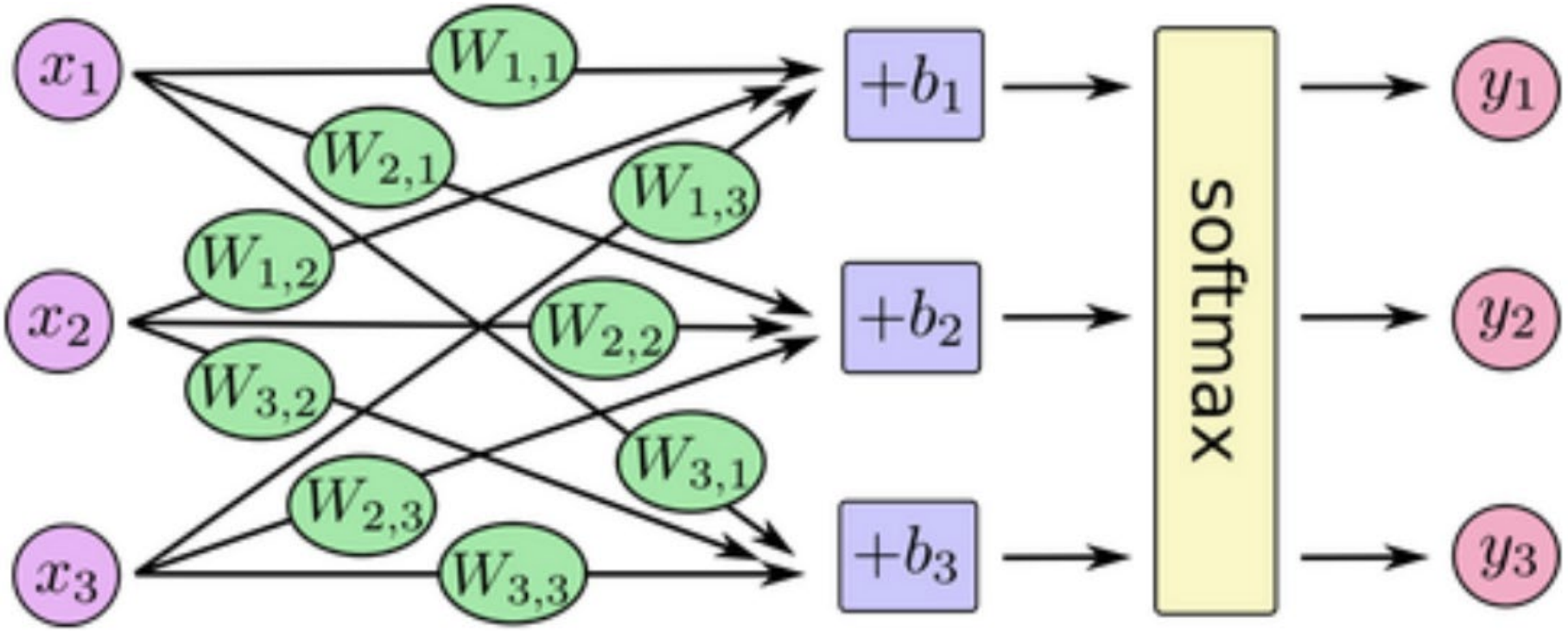
- The **softmax function** (aka normalized exponential), is defined as follows:

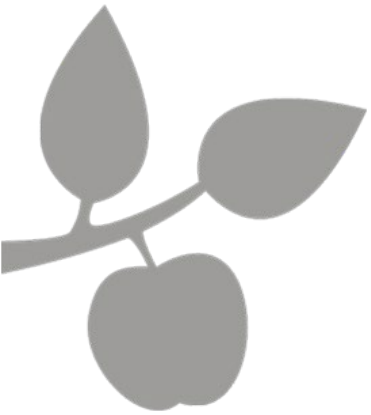
$$\text{softmax}(a_1, \dots, a_K) = \left(\frac{\exp a_1}{\sum_j^K \exp a_j}, \frac{\exp a_2}{\sum_j^K \exp a_j}, \dots, \frac{\exp a_K}{\sum_j^K \exp a_j} \right)$$

- We will learn later more about this function
- But it should be visible that it creates a valid distribution functions

➢ You will understand these slides later on.

Softmax Regression





Deep Feedforward Networks Part II

- **PART I**
  - What is a Neuron?
  - How to build a Network
- **Intermezzo: Some Math**
- **PART II**
  - Networks
  - Output Units
  - **Hidden Units**
  - Architecture Design

General Construction of a Hidden Unit

- Very Similar to an output unit
- Accepts a vector of inputs $\boldsymbol{x}$ and computes an affine transformation $\boldsymbol{h}' = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$
- Computes an element-wise non-linear function $g(\boldsymbol{h}')$
- Most hidden units are distinguished from each other by the choice of activation function $g(\boldsymbol{h}')$
  - We look at: ReLU, Sigmoid and tanh, and other hidden units

Choice of Hidden Unit

- We now look at how to choose the type of hidden unit in the hidden layers of the model
- Design of hidden units is an active research area that does not have many definitive guiding theoretical principles
- ReLU is an excellent default choice
- But there are many other types of hidden units available
- When to use which kind?
  - Impossible to predict in advance which will work best
  - Design process is trial and error

The ReLU

$$\boldsymbol{h} = g(\boldsymbol{W}^T \boldsymbol{x} + \boldsymbol{b})$$
$$g(x) = \max\{0, x\}$$

- Good practice to set all elements of $\boldsymbol{b}$ to a small value such as 0.1
  - This makes it likely that ReLU will be initially active for most training samples and allow derivatives to pass through
- Generalizations of ReLU
  - Perform comparably to ReLU and occasionally perform better
  - ReLU cannot learn on examples for which the activation is zero
  - Generalizations guarantee that they receive gradient everywhere

Generalizations of ReLU

- Three methods based on using a non-zero slope α_i when $z_i < 0$:

$$h_i = g(\boldsymbol{z}, \boldsymbol{\alpha})_i = \max(0, z_i) + \alpha_i \min(0, z_i)$$

- Absolute-value rectification:
  - fixes $\alpha_i = -1$ to obtain $g(z) = |z|$
- Leaky ReLU:
  - fixes α_i to a small value like 0.01
- Parametric ReLU or PReLU
  - treats α_i as a learnable parameter

Logistic Sigmoid

- Prior to introduction of ReLU, most neural networks used logistic sigmoid activation

$$g(z) = \sigma(z)$$

- Or the hyperbolic tangent

$$g(z) = \tanh(z)$$

- These activation functions are closely related because

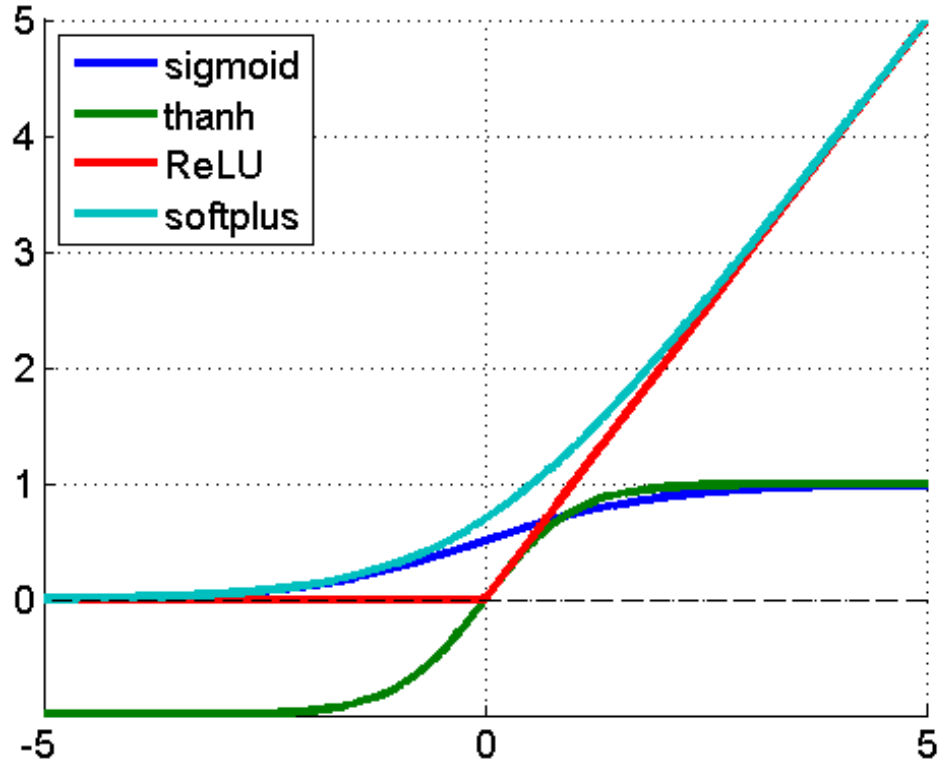
$$\tanh(z) = 2\sigma(2z) - 1$$

- Sigmoid units are used to predict probability that a binary variable is 1

Sigmoid Saturation

- Sigmoidals saturate across most of domain
  - Saturate to 1 when z is very positive and 0 when z is very negative
  - Strongly sensitive to input when z is near 0
  - Saturation makes gradient-learning difficult

- ReLU and Softplus increase for input >0



Sigmoid vs $tanh$ Activation

- Hyperbolic tangent typically performs better than logistic sigmoid

- It resembles the identity function more closely

$$\tanh(0) = 0 \quad \text{while} \quad \sigma(0) = 1 / 2$$

- Because tanh is similar to identity near 0, training a deep neural network

$$\hat{\boldsymbol{y}} = \boldsymbol{w}^T \tanh(\boldsymbol{U}^T \tanh(\boldsymbol{V}^T \boldsymbol{x}))$$

resembles training a linear model

$$\hat{\boldsymbol{y}} = \boldsymbol{w}^T \boldsymbol{U}^T \boldsymbol{V}^T \boldsymbol{x}$$

so long as the activations can be kept small

Other Activation Functions

- **Cosine**

$$\boldsymbol{h} = \cos(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

  - Feedforward networks on MNIST obtained error rate of less than 1%

- **Radial Basis**

$$h_i = \exp\left(-\frac{1}{\sigma^2}\left\|\boldsymbol{W}_{:j} - \boldsymbol{x}\right\|^2\right)$$

  - Becomes more active as $\boldsymbol{x}$ approaches a template $W_{:,i}$

- **Softplus**

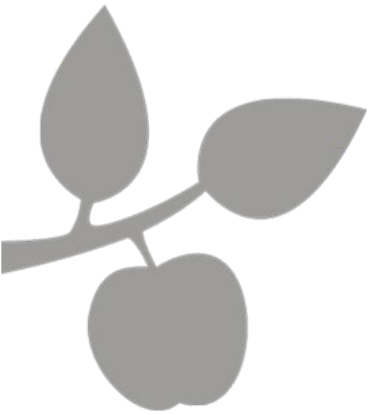
$$g(a) = \zeta(a) = \log(1 + e^a)$$

  - Smooth version of the rectifier

- **Hard tanh**

$$g(a) = \max(-1, \min(1, a))$$

  - Shaped similar to tanh and the rectifier but it is bounded



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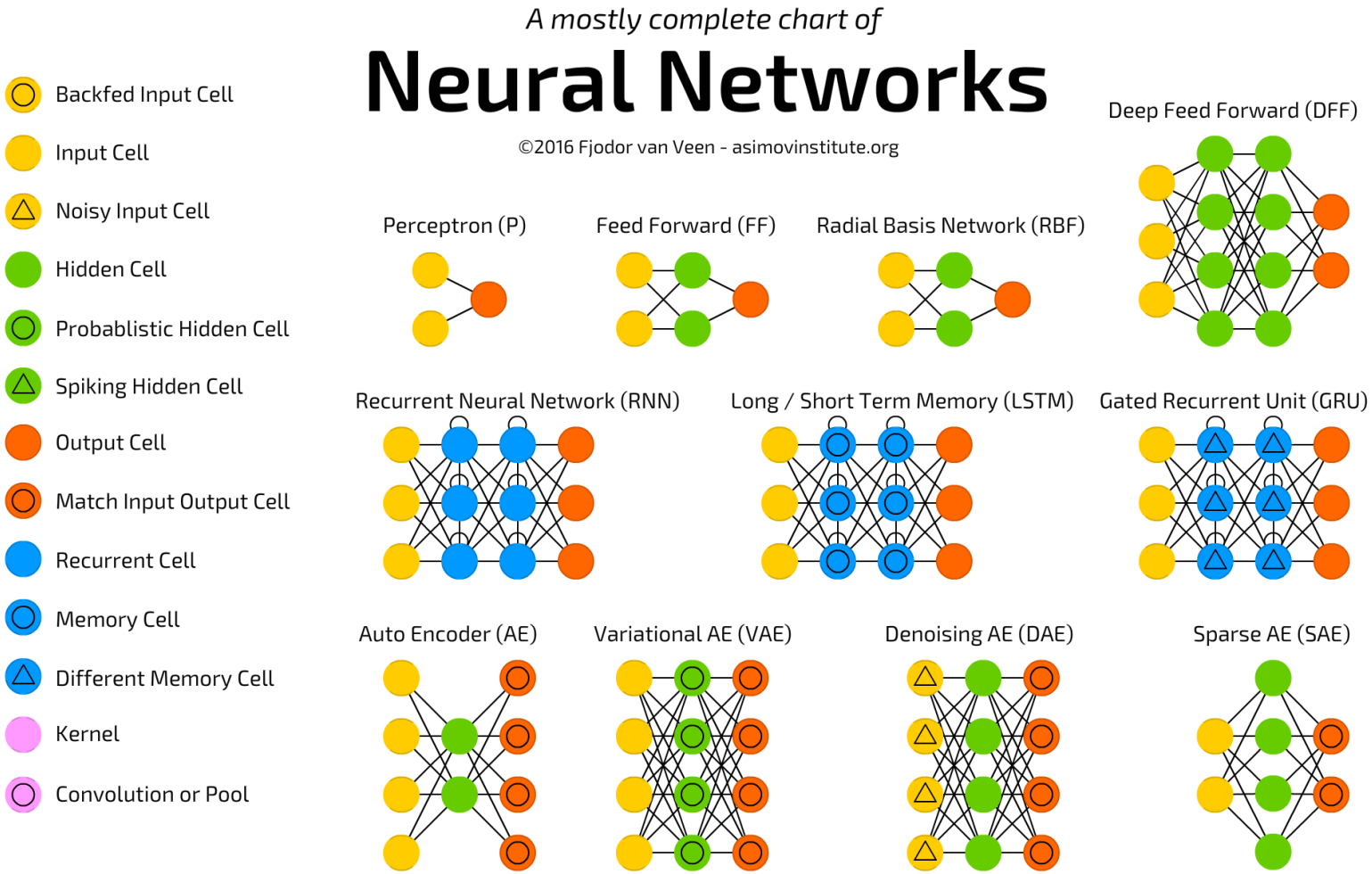
A mostly complete chart of Neural Networks



- https://towardsdatascience.com/the-mostly-complete-chart-of-neural-networks-explained-3fb6f2367464

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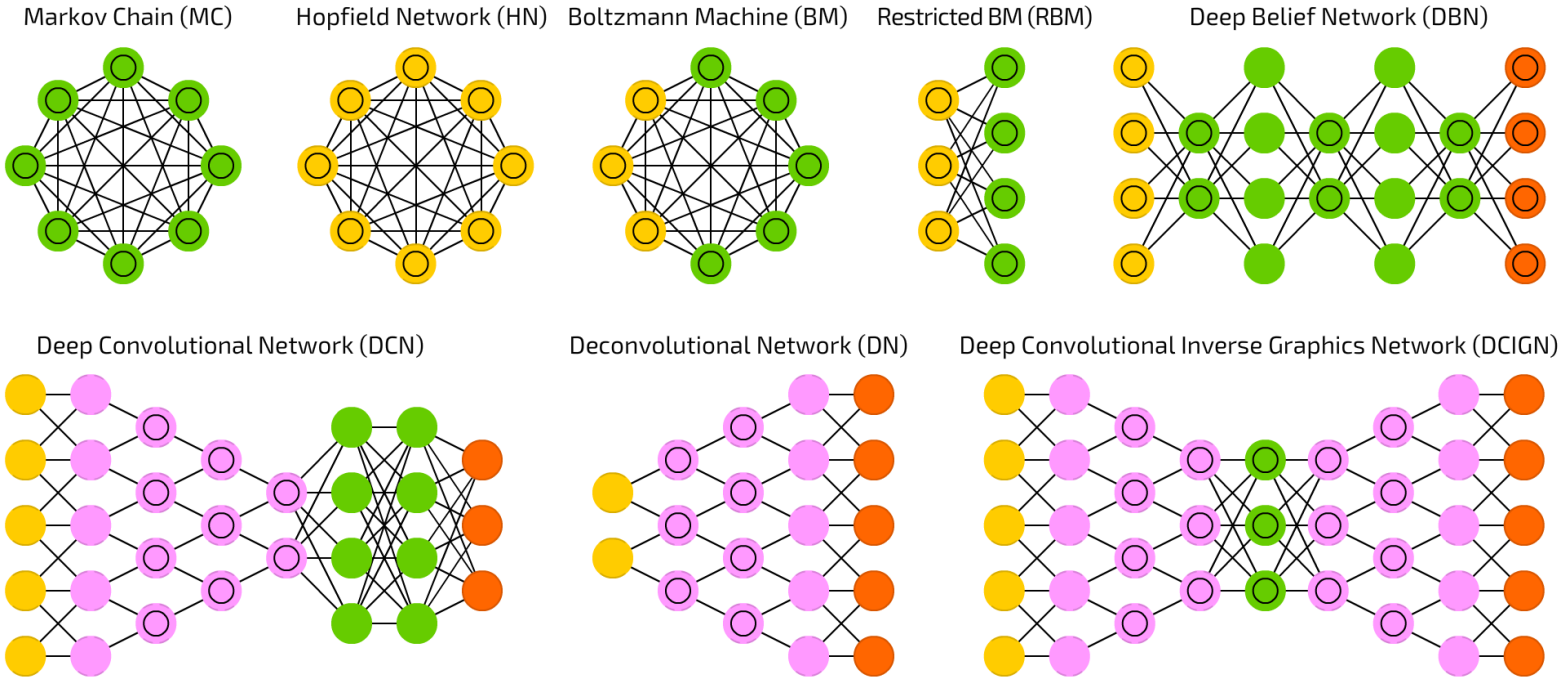

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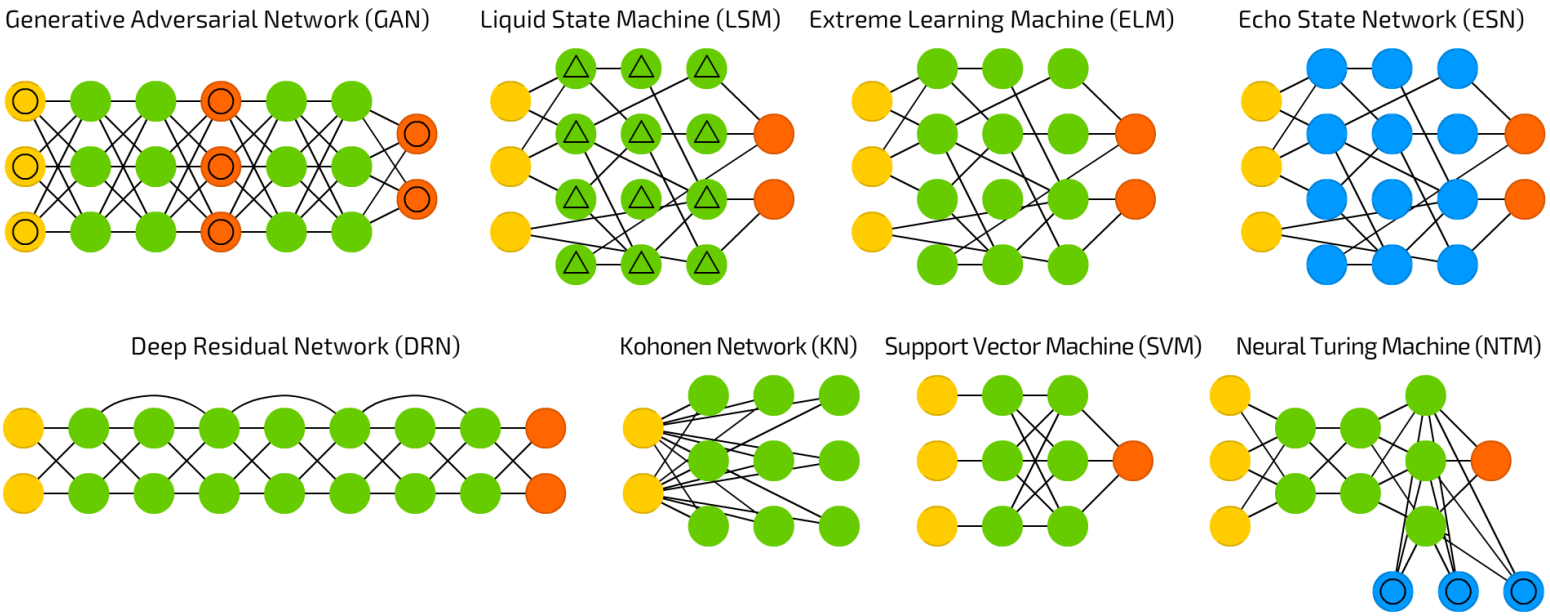

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Main Architectural Considerations

1. **Choice of depth of network**
2. **Choice of width of each layer**

- Deeper networks have
  - Far fewer units in each layer
  - Far fewer parameters
  - Often generalize well to the test set
  - But are often more difficult to optimize

- Ideal network architecture must be found via experimentation guided by validation set error

On the Power of Neural Networks

- A linear model, mapping from features to outputs via matrix multiplication, can by definition represent only linear functions.
  - Easy to learn
  - Cost function results in convex optimization problem

The **universal approximation theorem** states that a feedforward network with a linear output layer and at least one hidden layer with any "squashing" activation function and enough units (e.g. sigmoid) can approximate any Borel measurable function (with some restrictions).

- We don't need specialized model families for approximating functions
- However, it does not state how to learn and how to design the appropriate network

Implication of Theorem

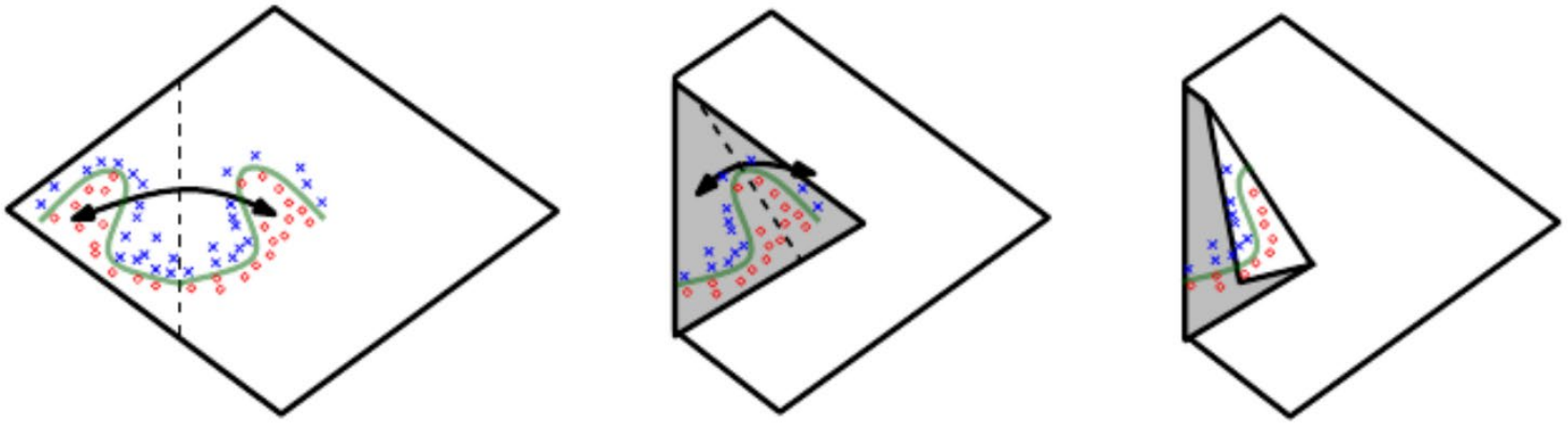
- Whatever function we are trying to learn, a large MLP will be able to represent it
- However we are not guaranteed that the training algorithm will learn this function
  - Optimizing algorithms may not find the parameters
  - May choose wrong function due to over-fitting
- No Free Lunch: There is no universal procedure for examining a training set of samples and choosing a function that will generalize to points not in training set

Function Families and Depth

- Some families of functions can be represented efficiently in a deep network but require much larger networks if the model is shallow
- In some cases no. of hidden units required by shallow model is exponential in n
- Piecewise linear networks (which can be obtained from rectifier nonlinearities or maxout units) can represent functions with a no. of regions that is exponential in d

Advantage of deeper networks

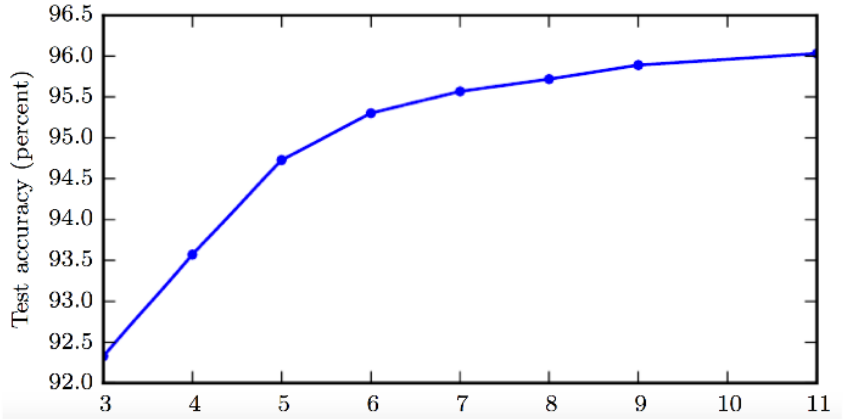
- Absolute value rectification creates mirror images of function computed on top of some hidden unit, wrt the input of that hidden unit.
- Each hidden unit specifies where to fold the input space in order to create mirror responses.
- By composing these folding operations we obtain an exponentially large no. of piecewise linear regions which can capture all kinds of repeating patterns



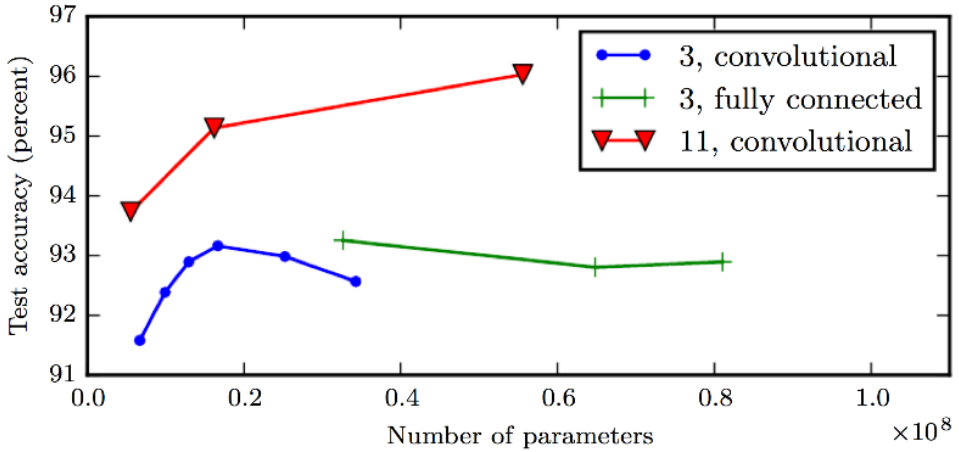
Intuition of Depth

- Any time we choose a ML algorithm we are implicitly stating a set of beliefs about what kind of functions that algorithm should learn
- Choosing a deep model encodes a belief that the function should be a composition several simpler functions
- The learning problem consists of discovering a set of underlying factors of variation that can in turn be described in terms of other, simpler underlying factors of variation.
- Empirically: Deeper Networks perform better ☺

Deeper Networks



Test accuracy consistently increases with depth



Increasing parameters without increasing depth is not as effective

Other architectural considerations

- Most important specialized architectures are
- Convolutional Networks
  - Used heavily for computer vision
- Recurrent Neural Networks
  - Used for sequence processing
  - Have their own architectural considerations
- Non-chain architectures
  - Skipping going from layer i to layer i+2 or higher