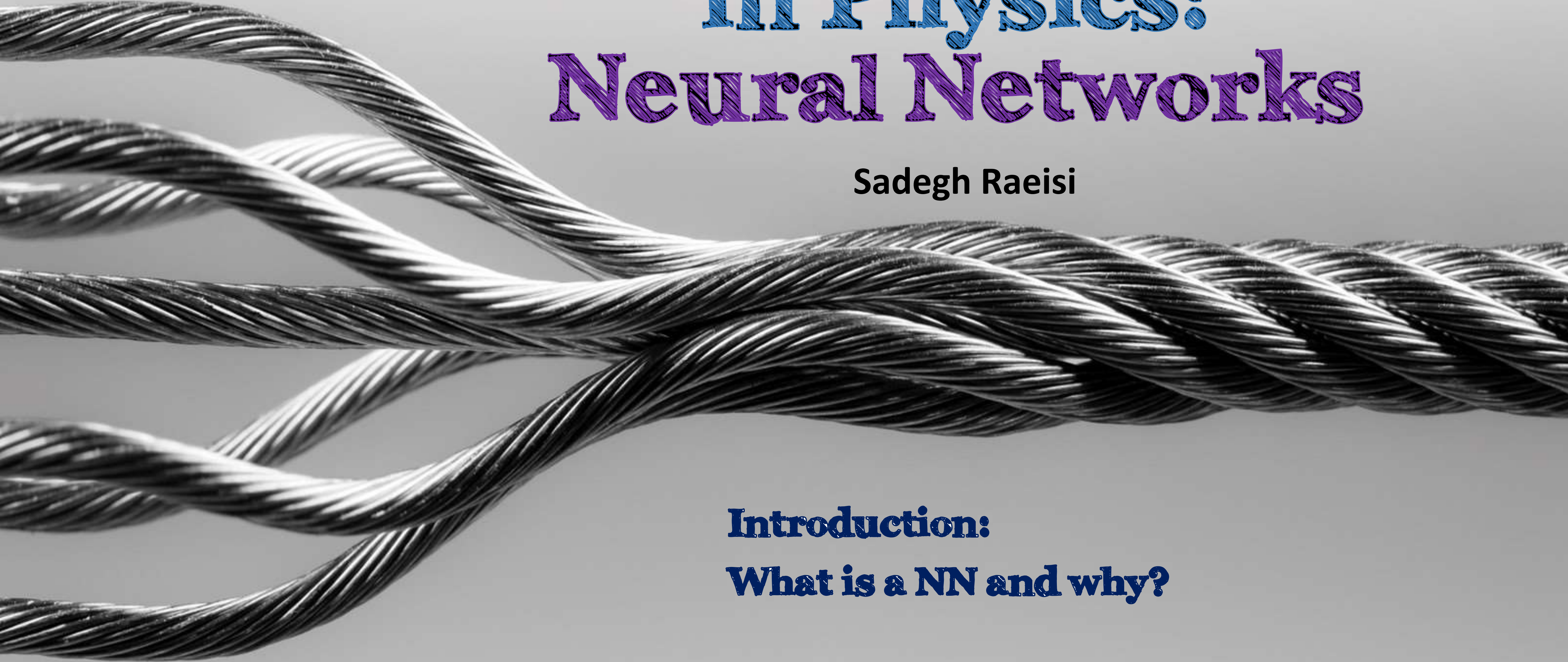


Machine Learning in Physics: Neural Networks

Sadegh Raeisi

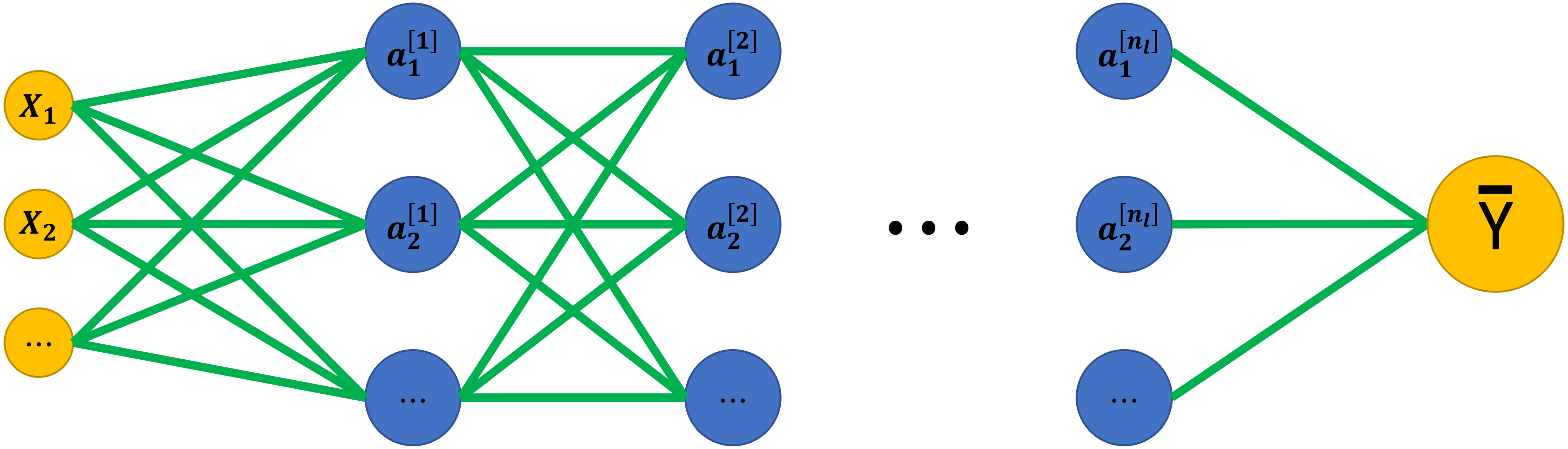
Introduction:
What is a NN and why?

Plan for the next part

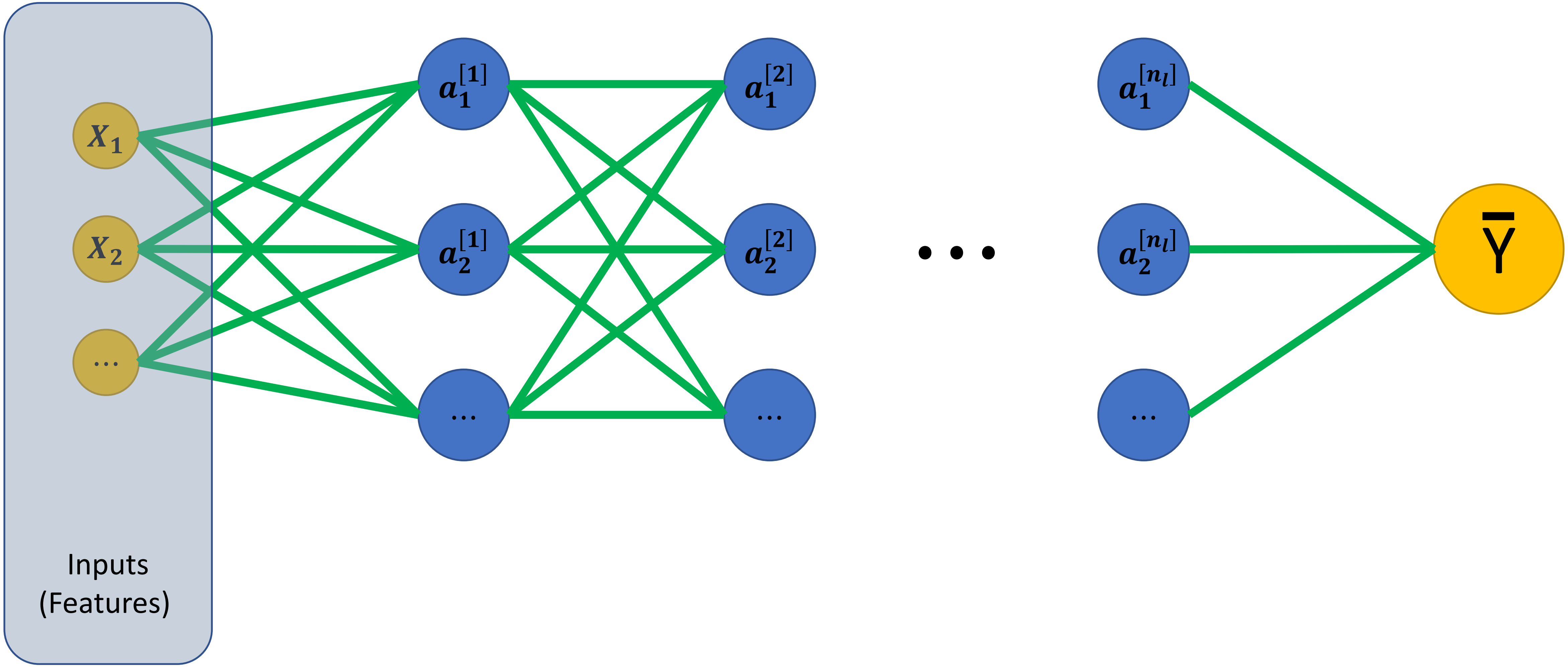
- Intro to NN
  - Structure
  - Intuition
  - Universality of NN
- Back propagation
- Hands-on example
- Convolutional NN
- Recurrent NN
- …

What is a NN?

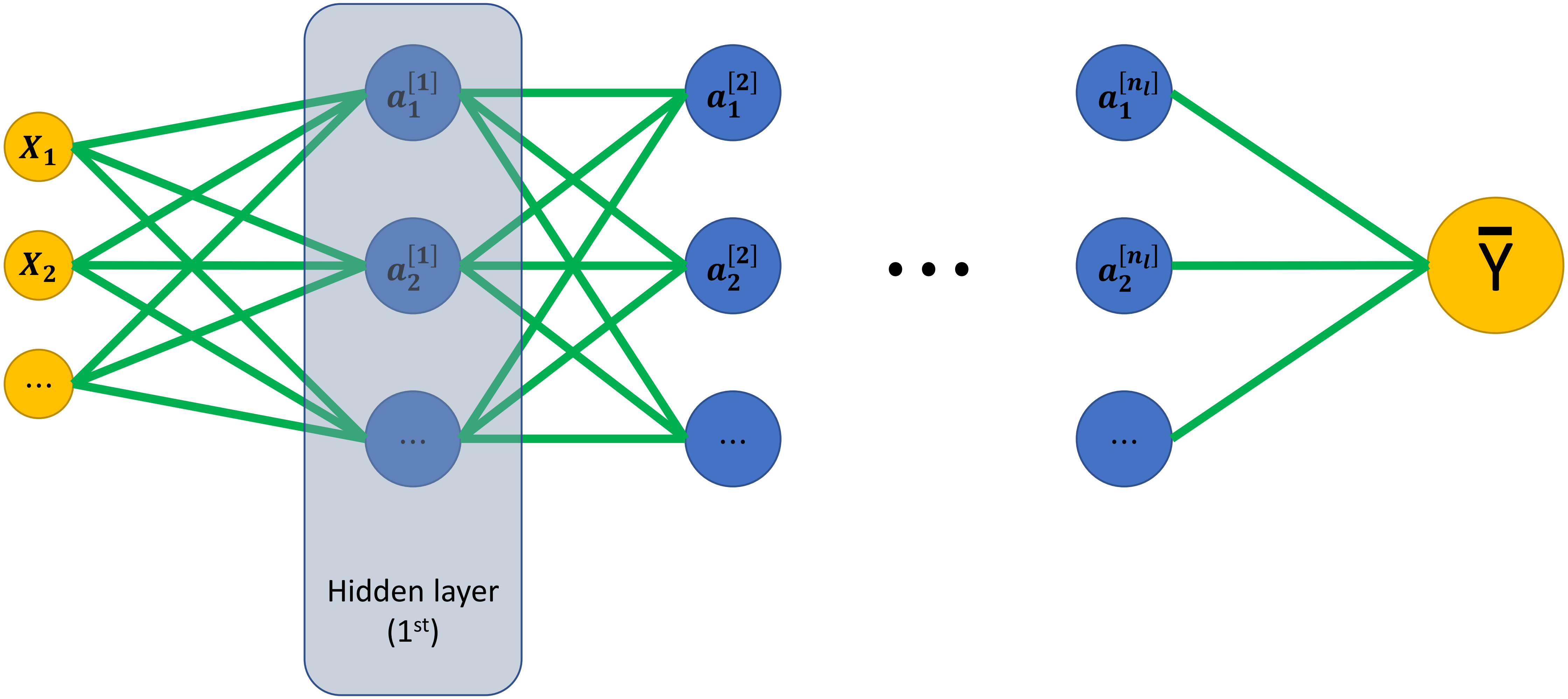
Structure and terminology



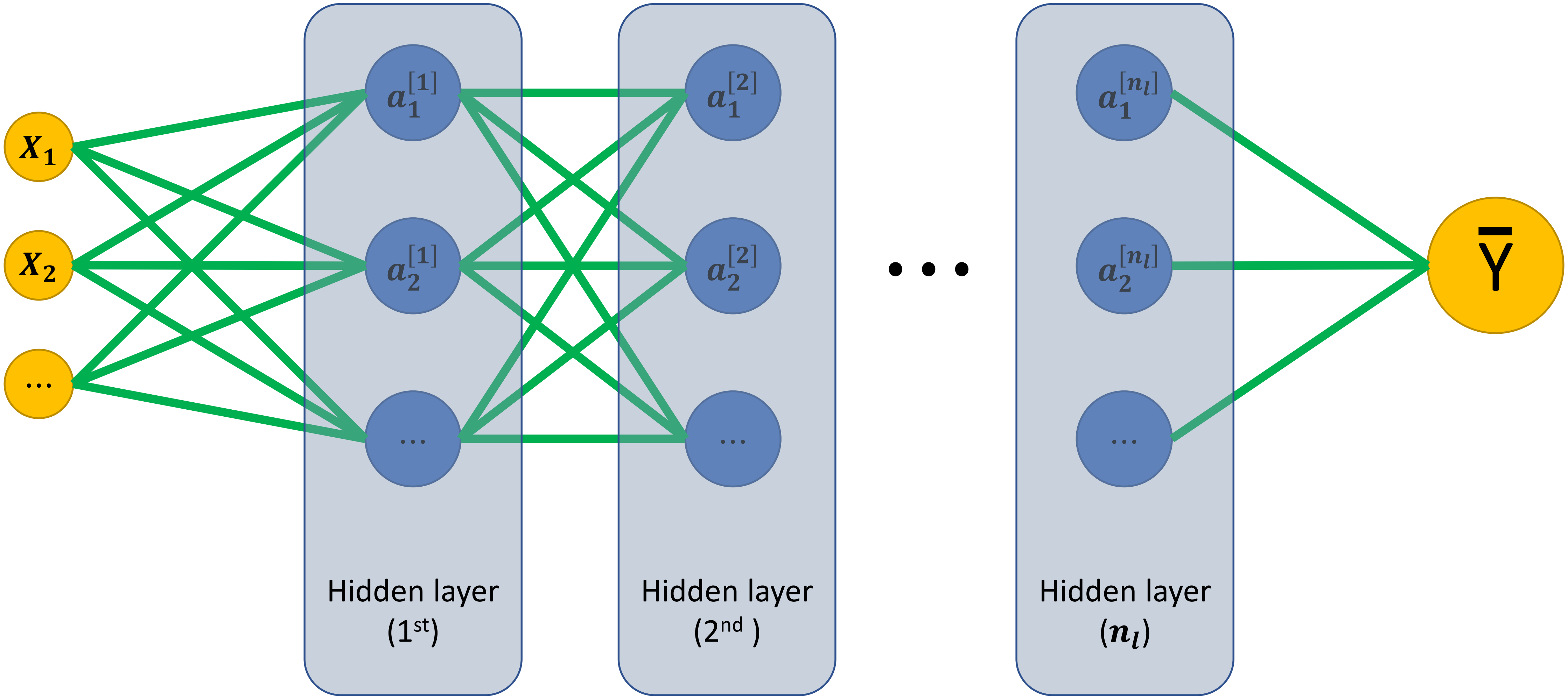
Structure and terminology



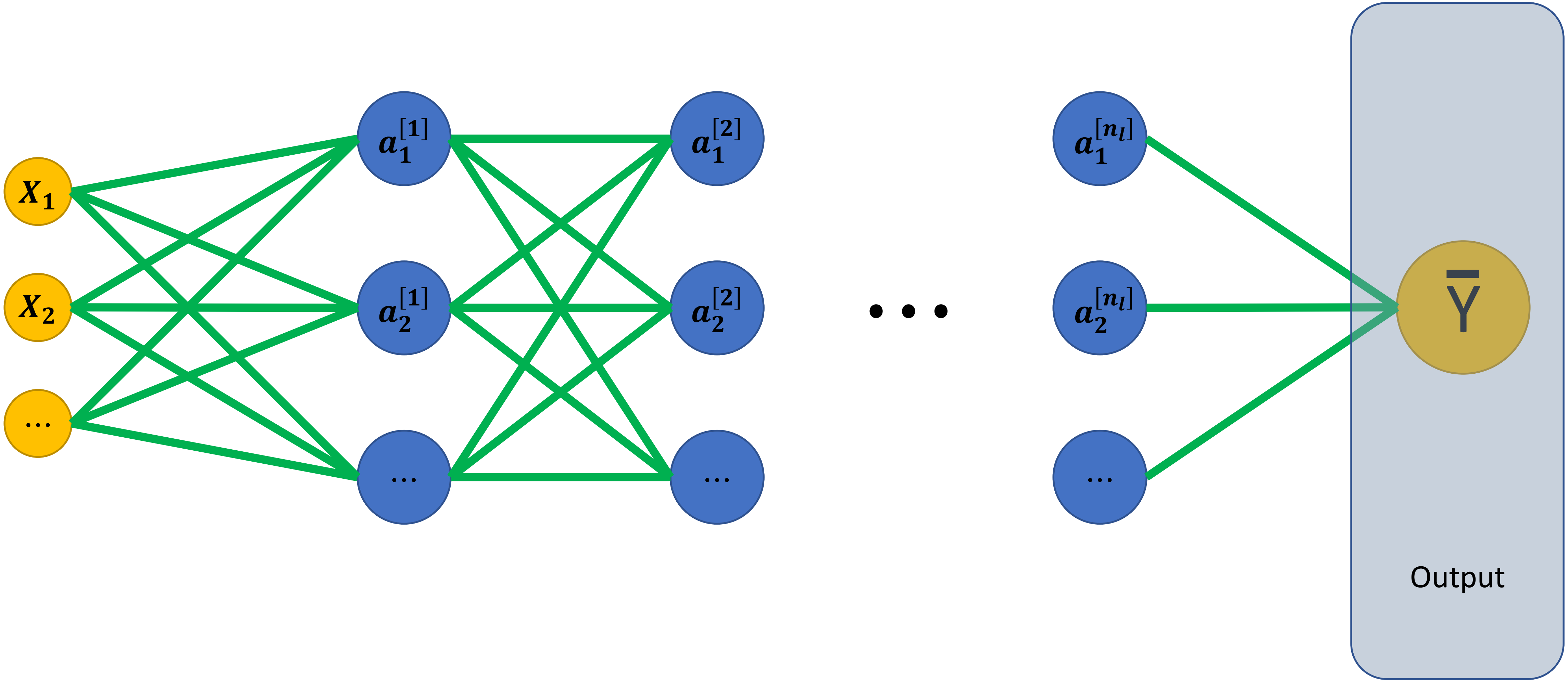
Structure and terminology



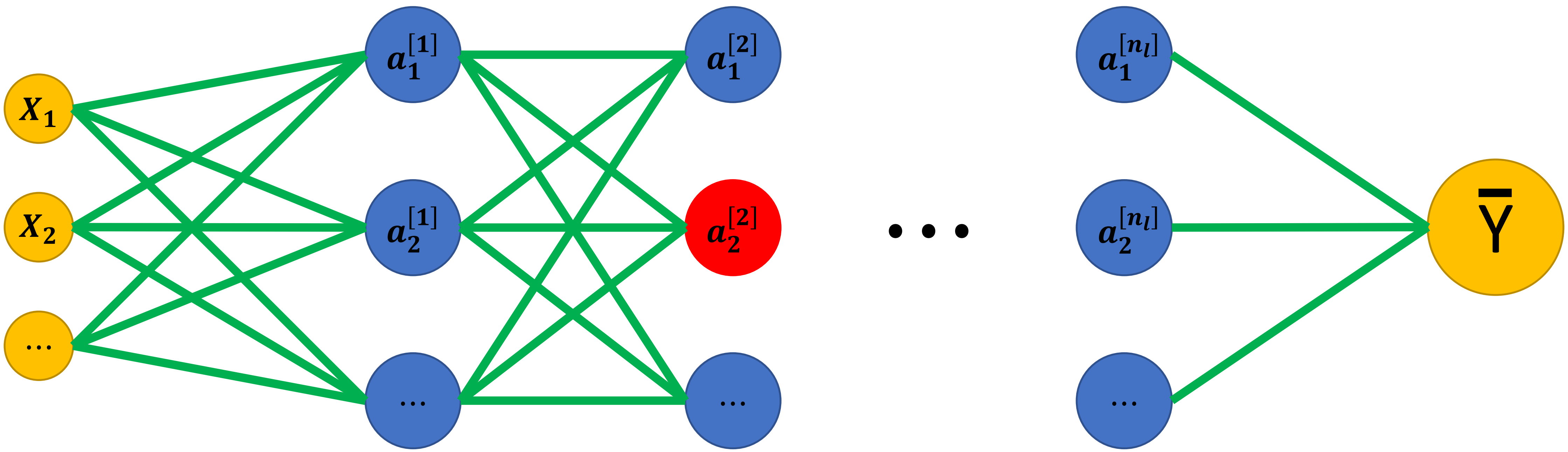
Structure and terminology



Structure and terminology

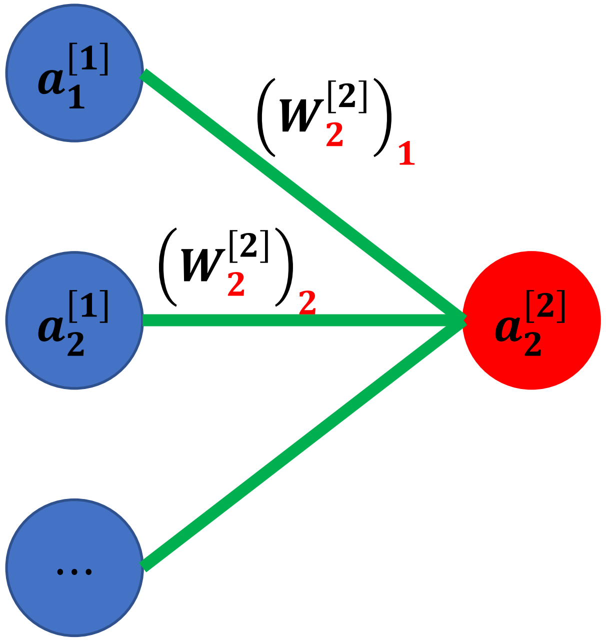


Structure and terminology



A node

Structure and terminology



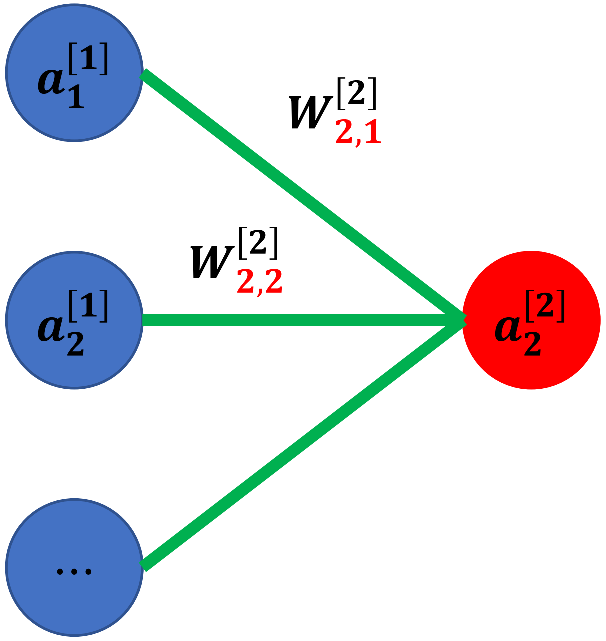
$$z_2^{[2]} = \left(W_2^{[2]}\right)_1 a_1^{[1]}$$

$$+ \left(W_2^{[2]}\right)_2 a_2^{[1]}$$

$$+ \cdots$$

$$a_2^{[2]} = f_{act}\left(z_2^{[2]}\right)$$

Structure and terminology



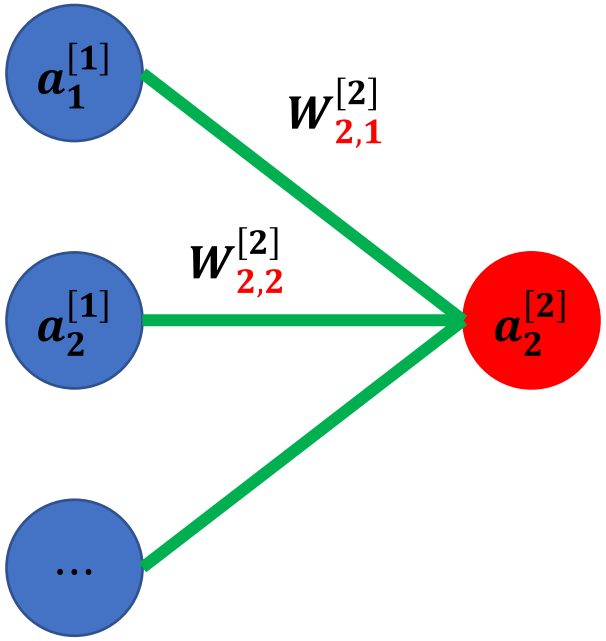
$$z_2^{[2]} = W_{2,1}^{[2]}\ a_1^{[1]}$$

$$+W_{2,2}^{[2]}\ a_2^{[1]}$$

$$+\cdots$$

$$a_2^{[2]} = f_{act}\left(z_2^{[2]}\right)$$

Structure and terminology



Linear combination of previous nodes

A node in layer l

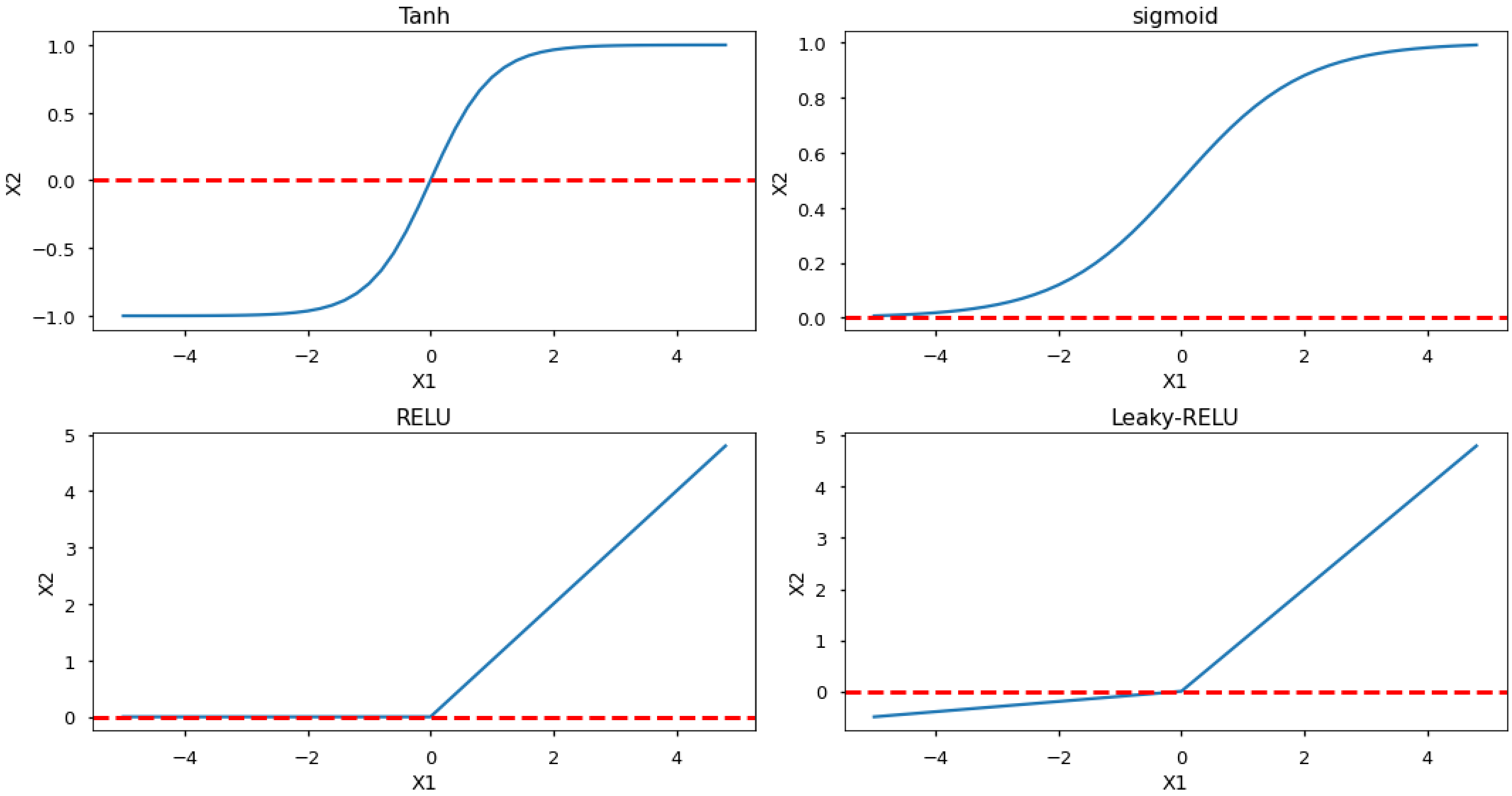
$$a_i^{[l]} = f_{act}^{[l]}\left(\sum_j W_{i,j}^{[l]}\, a_j^{[l-1]} + B_i\right)$$

Activation function

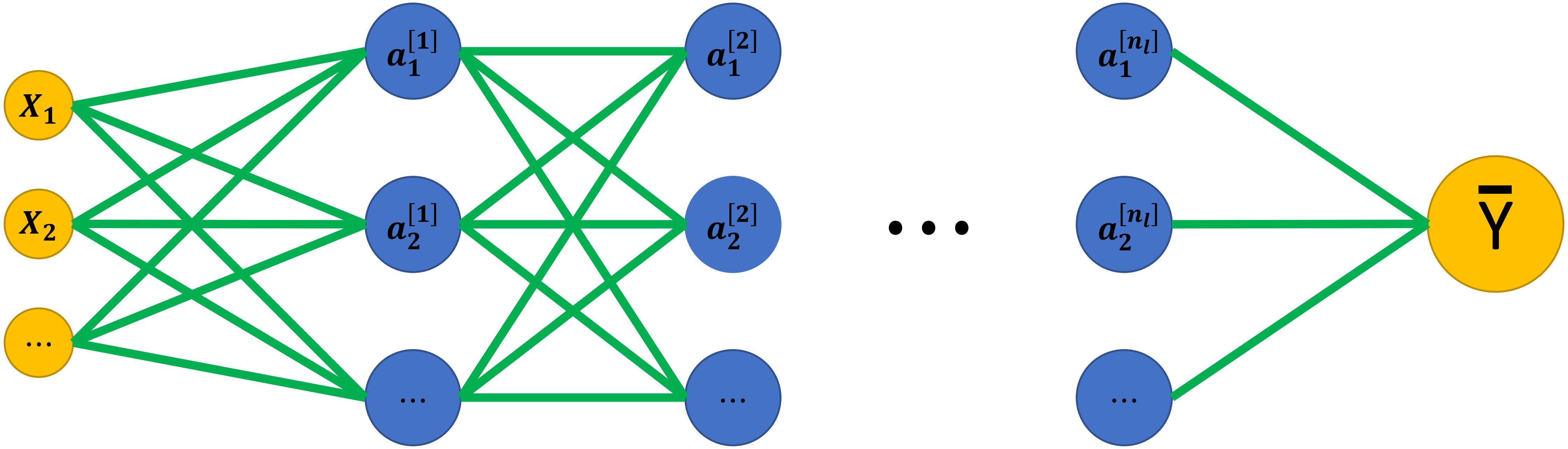
Weights

Bias

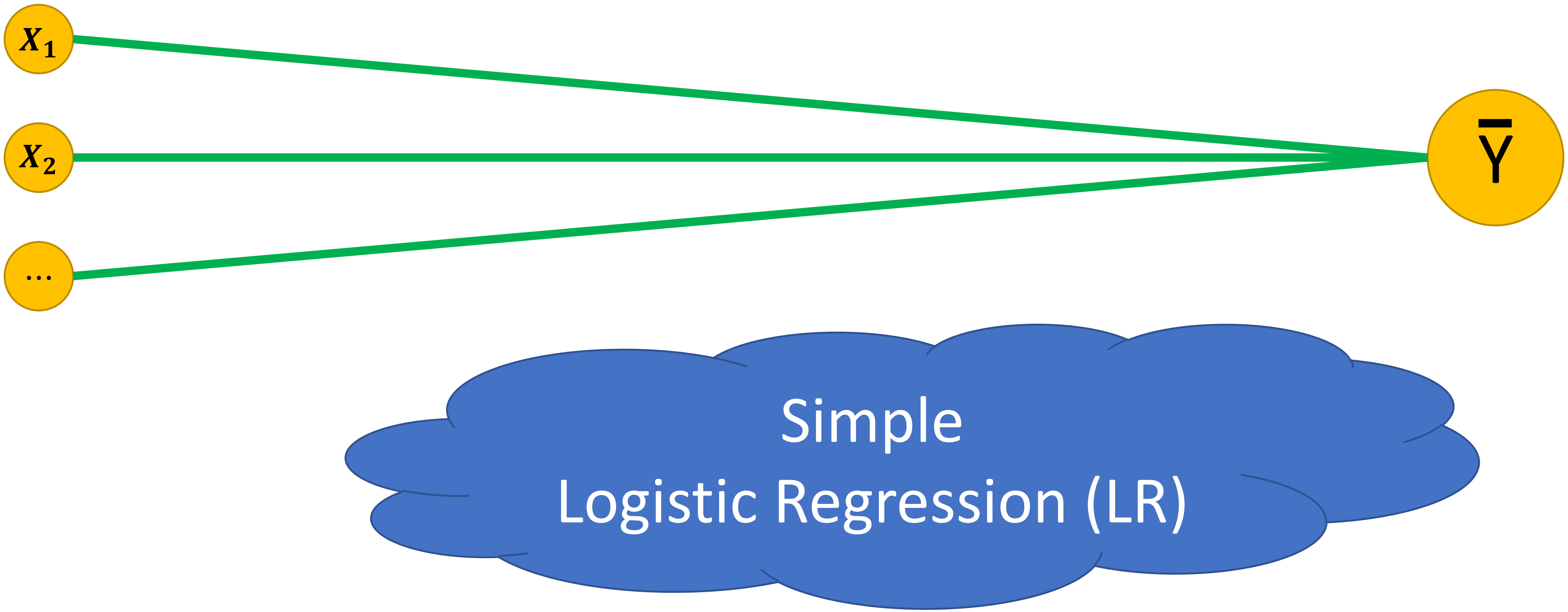
Activation Functions



What would happen without activation func?



What would happen without activation func?



What are the parameters?

What are the hyper-parameters?

Notation

Notation

$$\boldsymbol{z}_i^{[l]} = \sum_j \boldsymbol{W}_{i,j}^{[l]} \boldsymbol{a}_j^{[l-1]} + \boldsymbol{B}_i^{[l]}$$

$$\boldsymbol{a}_i^{[l]} = \boldsymbol{f}_{act}^{[l]}\left(\boldsymbol{z}_i^{[l]}\right)$$

Notation

$\boldsymbol{W}^{[l]}$: Weights in layer l

$\boldsymbol{B}^{[l]}$: Bias in layer l

$\boldsymbol{Z}^{[l]}$: Linear outcome in layer l

$\boldsymbol{f}_{act}^{[l]}$: Activation func. in layer l

$\boldsymbol{A}^{[l]}$: Full outcome in layer l

$$\boldsymbol{Z}^{[l]} = \boldsymbol{W}^{[l]} . \boldsymbol{A}^{[l-1]} + \boldsymbol{B}^{[l]}$$

$$\boldsymbol{A}^{[l]} = \boldsymbol{f}_{act}^{[l]}(\boldsymbol{Z}^{[l]})$$

Notation

$$Z^{[l]} = W^{[l]}.A^{[l-1]} + B^{[l]}$$

$$A^{[l]} = f_{act}^{[l]}(Z^{[l]})$$

$n^{[l]}$: #nodes in layer l

$W^{[l]}$: Weights in layer l

$W^{[l]}: (n^{[l]}, n^{[l-1]})$

$B^{[l]}$: Bias in layer l

$B^{[l]}: (n^{[l]})$

$Z^{[l]}$: Linear outcome in layer l

$Z^{[l]}: (n^{[l]}, n_s)$

$f_{act}^{[l]}$: Activation func. in layer l

$A^{[l]}$: Full outcome in layer l

$A^{[l]}: (n^{[l]}, n_s)$

Notation

$$\boldsymbol{Z}^{[l]} = \boldsymbol{W}^{[l]} . \boldsymbol{A}^{[l-1]} + \boldsymbol{B}^{[l]}$$

$$\boldsymbol{A}^{[l]} = \boldsymbol{f}_{act}^{[l]}(\boldsymbol{Z}^{[l]})$$

$$\boldsymbol{W}^{[l]} : \left(n^{[l]}, n^{[l-1]}\right)$$

$$\boldsymbol{B}^{[l]} : \left(n^{[l]}\ \right)$$

$$\boldsymbol{Z}^{[l]} : \left(n^{[l]}, n_s\right)$$

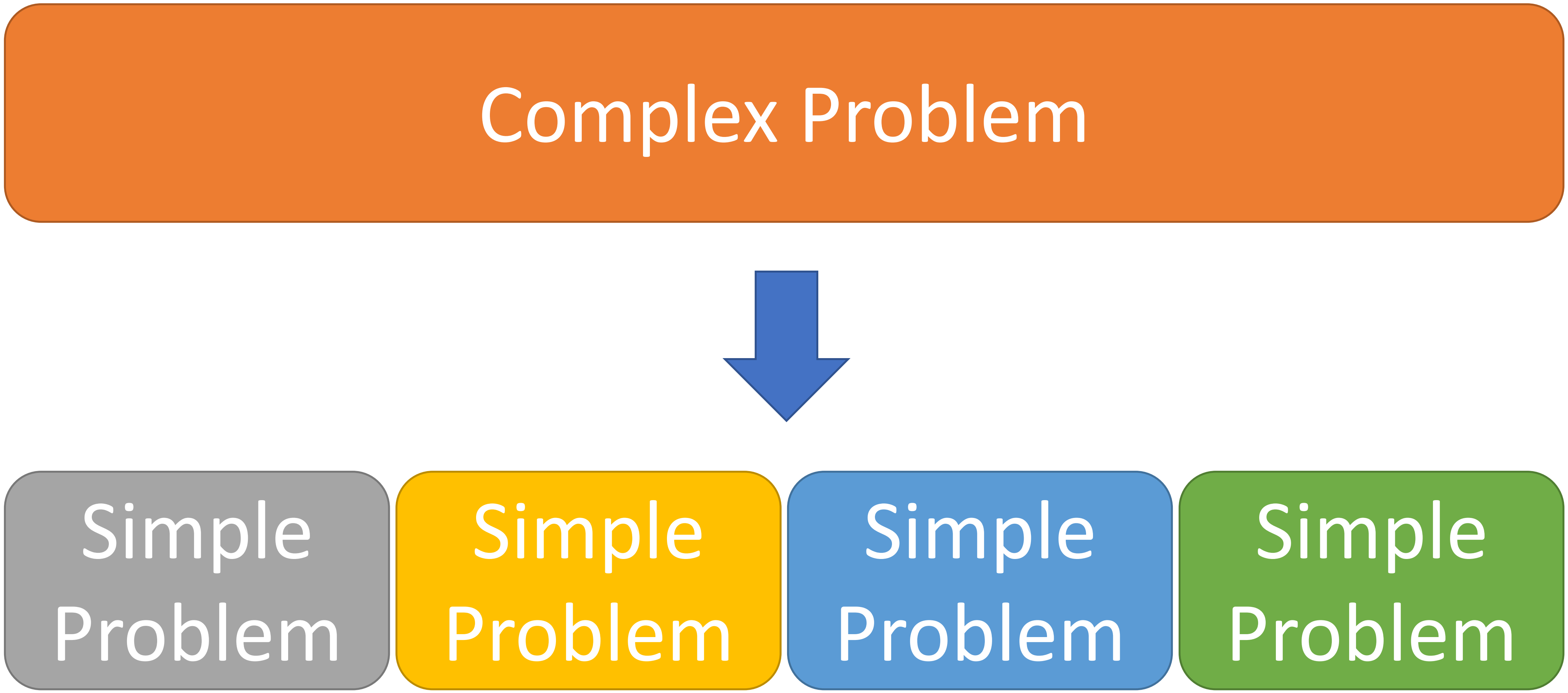
$$\boldsymbol{A}^{[l]} : \left(n^{[l]}, n_s\right)$$

Why?

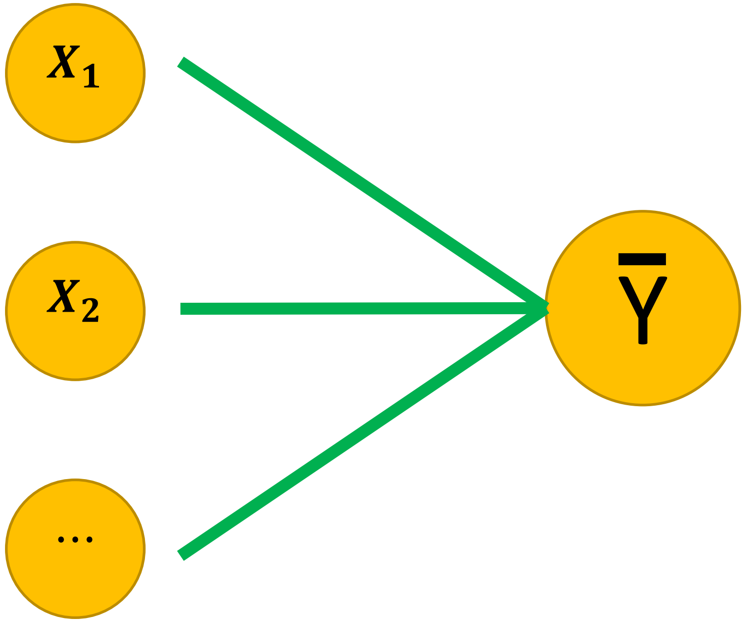
The Logic of using a layered model

Why do we need to do layers?

Reductionism: how we solve problems …



Let’s take a step back and take a look at Logistic Regression.



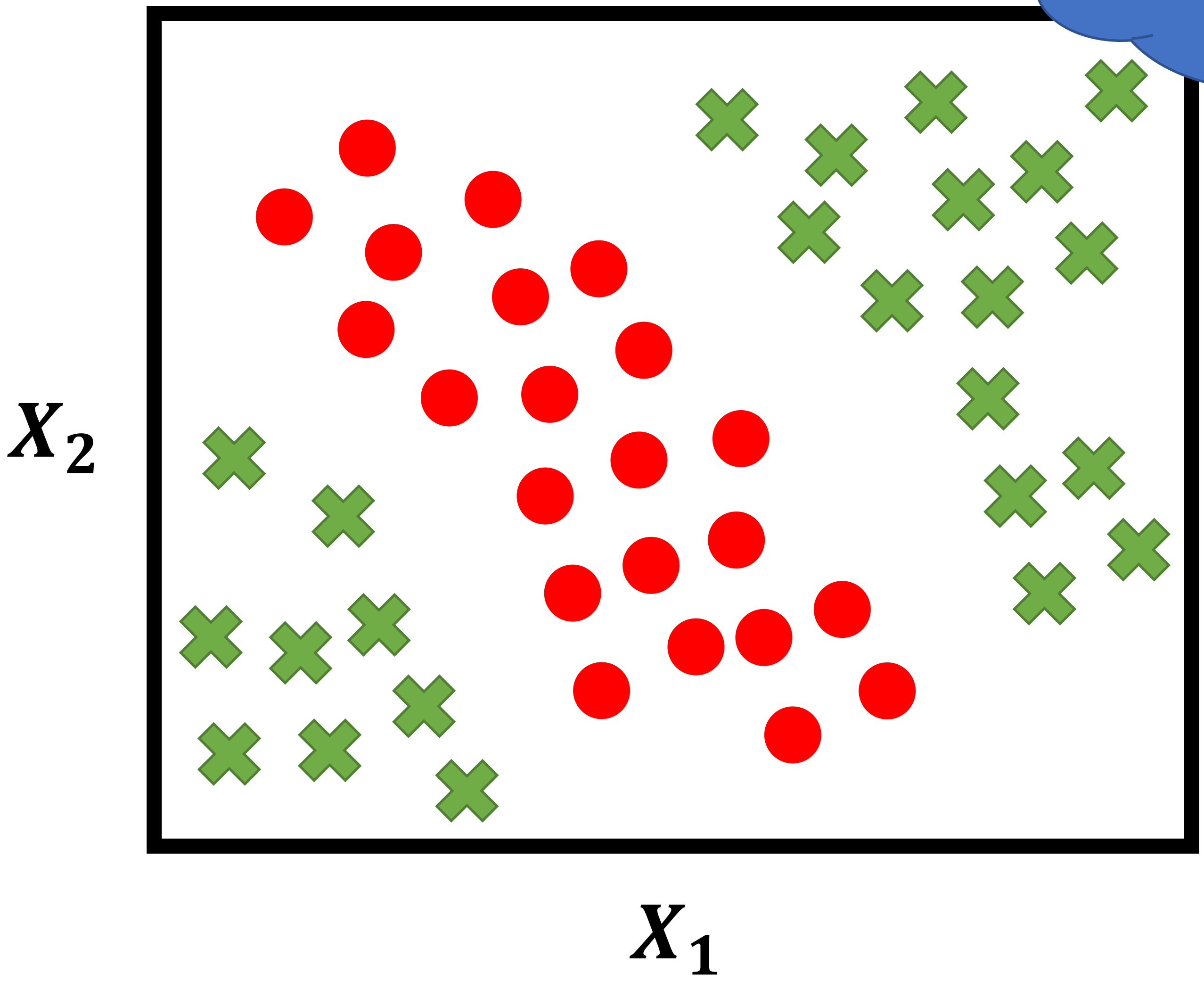
$$= \text{sigmoid}\left(\sum_{j} \boldsymbol{W}_{j}\ \boldsymbol{X}_{j}\right)$$

Linear

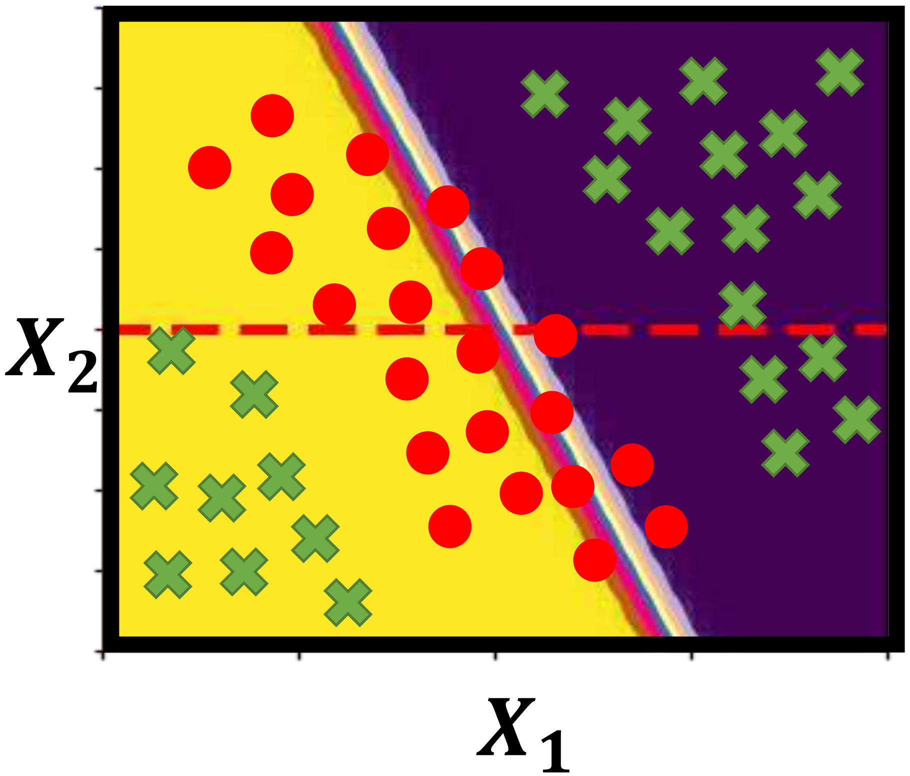
Consider the following classification

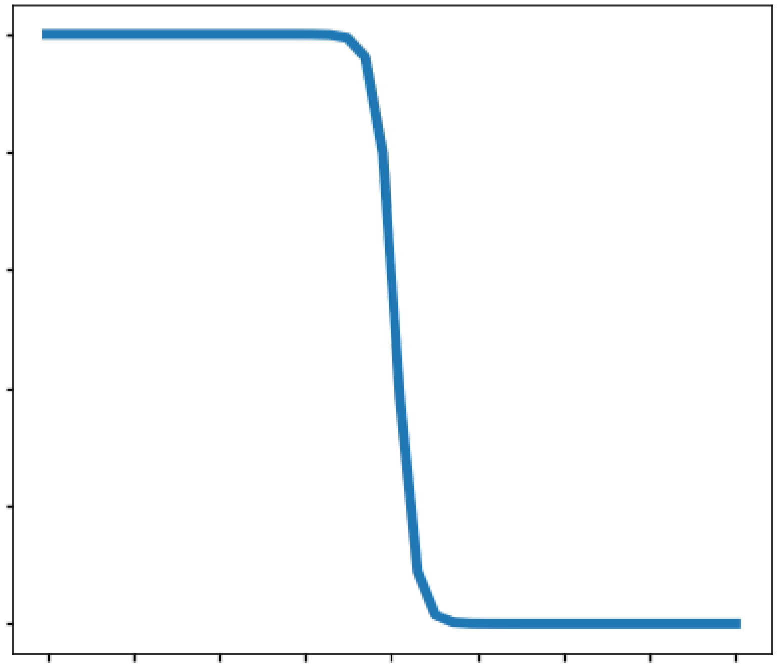
Example

How well would LR do on this?

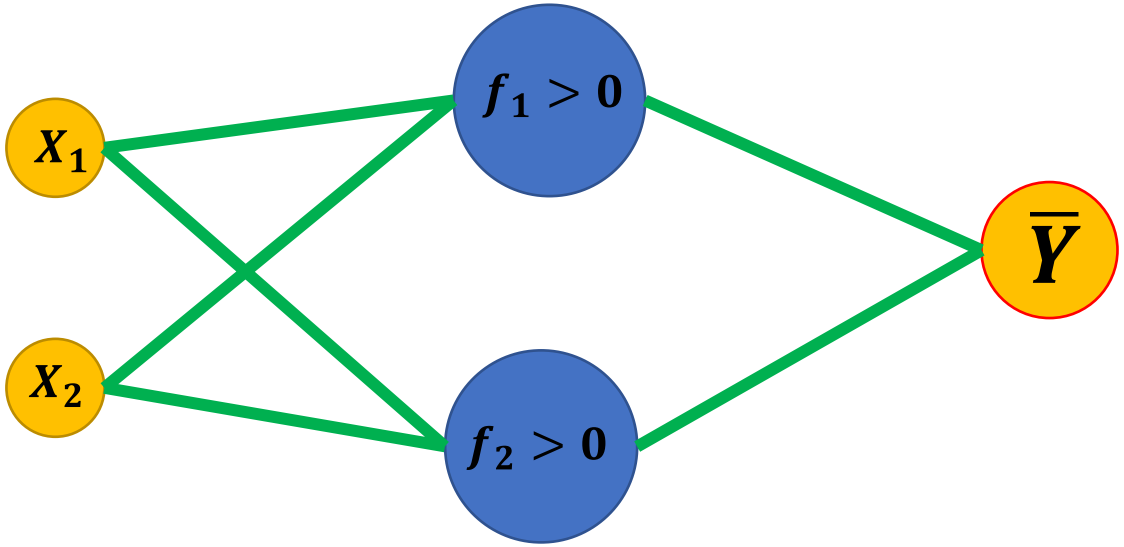


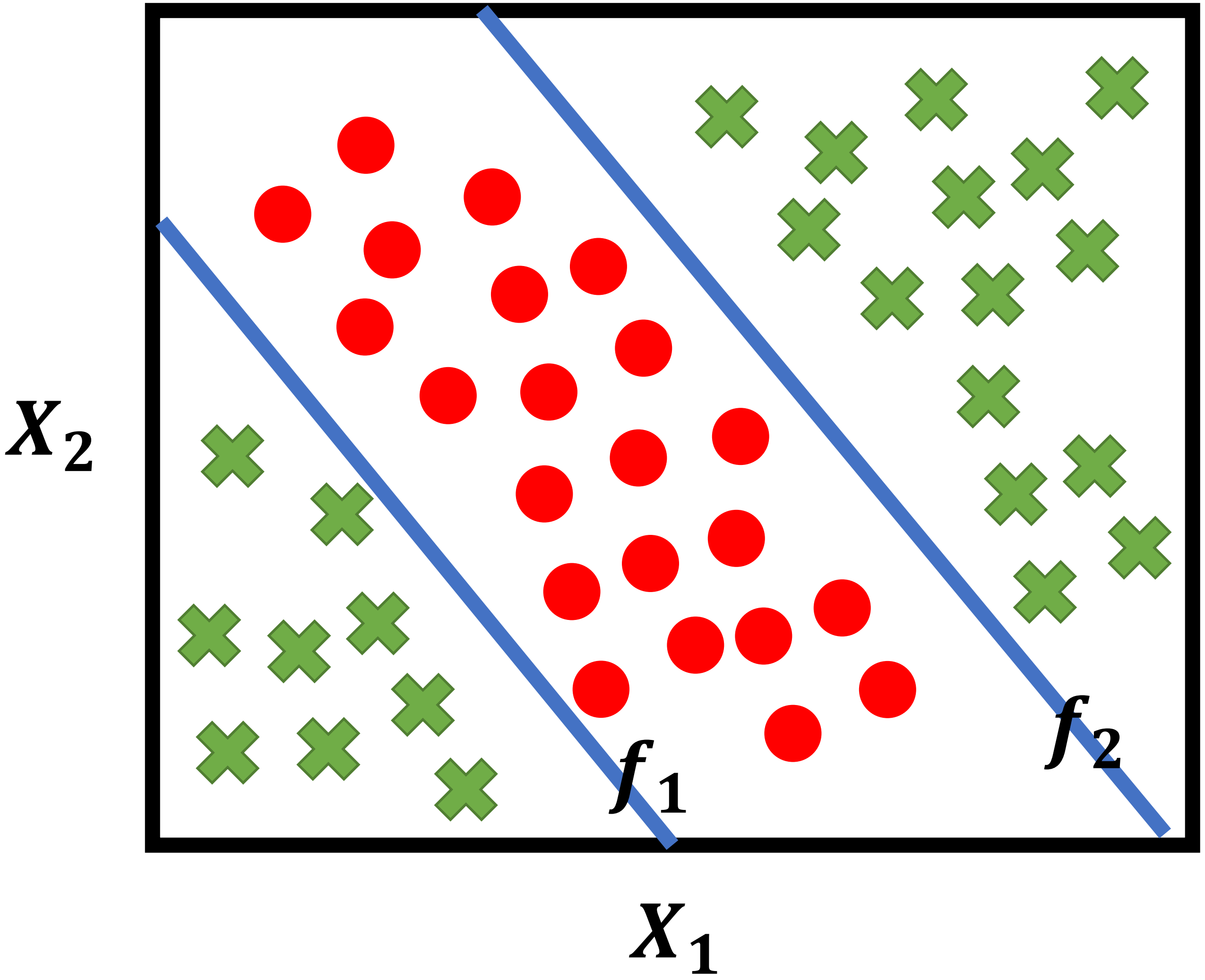
Example





Example: what is the solution





Example: NMR spectrum

Universality of NN:

Universal approximation theorem

- Hornik, Kurt; Tinchcombe, Maxwell; White, Halbert (1989). *Multilayer Feedforward Networks are Universal Approximators*. *Neural Networks*. **2**. Pergamon Press. pp. 359–366.

Universality of NN:

- Arbitrary width and Sigmoid, George Cybenko 89

Depth

- Enough depth, can reduce the width to n+c

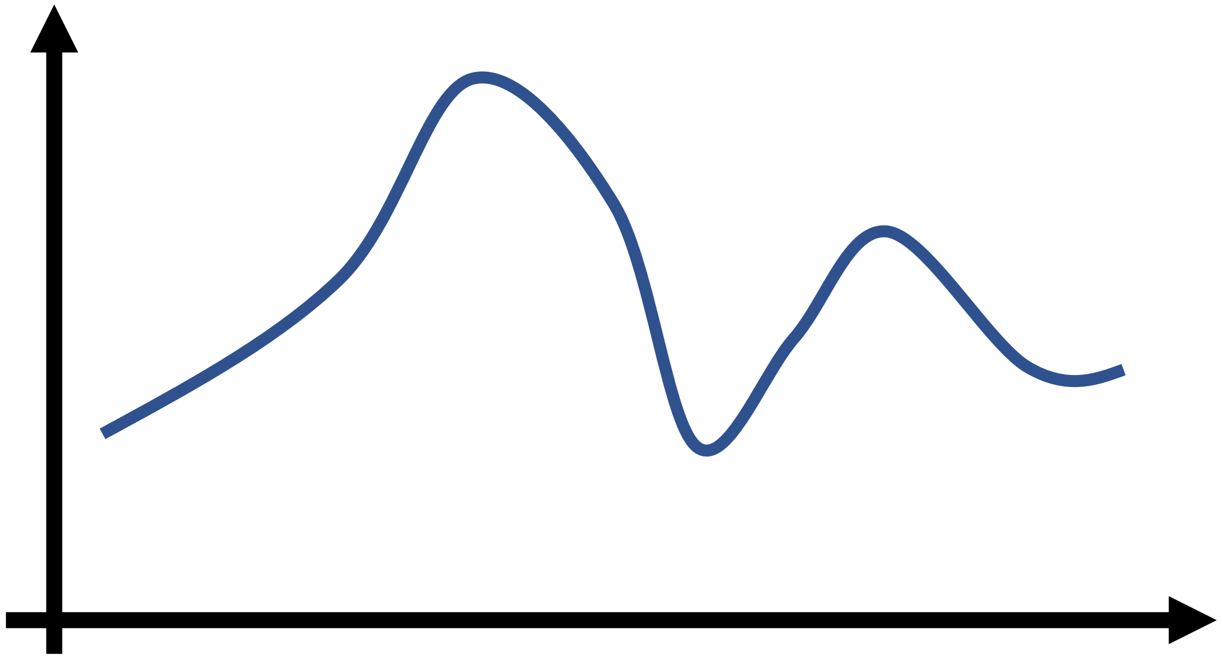
Activation Funciton

- Any activation function, Kurt Hornik 91
- Non-polynomial activation func are universal, Moshe Leshno et al 93

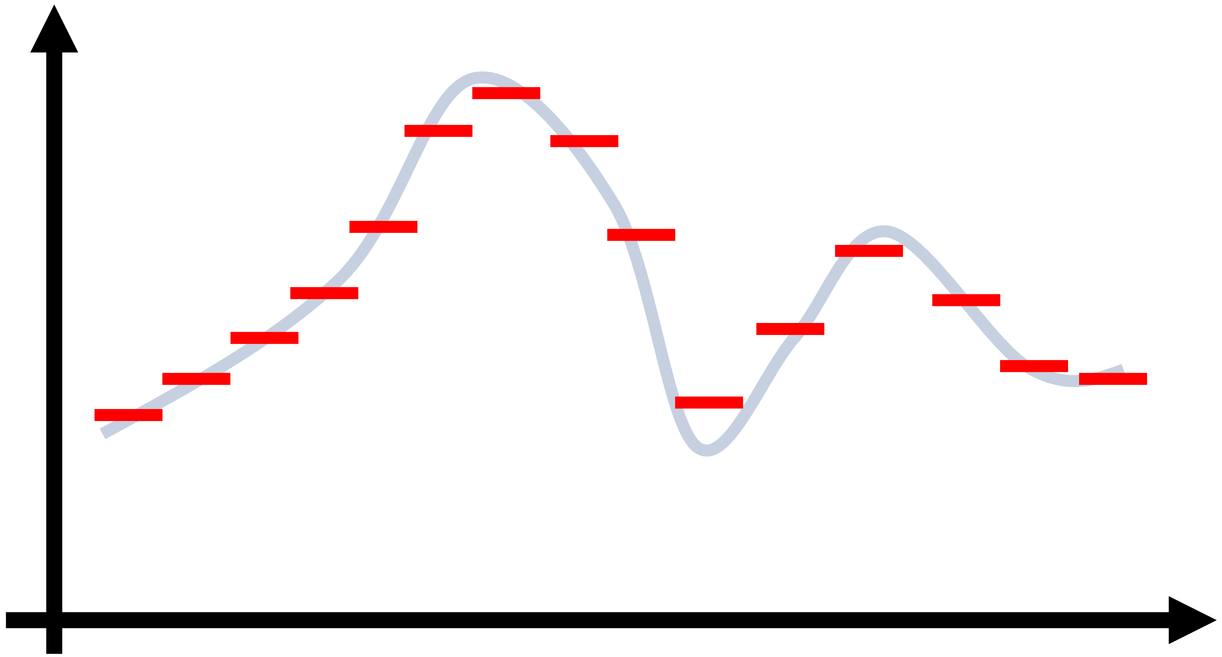
[1905.08539] Universal Approximation with Deep Narrow Networks (arxiv.org)

Universal approximation theorem - Wikipedia

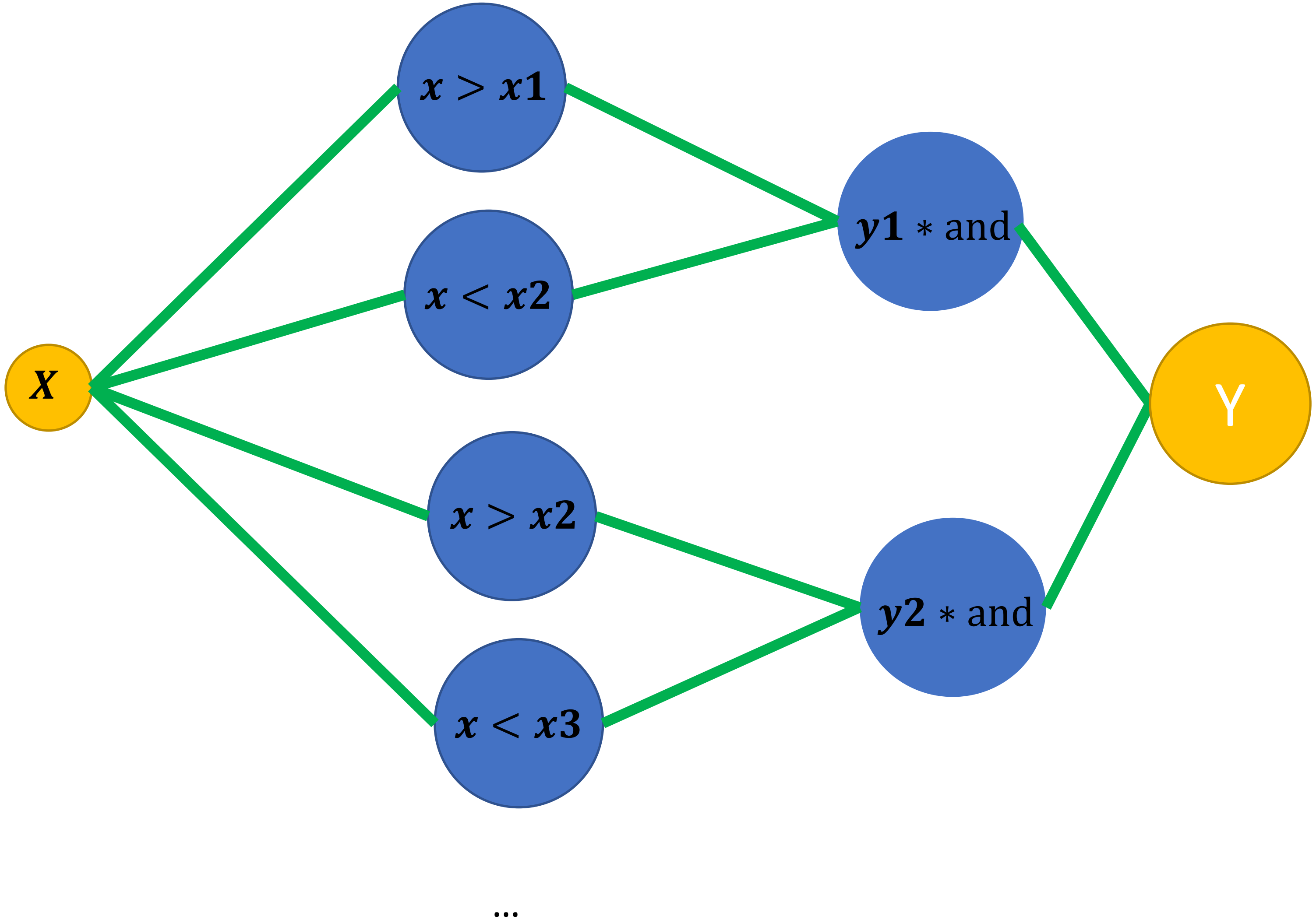
Universality of NN: Intuition

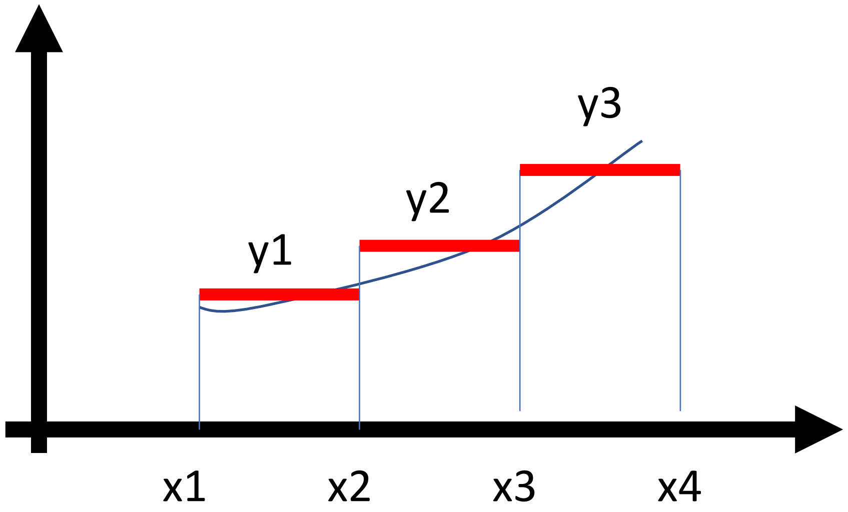


Universality of NN: Intuition



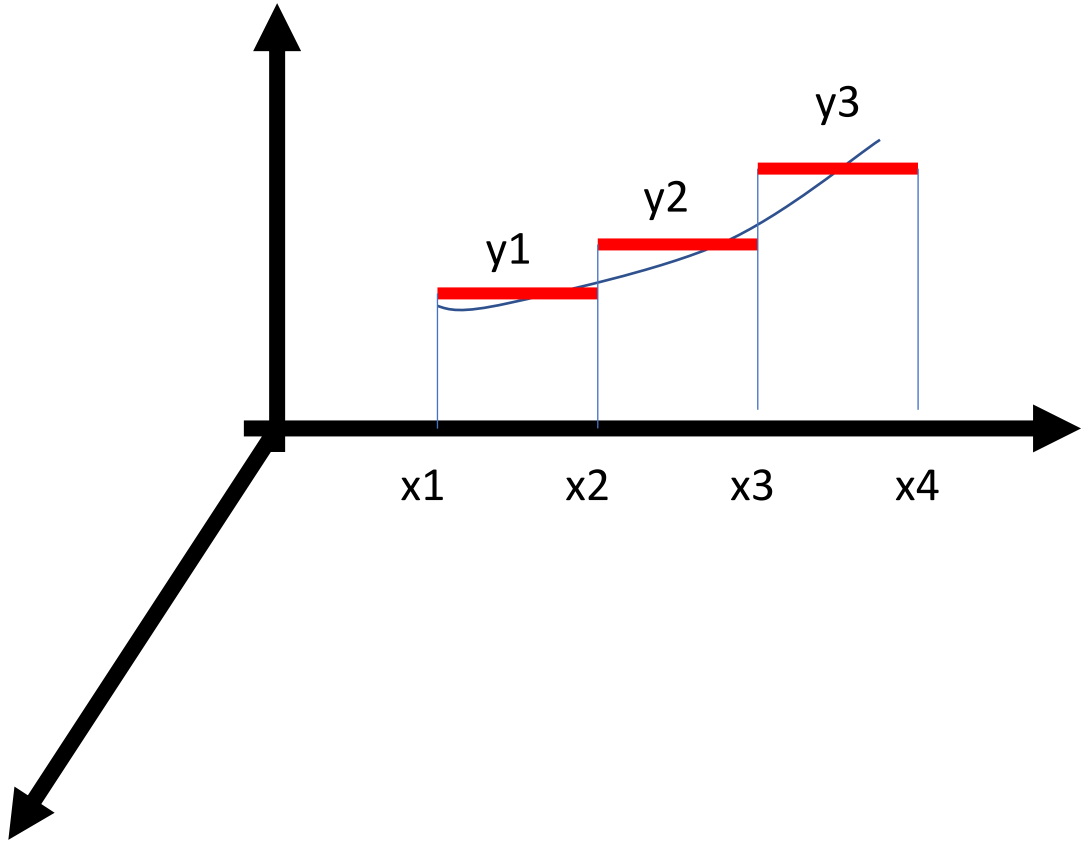
Universality of NN: Intuition





How does the depth help?

How does the number of features affect this?



What does the universality tell us?

Bias

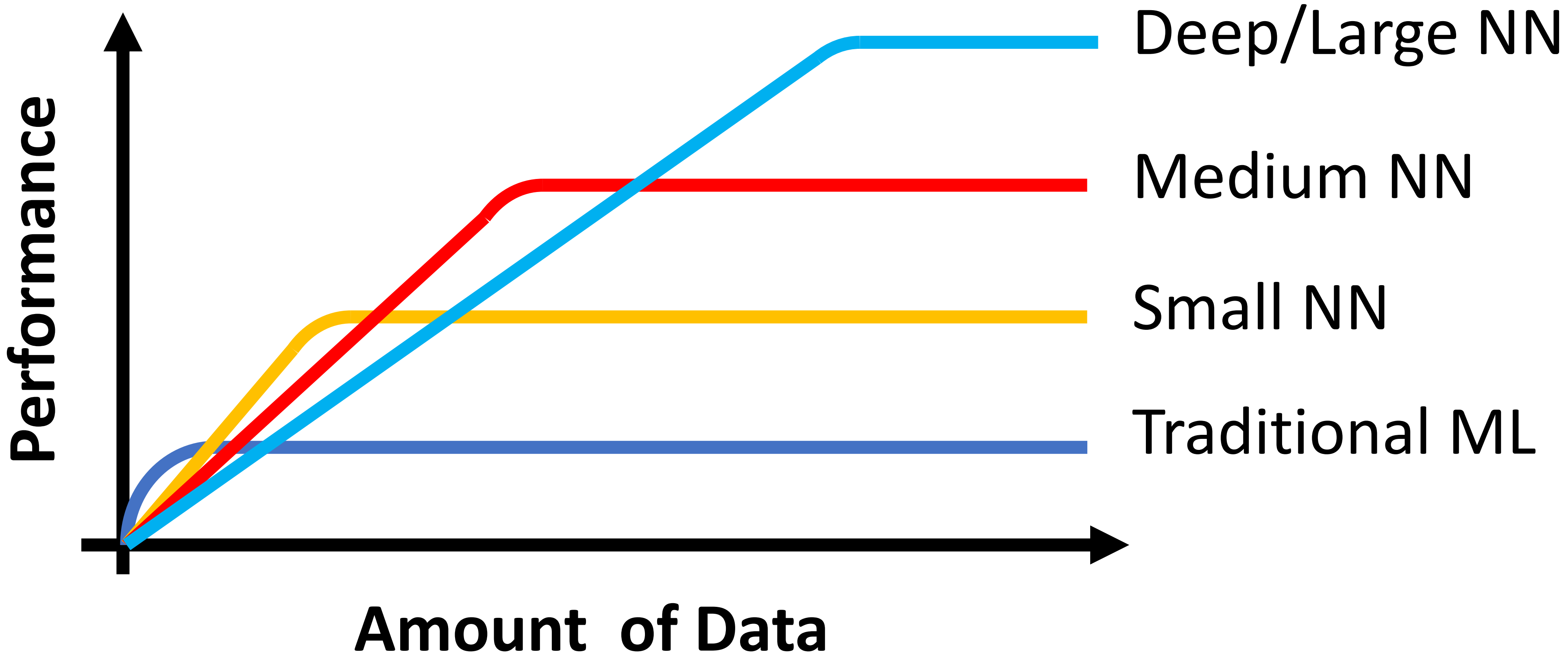
can be **arbitrary small**

if we allow for **enough number of nodes or depth**.

What do you think is going to happen to variance?

How can we deal with the increase in variance?

Data for NN


Deep/Large NN
Medium NN
Small NN
Traditional ML
Performance
Amount of Data

Summary

- Introduced NN
- Notation
- Universality of NN

Next …