Lecture 2: Neural Networks Design

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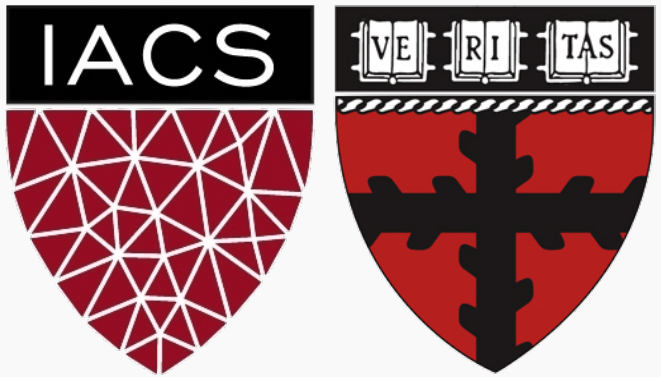
Institute for Applied Computational Science
Harvard

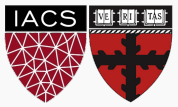


Outline

Anatomy of a NN

Design choices

- Activation function
- Loss function
- Output units
- Architecture
- Optimizer



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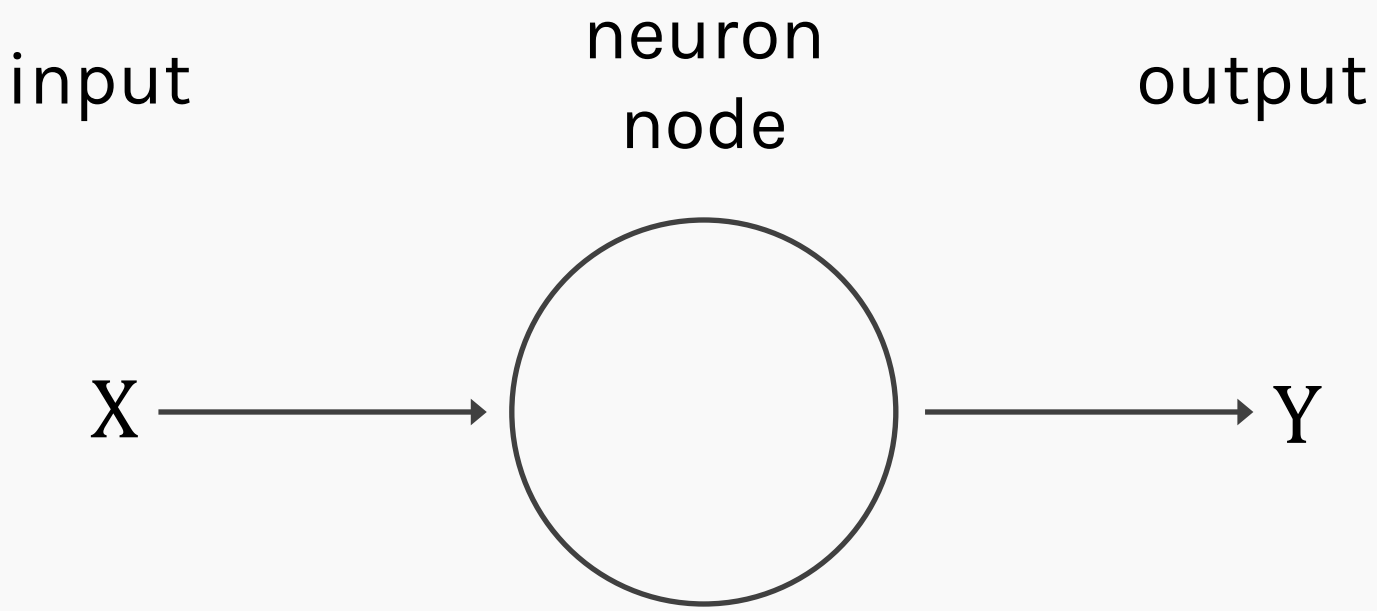
Anatomy of artificial neural network (ANN)



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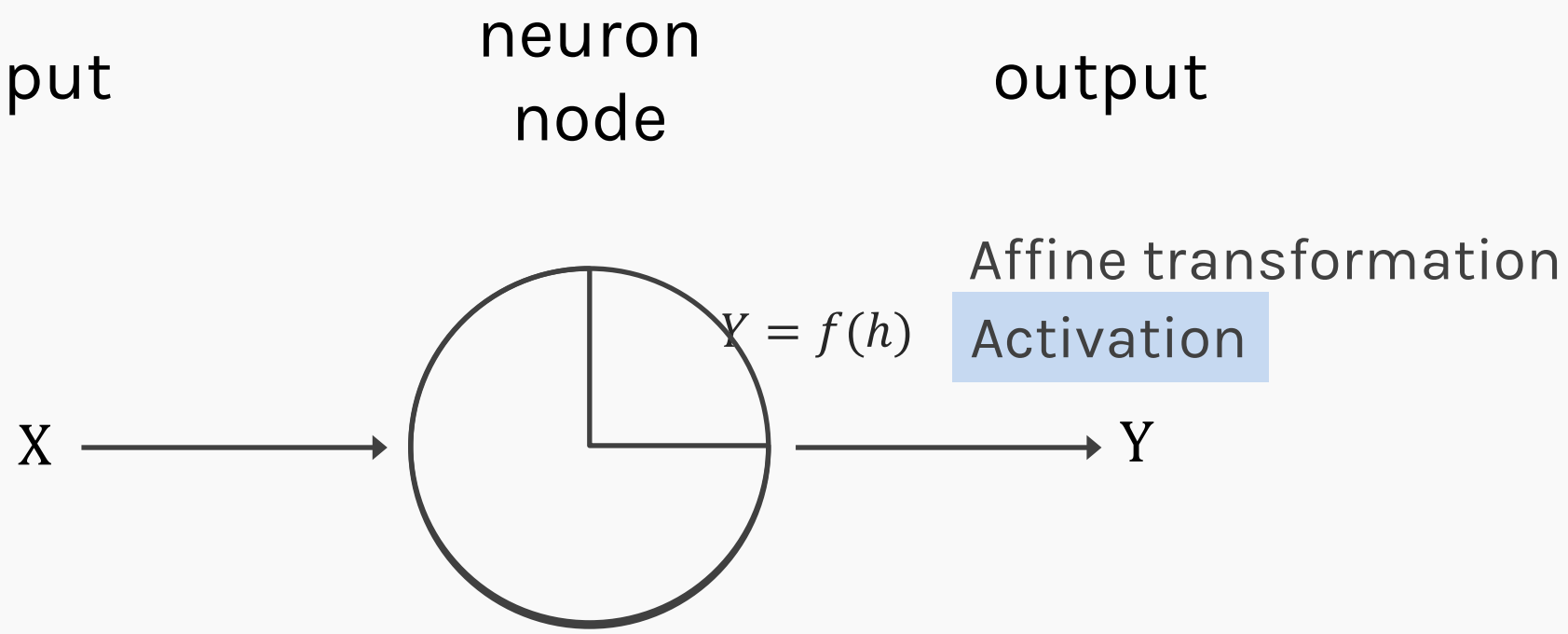

We will talk later about the choice of activation function. So far we have only talked about sigmoid as an activation function but there are other choices.

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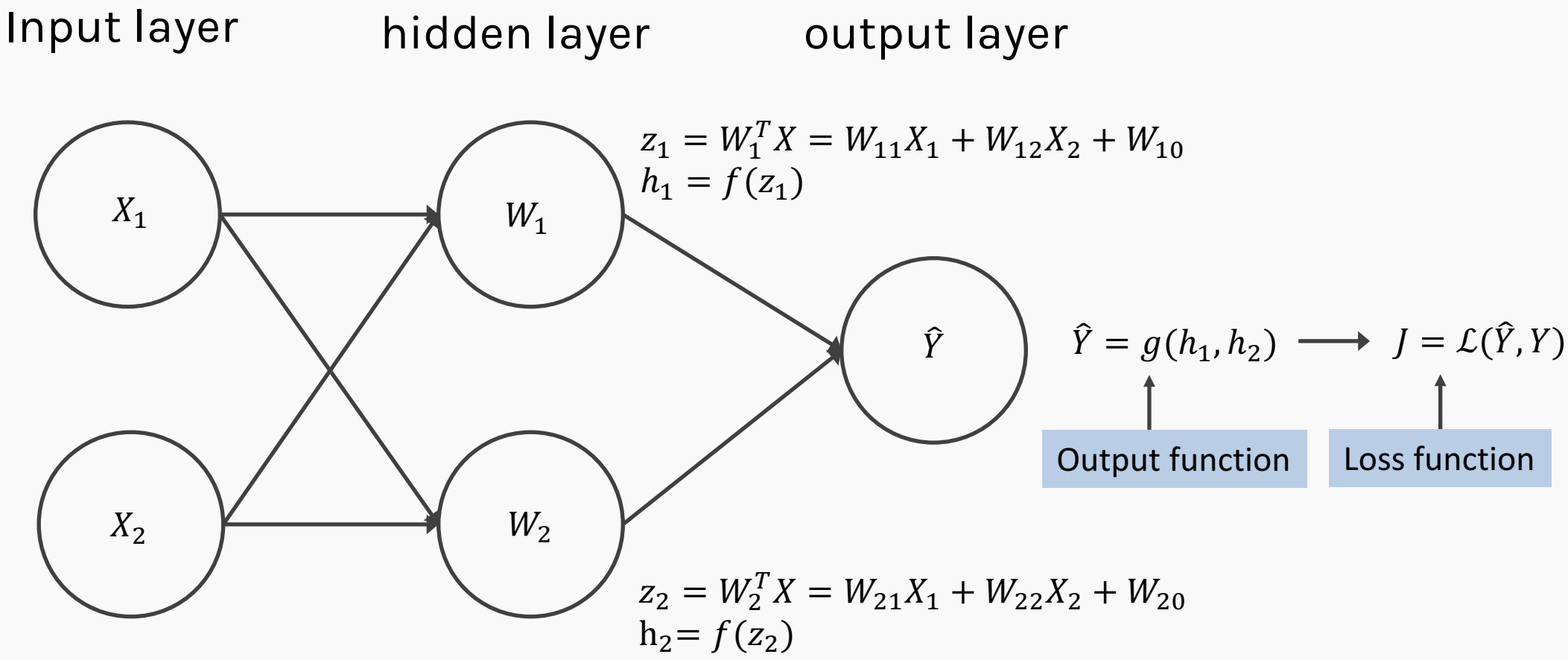

We will talk later about the choice of the output layer and the loss function. So far we consider sigmoid as the output and log-bernouli.

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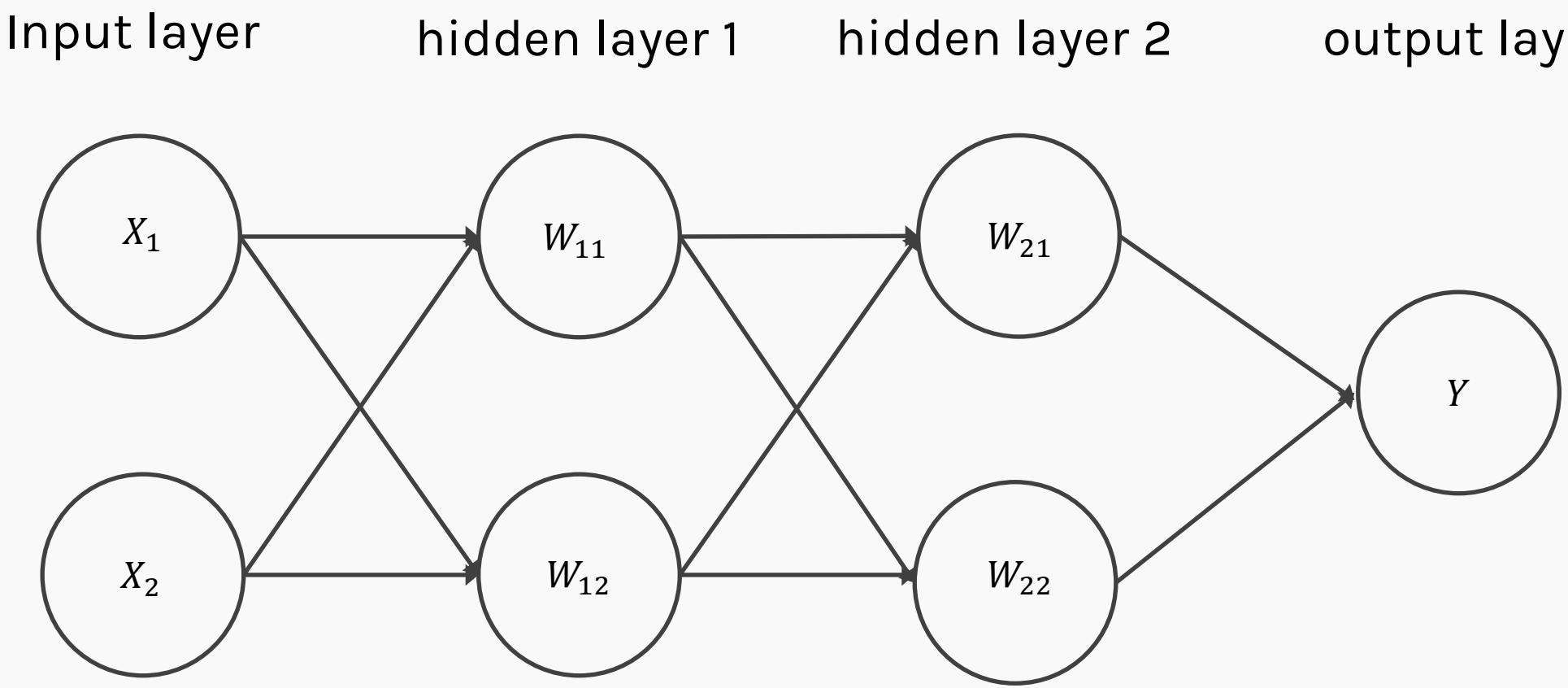

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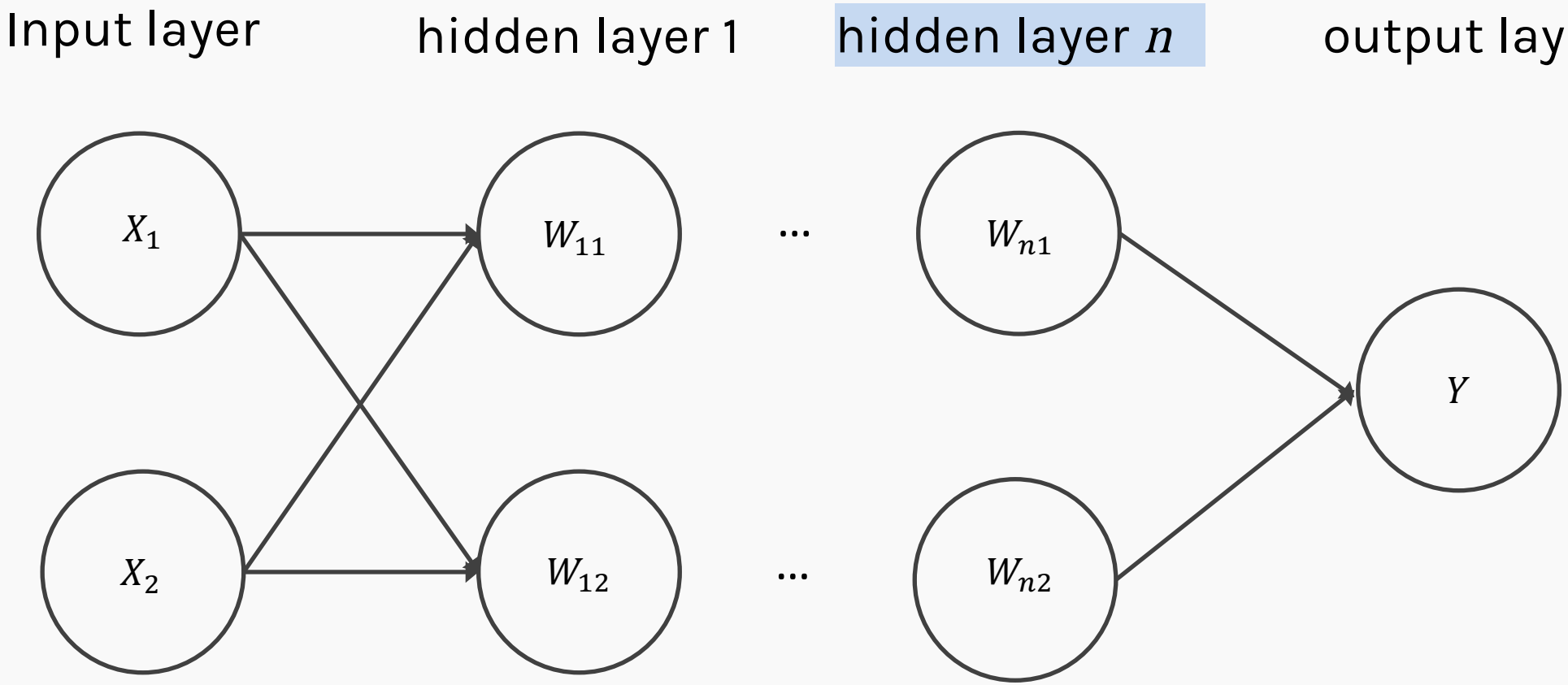


We will talk later about the choice of the number of layers.

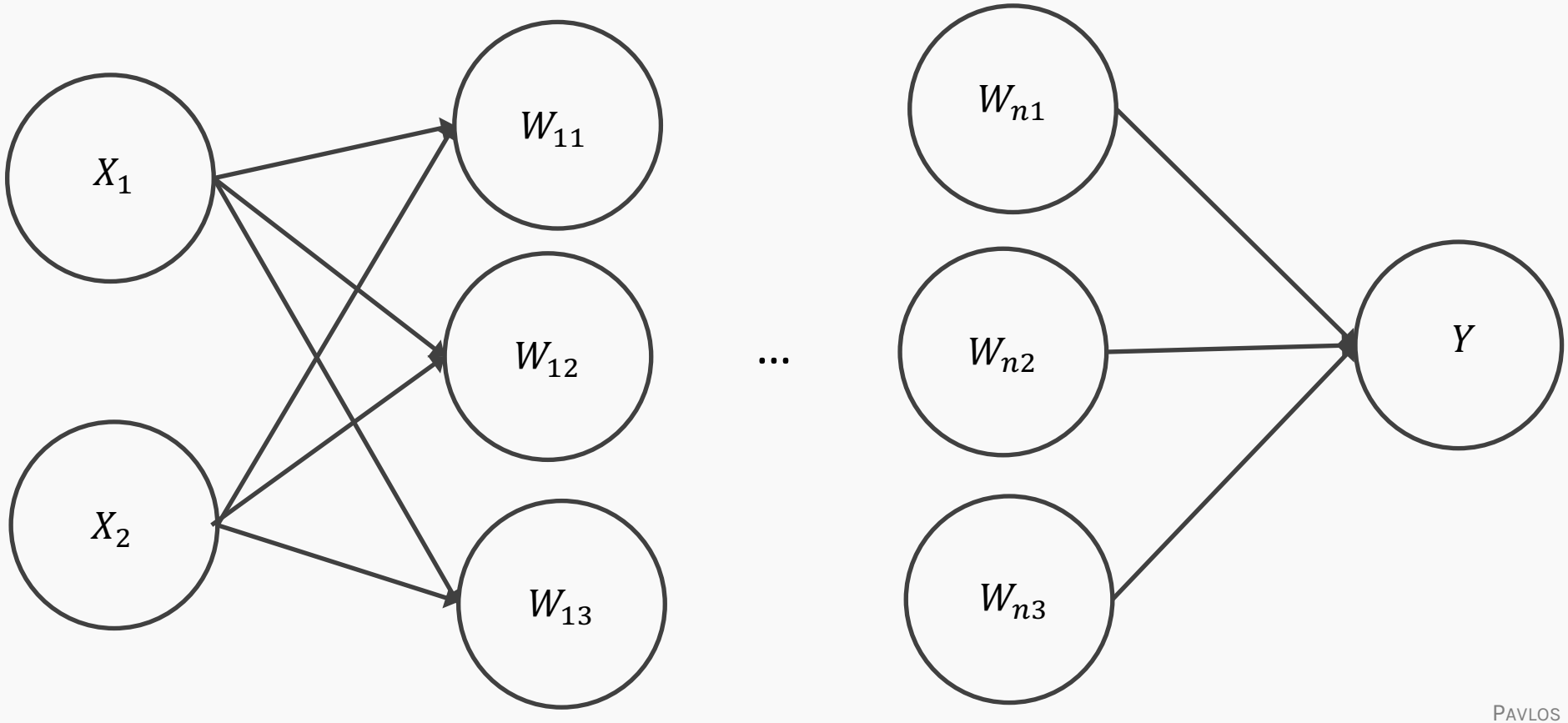
Anatomy of artificial neural network (ANN)

Input layer

hidden layer 1,
3 nodes

hidden layer n
3 nodes

output layer



Anatomy of artificial neural network (ANN)

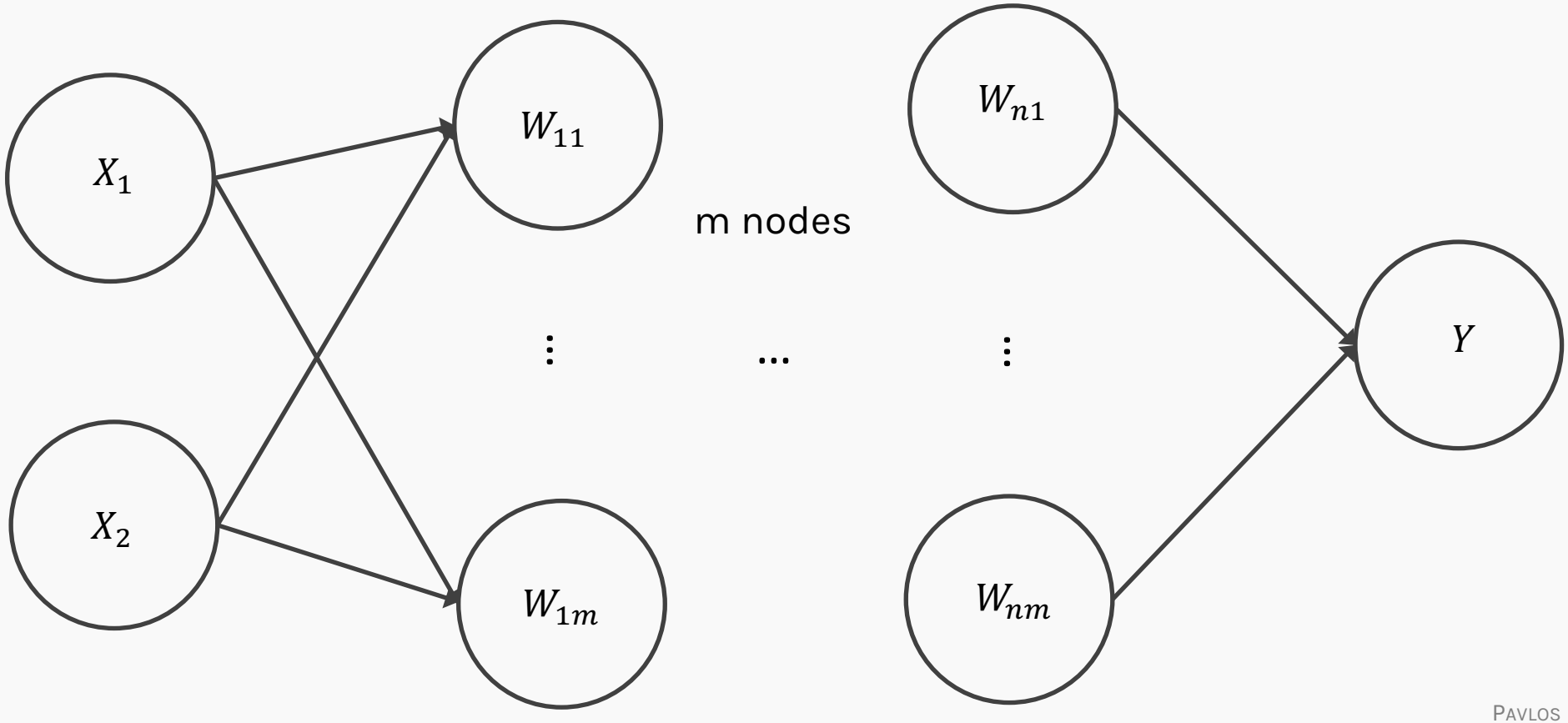
Input layer

hidden layer 1,

m nodes

hidden layer n

output layer



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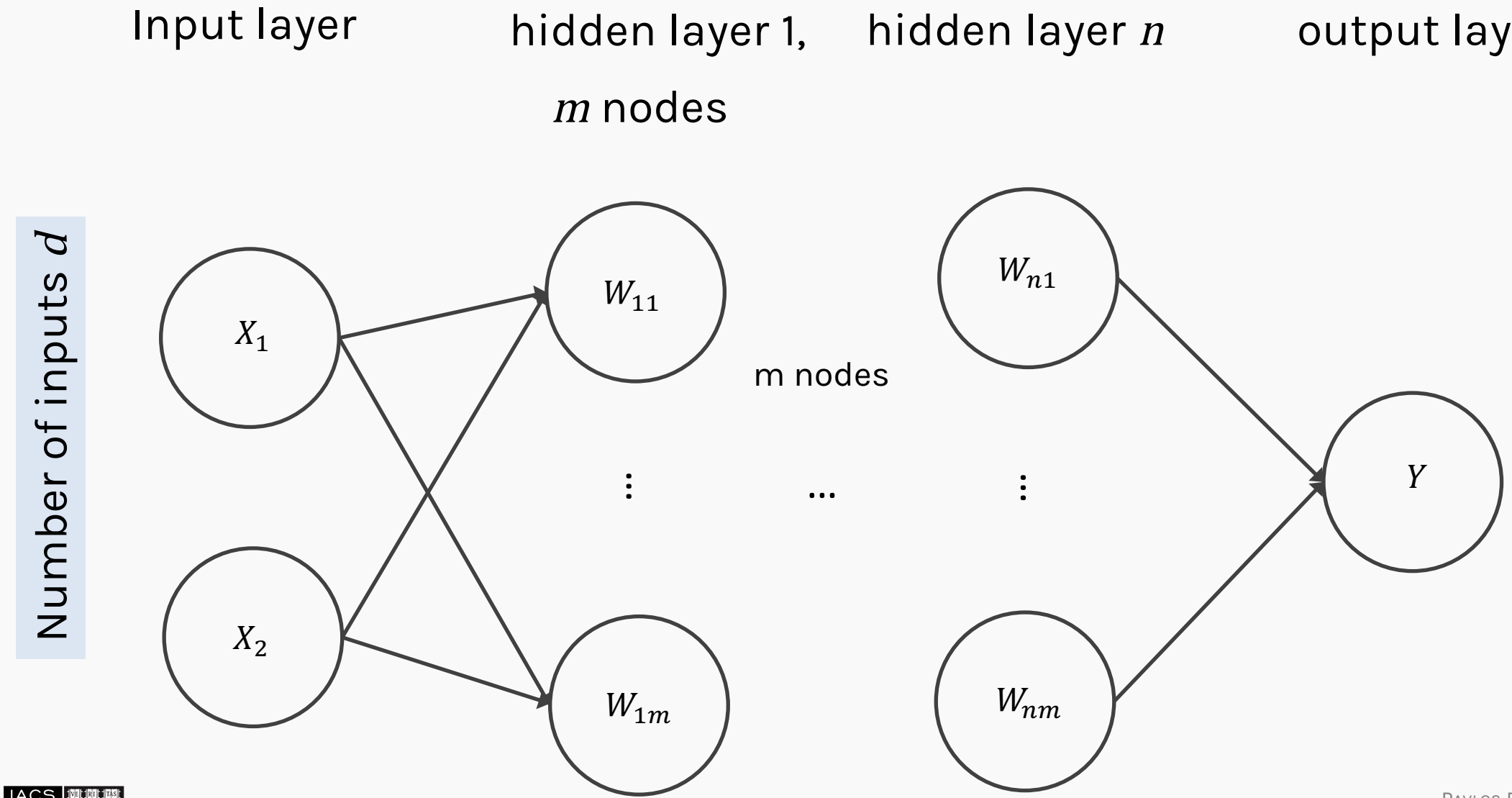
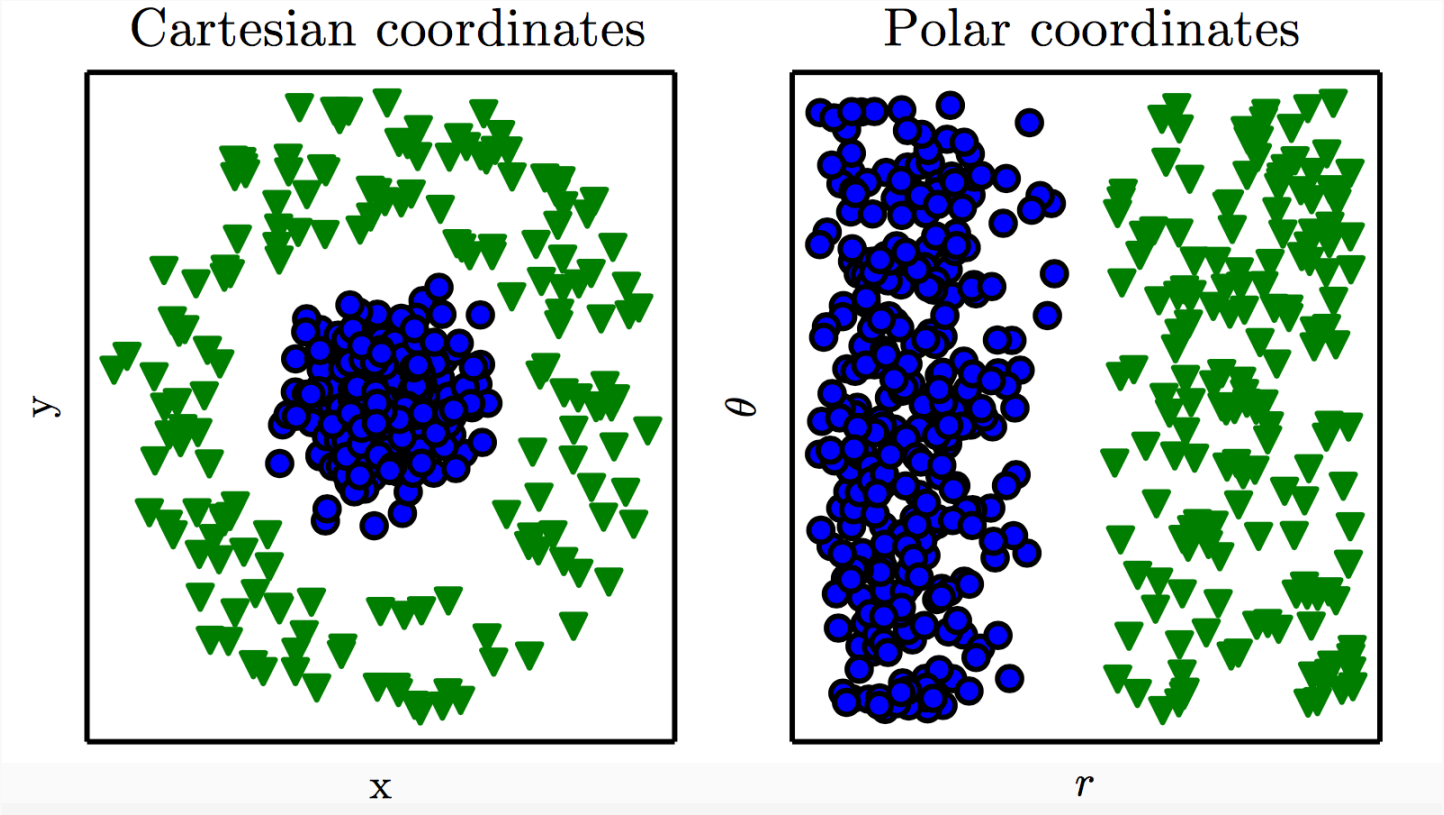


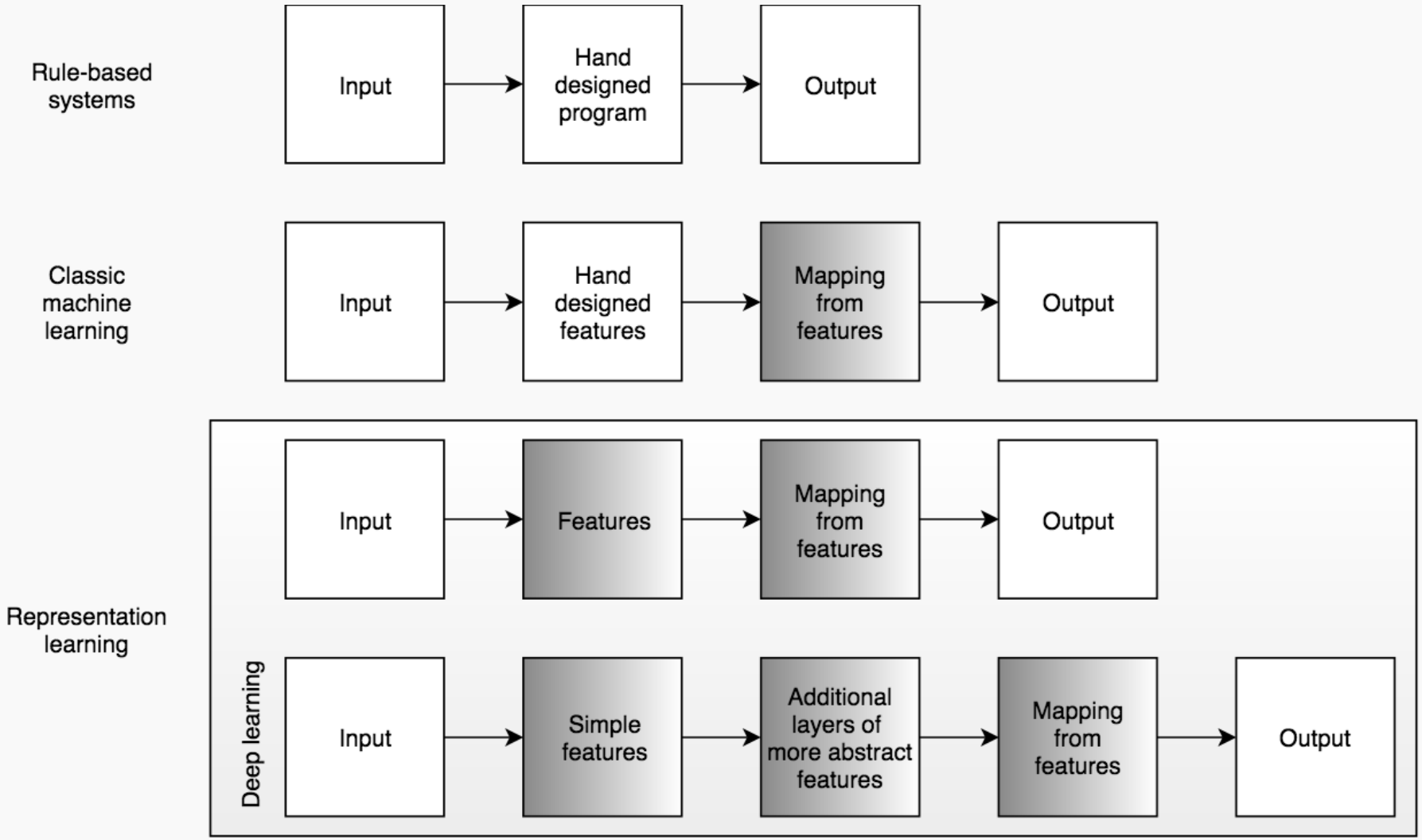
Number of inputs is specified by the data

Why layers? Representation

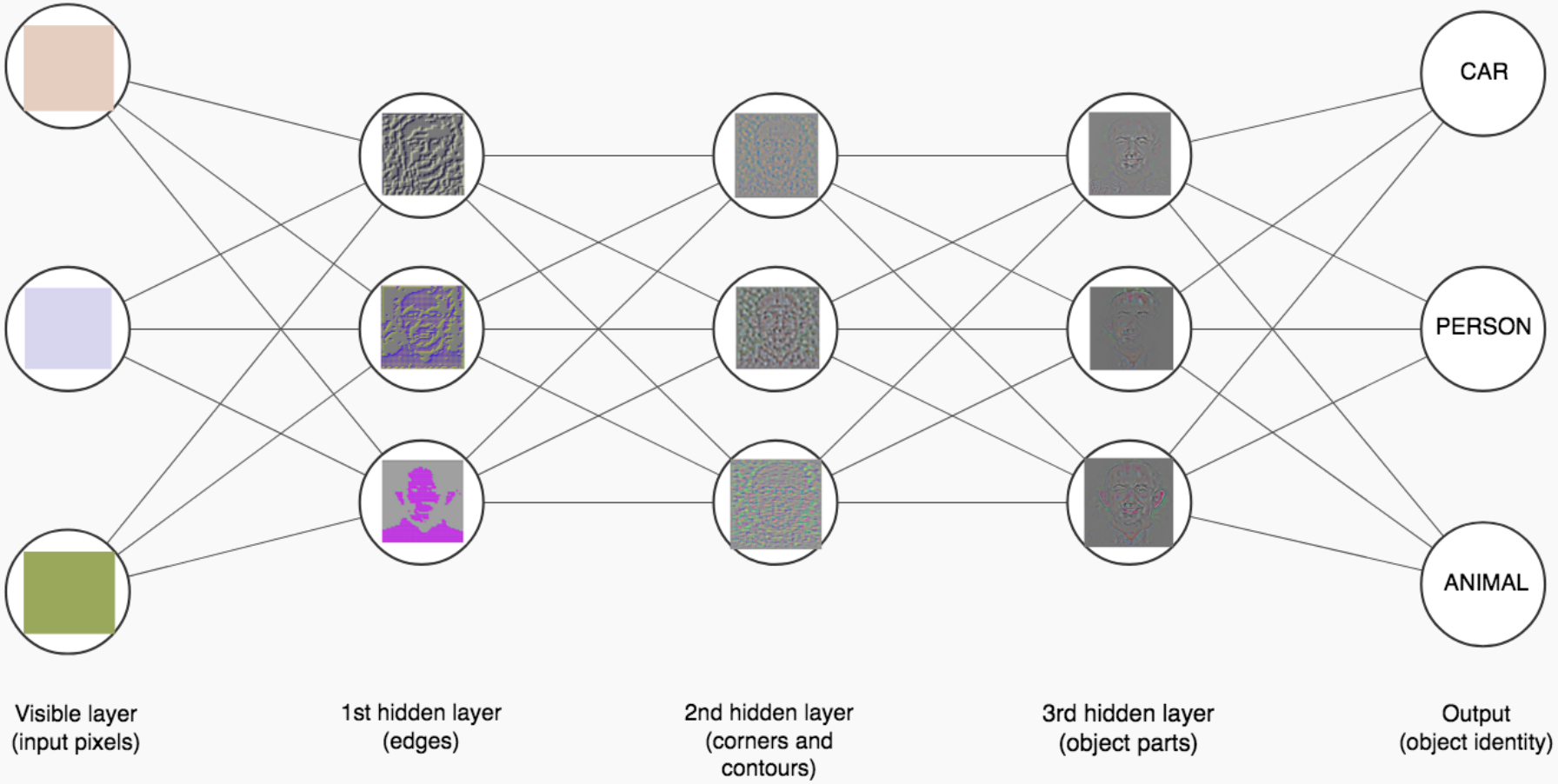
Representation Matters



Learning Multiple Components



Depth = Repeated Compositions



Neural Networks

Hand-written digit recognition: MNIST data

Design Choices

Activation function

Loss function

Output units

Architecture

Optimizer

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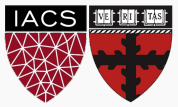


Activation function

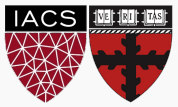
$$h = f(W^T X + b)$$

The activation function should:

- Ensures not linearity
- Ensure gradients remain large through hidden unit

Common choices are

- Sigmoid
- Relu, leaky ReLU, Generalized ReLU, MaxOut
- softplus
- tanh
- swish



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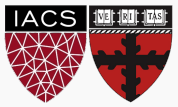

Beyond Linear Models

Linear models

- Can be fit efficiently (via convex optimization)
- Limited model capacity

Alternative:

$$f(x) = w^T \phi(x)$$

Where ϕ is a *non-linear transform*

Traditional ML

Manually engineer ϕ

- Domain specific, enormous human effort

Generic transform

- Maps to a higher-dimensional space
- Kernel methods: e.g. RBF kernels
- Over fitting: does not generalize well to test set
- Cannot encode enough prior information

Deep Learning

- Directly learn ϕ

$$f(x;\theta) = W^T \phi(x;\theta)$$

- where θ are parameters of the transform
- ϕ defines hidden layers
- Non-convex optimization
- Can encode prior beliefs, generalizes well

Activation function

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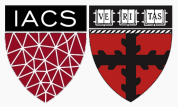
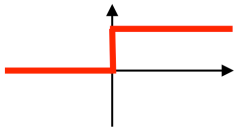
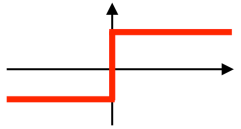
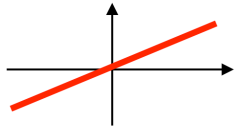
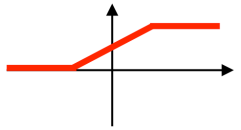
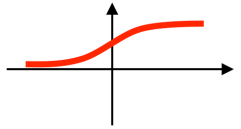
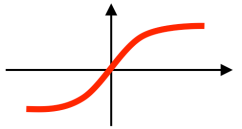
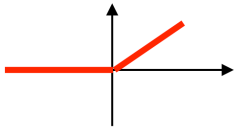
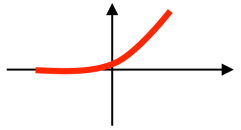
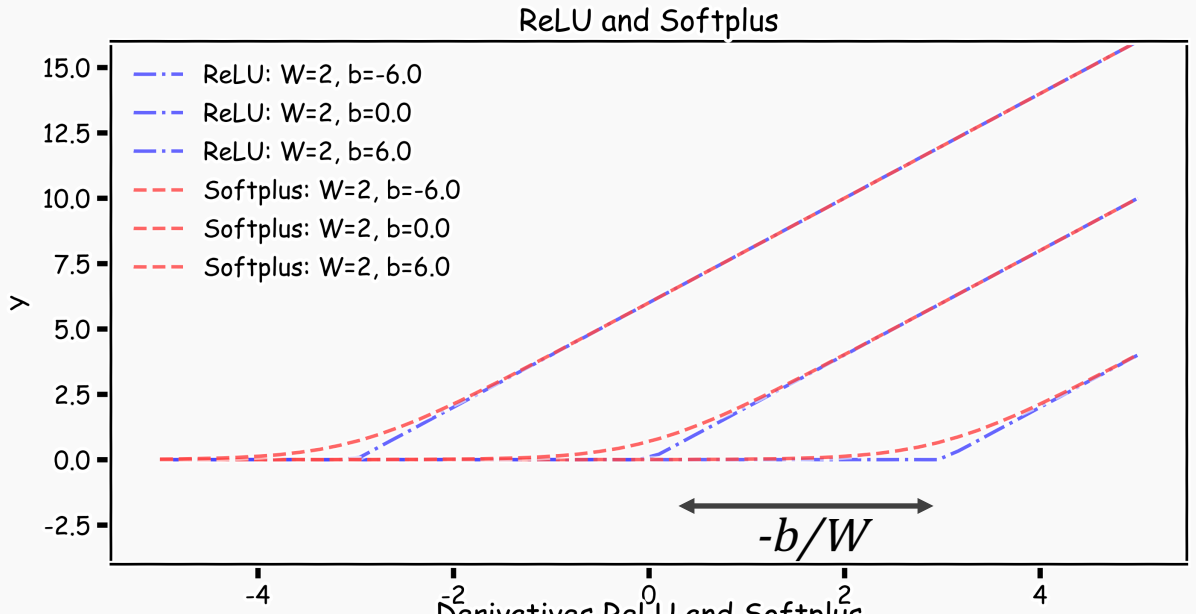
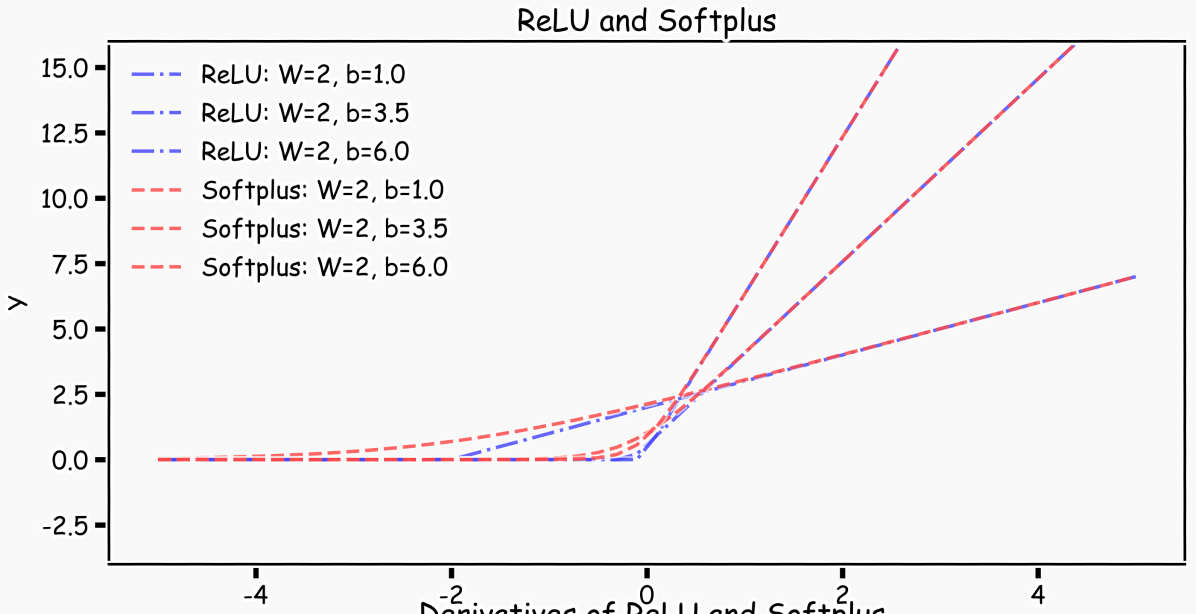
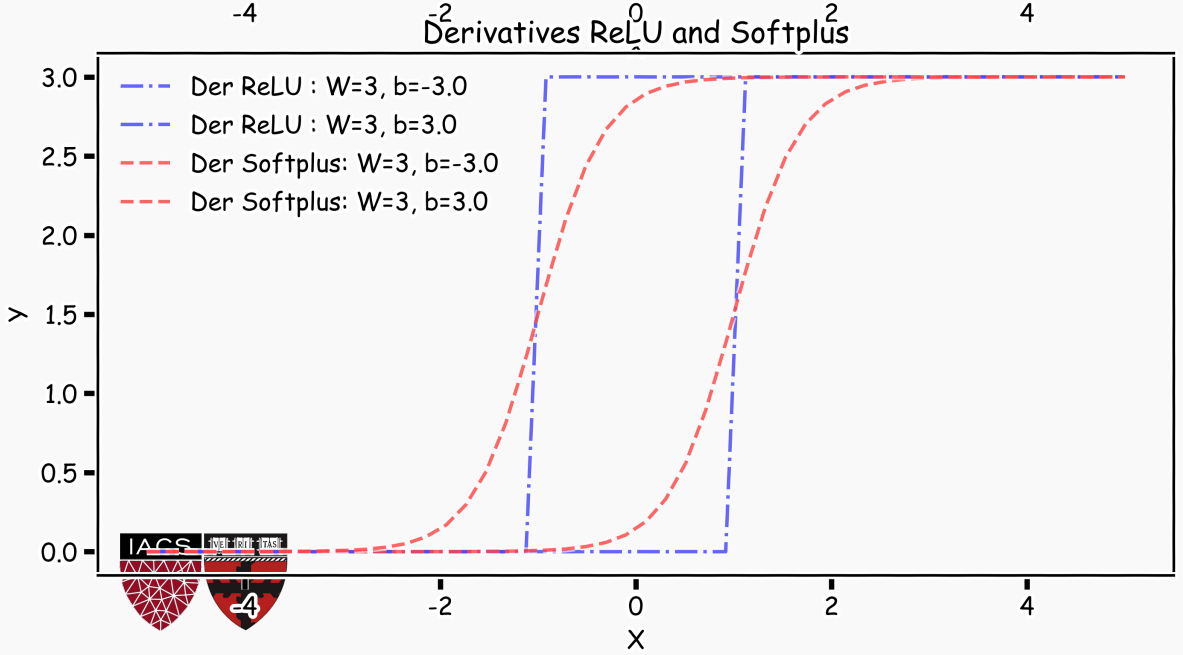


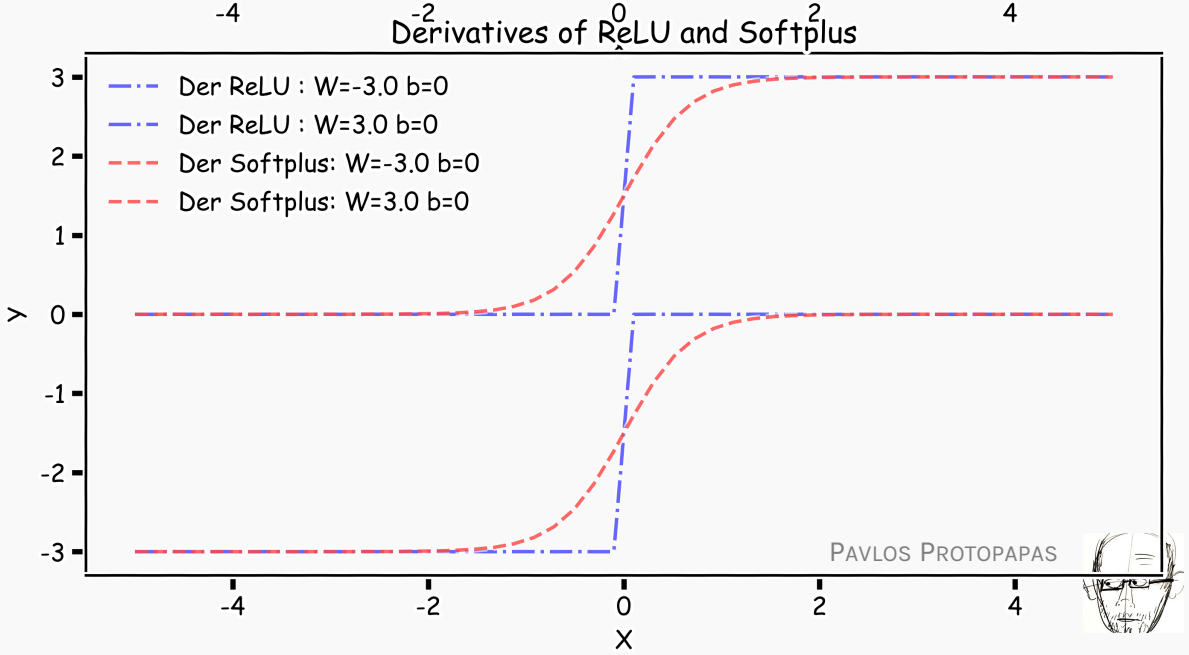
Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 0.5, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}}$	Multi-layer Neural Networks	
Rectifier, ReLU (Rectified Linear Unit)	$\phi(z) = max(0, z)$	Multi-layer Neural Networks	
Rectifier, softplus	$\phi(z) = \ln(1 + e^{z})$	Multi-layer Neural Networks	

Relu and Softplus







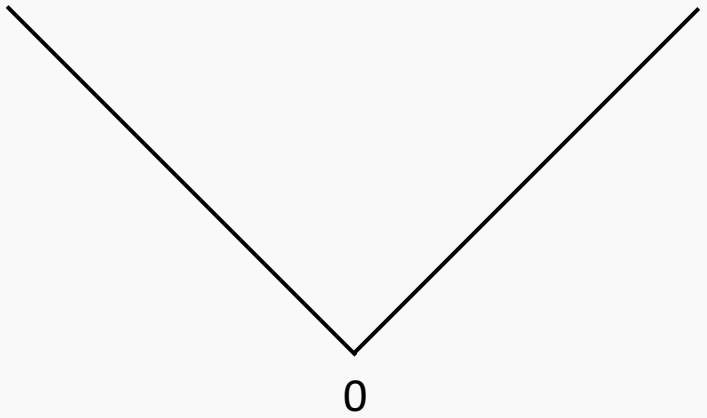


Generalized ReLU

Generalization: For $\alpha_i > 0$

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

E.g. Absolute value ReLU: $\alpha_i = -1 \Rightarrow g(z) = |z|$

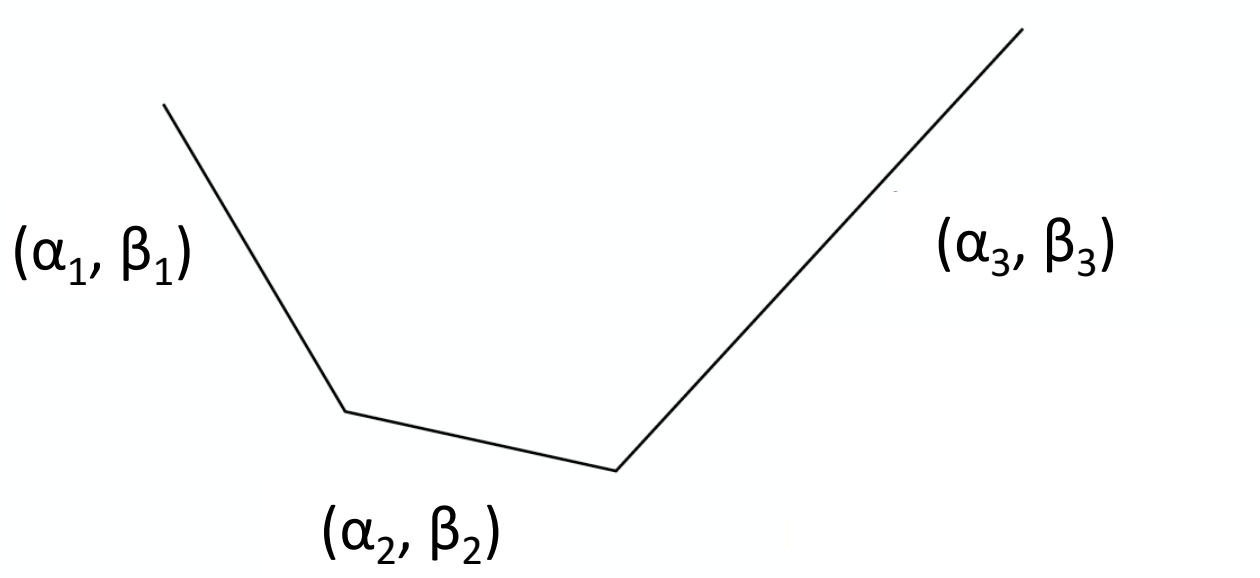


Maxout

Directly learn the activation function

- Max of k linear functions

$$g(z) = \max_{i \in \{1,\ldots,k\}} \alpha_i z_i + \beta_i$$



Design Choices

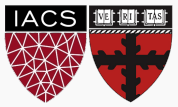
Activation function

Loss function

Output units

Architecture

Optimizer



Loss Function

Cross-entropy between training data and model distribution (i.e. negative log-likelihood)

$$J(W) = -\mathbb{E}_{x,y\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(\text{y}|\text{x})$$

Do not need to design separate loss functions.

Gradient of cost function must be large enough

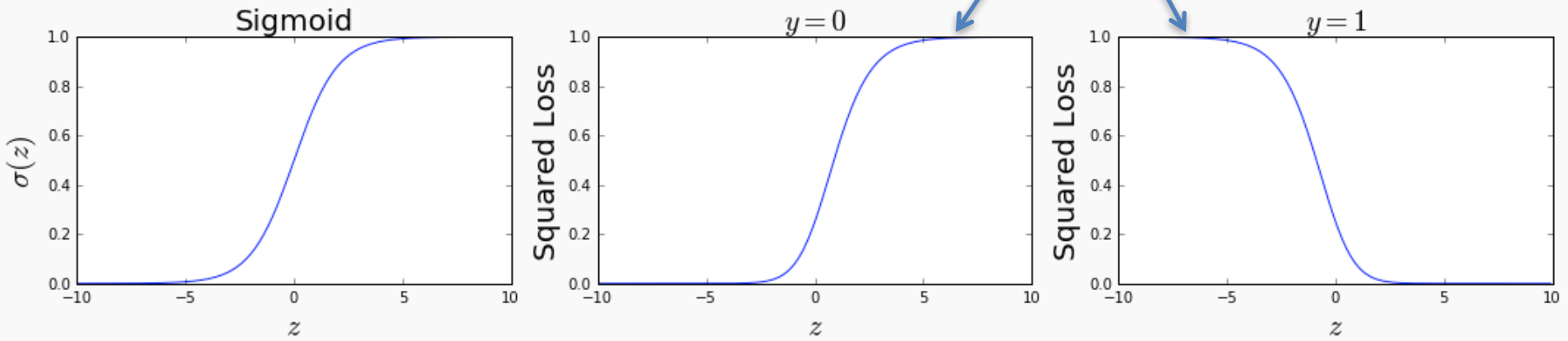
Cost Function

Example: sigmoid output + squared loss

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

$$L_{sq}(y,z) = (y - \sigma(z))^2$$

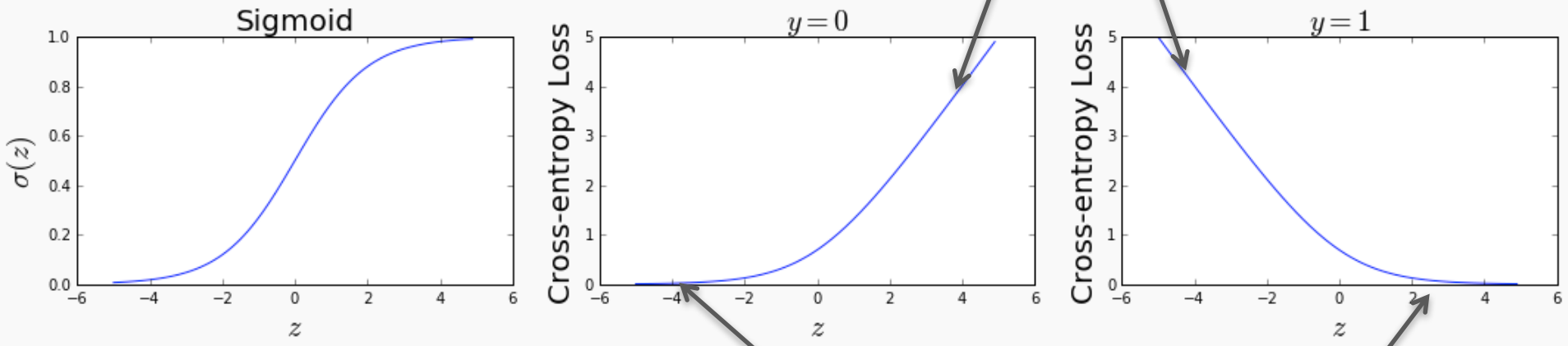
Flat surfaces



Cost Function

Example: sigmoid output + cross-entropy loss

$$L_{ce}(y,z) = -(y\log(z) + (1-y)\log(1-z))$$



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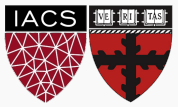
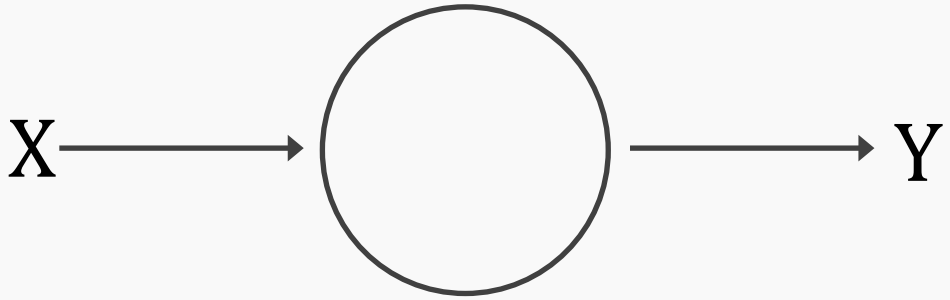


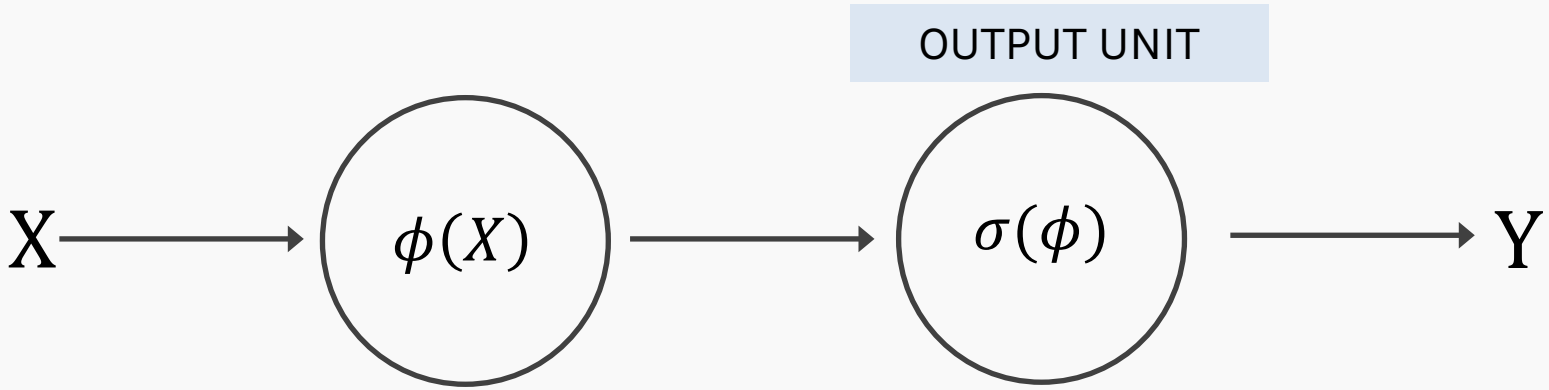
Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary			

Link function

$$X \Longrightarrow \phi(X) = W^T X \Longrightarrow P(y=0) = \frac{1}{1+e^{\phi(X)}}$$





Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary Cross Entropy

Output Units

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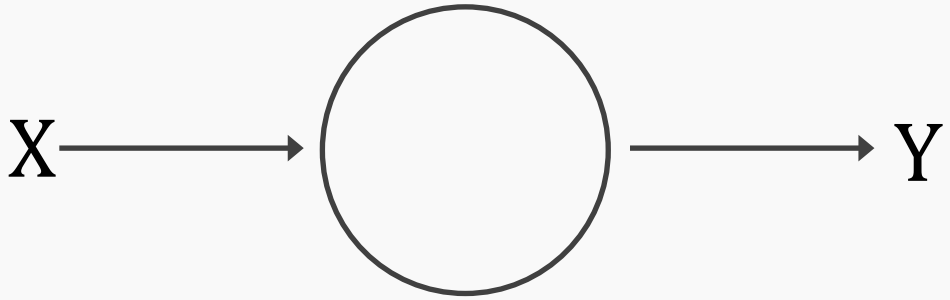
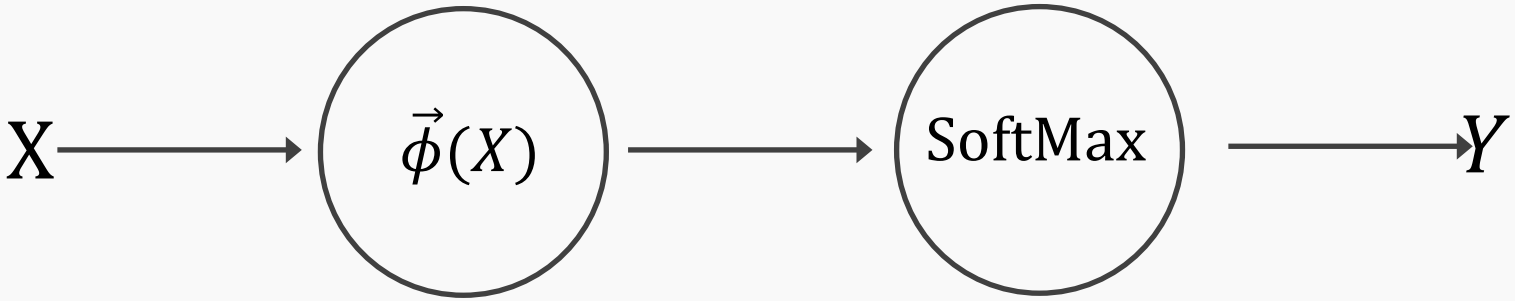
Discrete			

Link function multi-class problem



OUTPUT UNIT



$$Y = \frac{e^{\phi_k(X)}}{\sum_{k=1}^{K} e^{\phi_k(X)}}$$

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Discrete	Multinoulli	Softmax	Cross Entropy

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Continuous	Gaussian	Linear	MSE

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Continuous	Arbitrary	-	GANS

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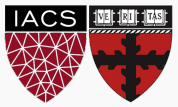
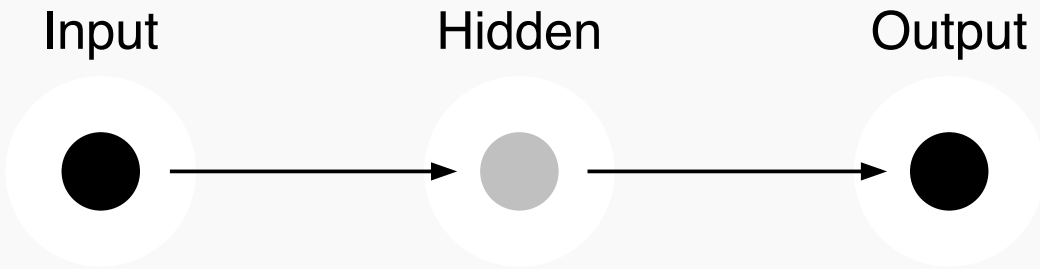
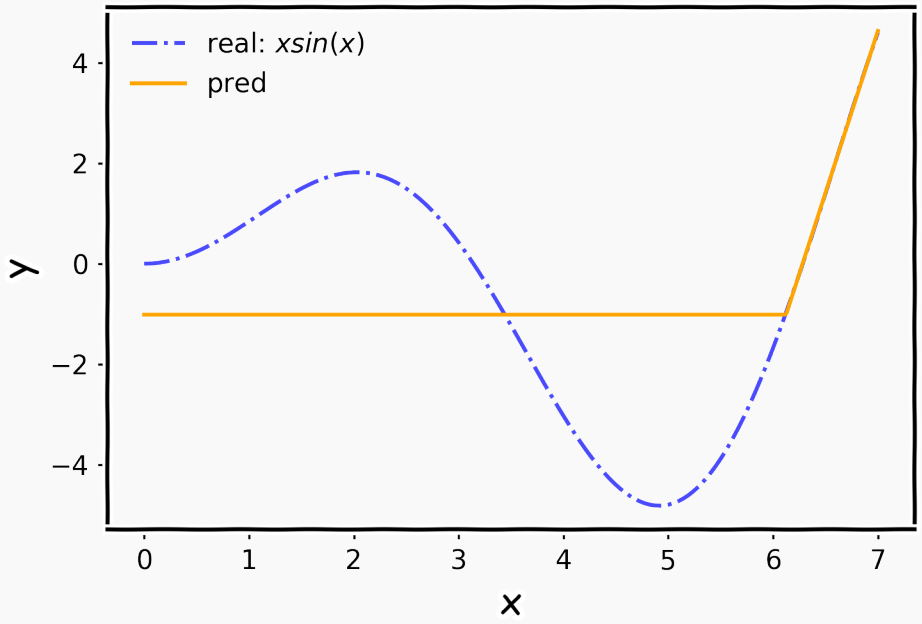
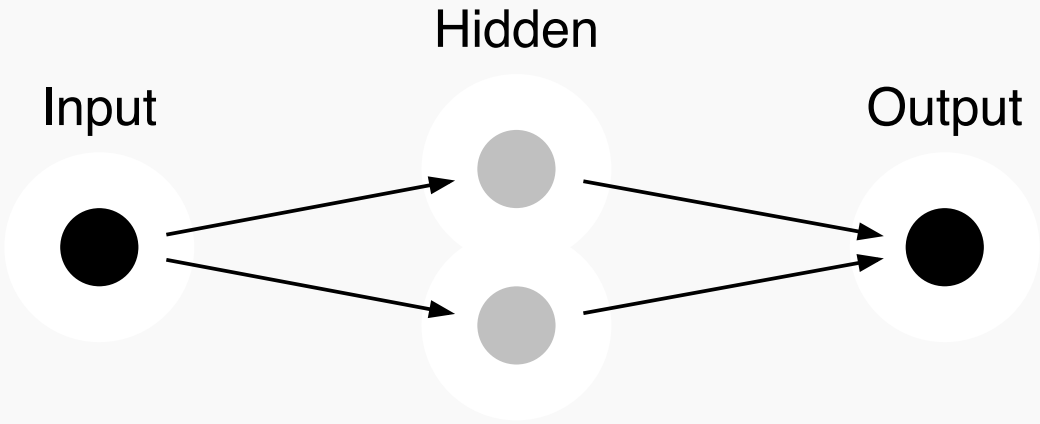


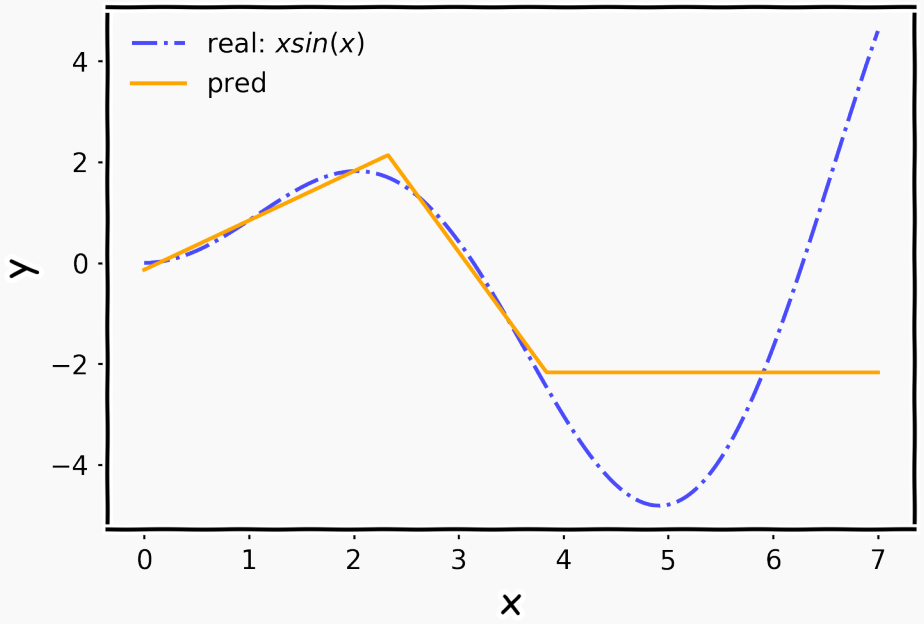
NN in action.



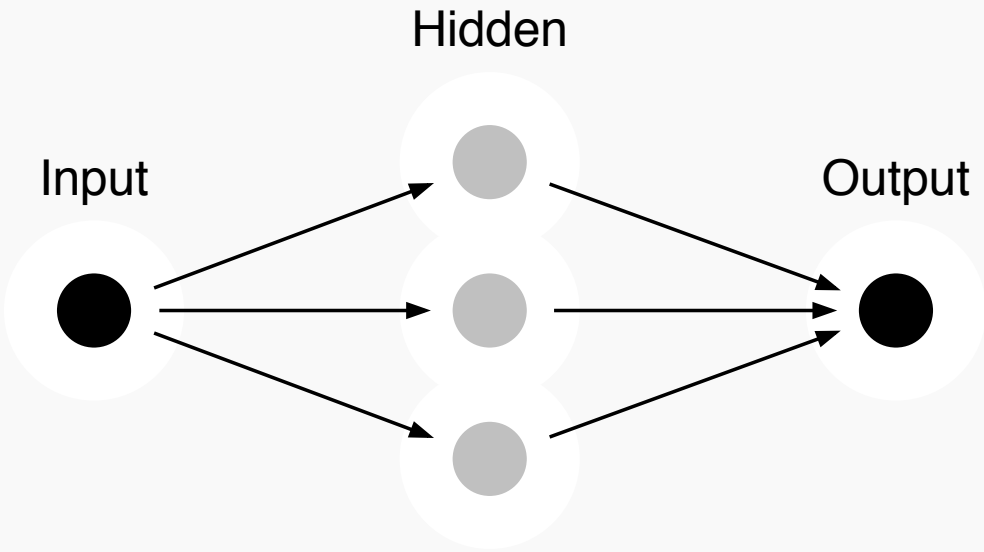


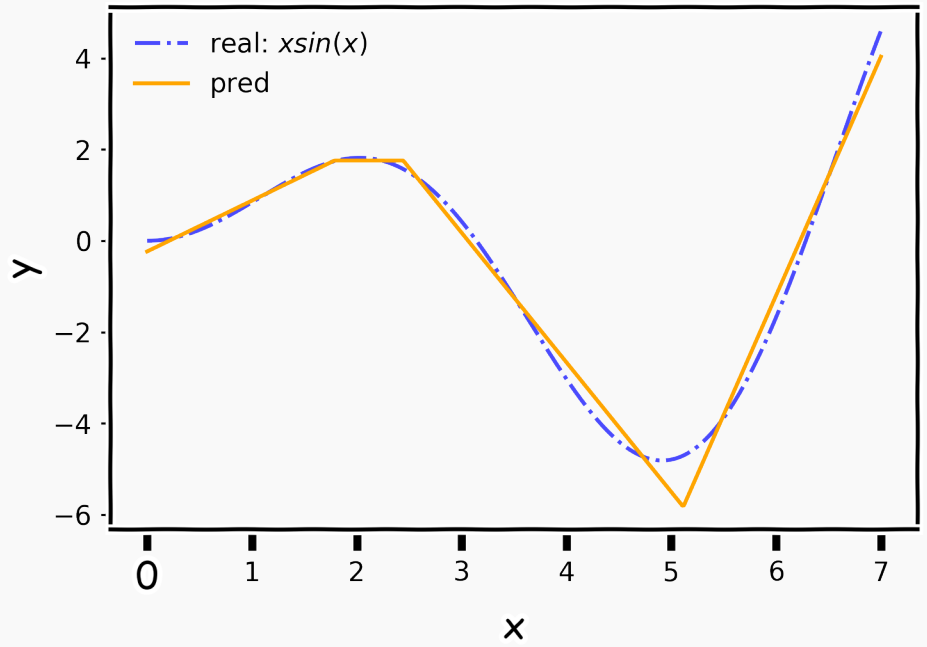
NN in action.



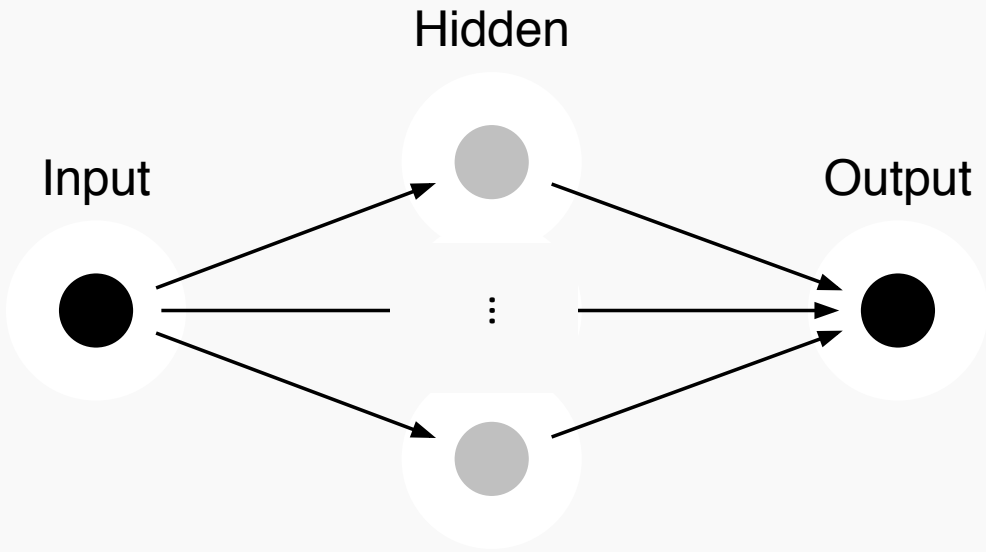


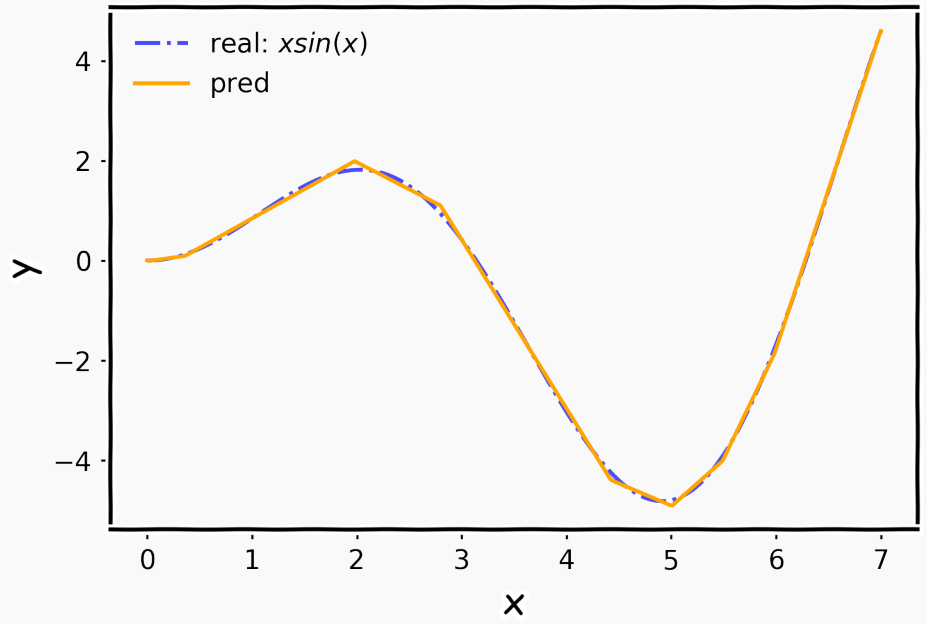
NN in action.



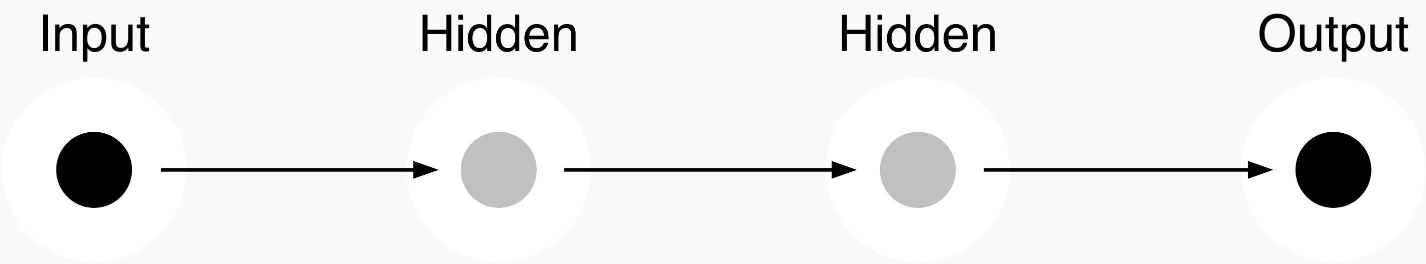


NN in action.





NN in action.


Input
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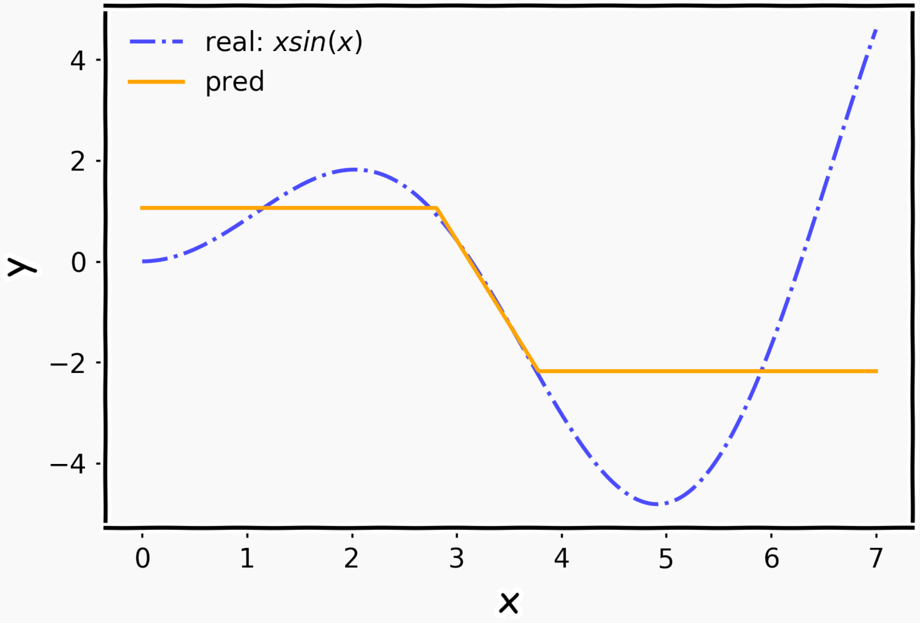
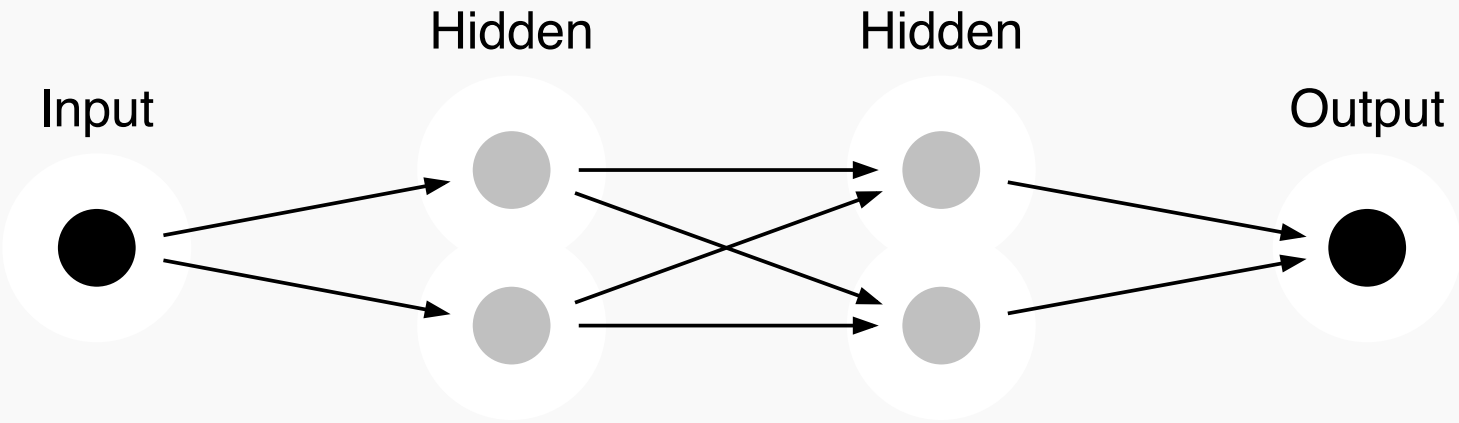
Hidden
Output


real: $xsin(x)$
pred
4
2
0
−2
−4
y
0
1
2
3
4
5
6
7
x

NN in action.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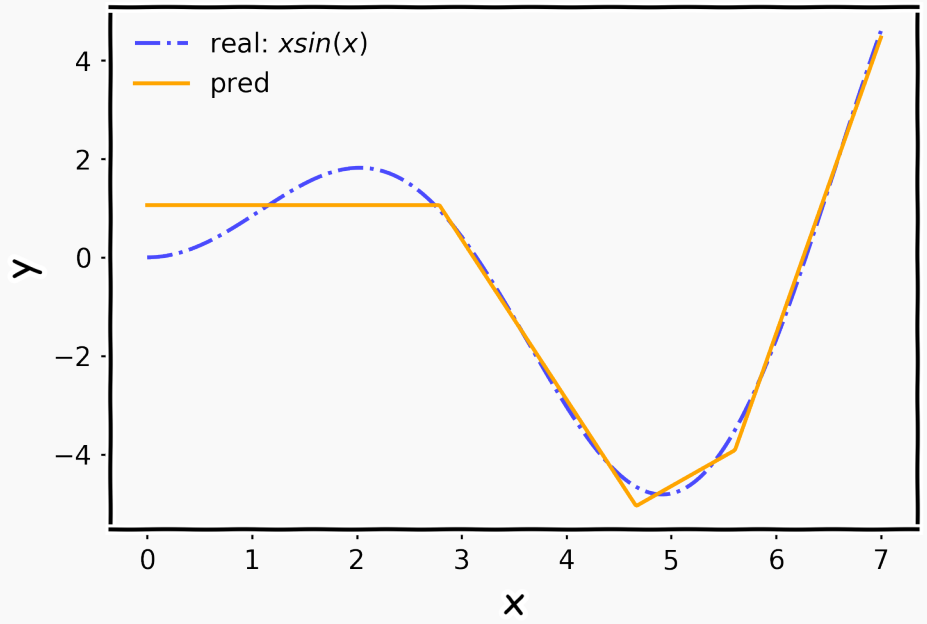
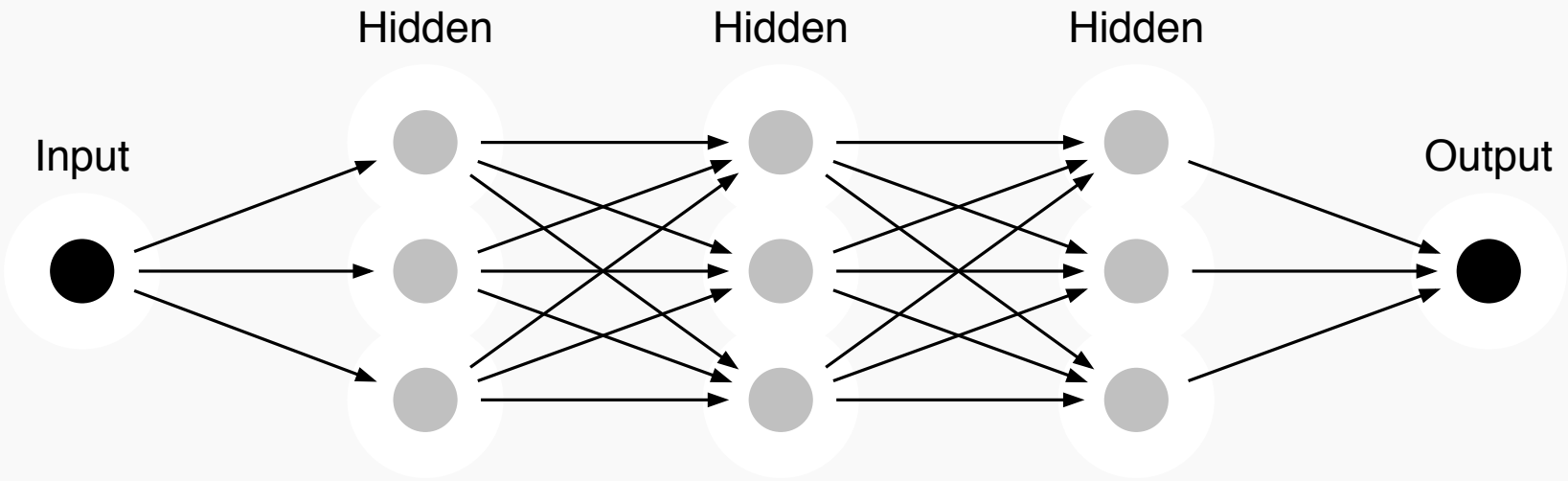

real: xsin(x)
pred
4
2
0
−2
−4
y
0
1
2
3
4
5
6
7
x

NN in action.


Hidden
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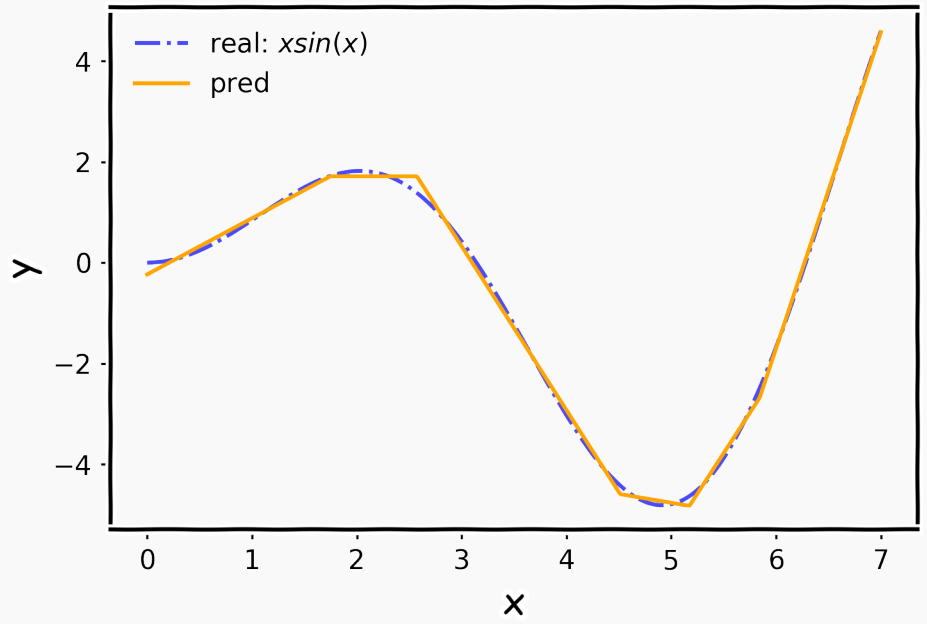
Input
Output


real: xsin(x)
pred
4
2
0
−2
−4
y
0
1
2
3
4
5
6
7
x

Universal Approximation Theorem

Think of Neural Network as function approximation.

$$Y = f(x) + \epsilon$$

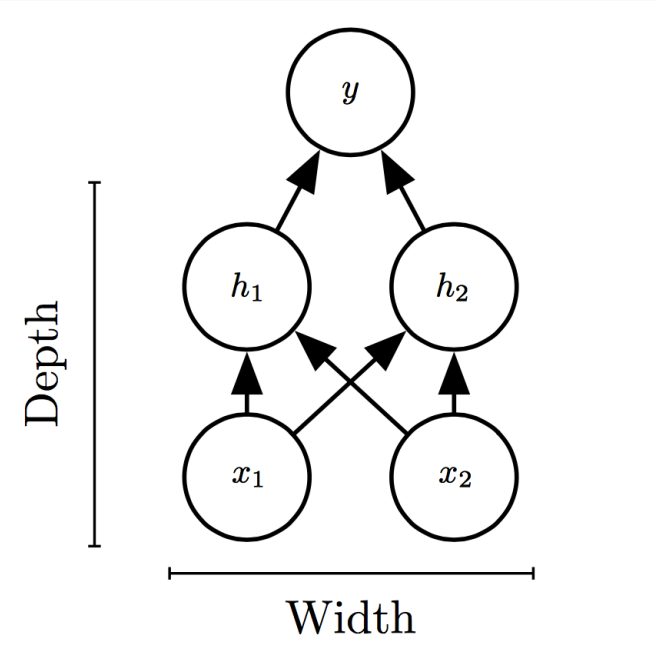
$$Y = \hat{f}(x) + \epsilon$$

NN: $\Longrightarrow \hat{f}(x)$

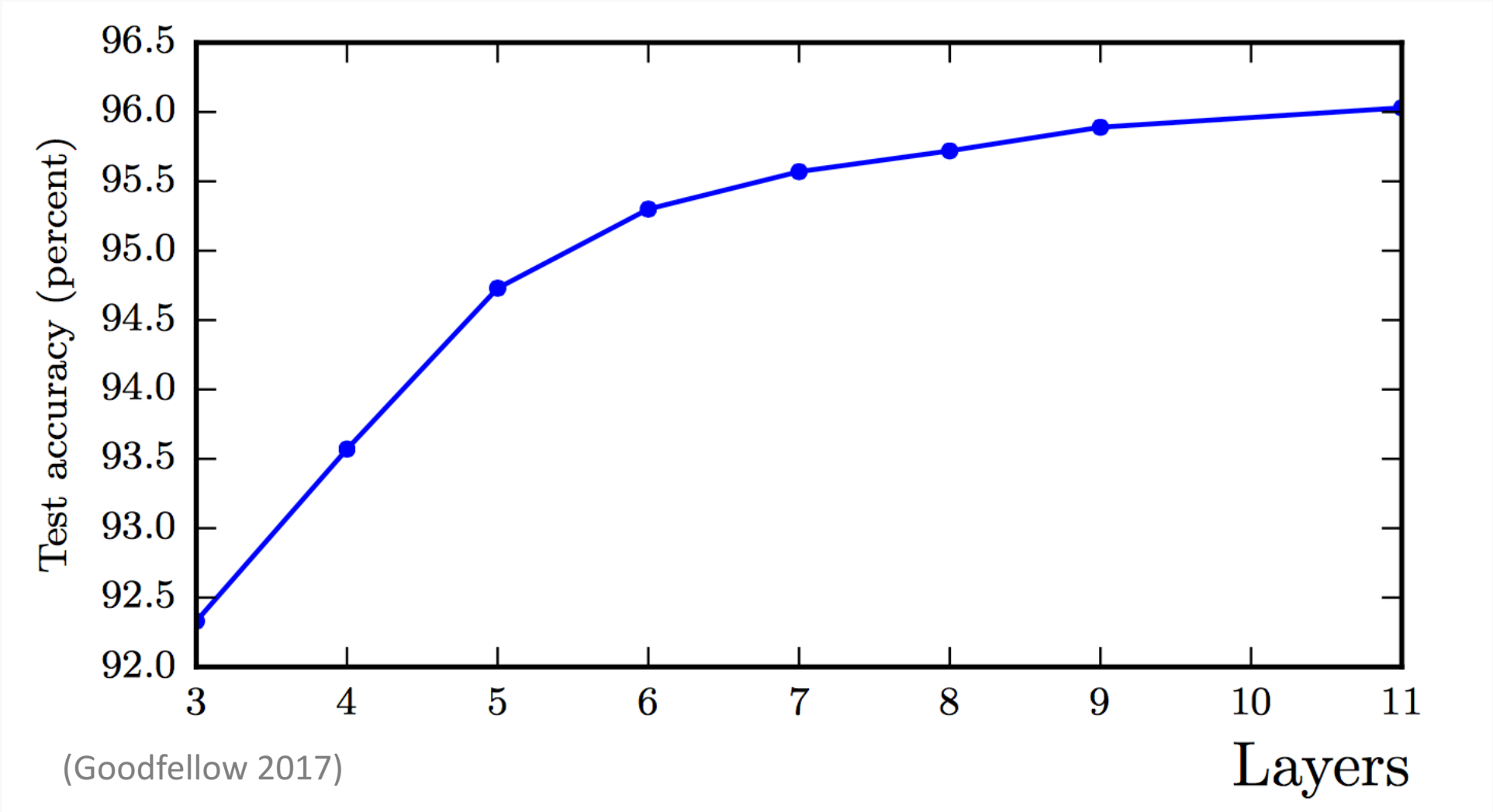
One hidden layer is enough to *represent* an approximation of any function to an arbitrary degree of accuracy

So why deeper?

- Shallow net may need (exponentially) more width
- Shallow net may overfit more

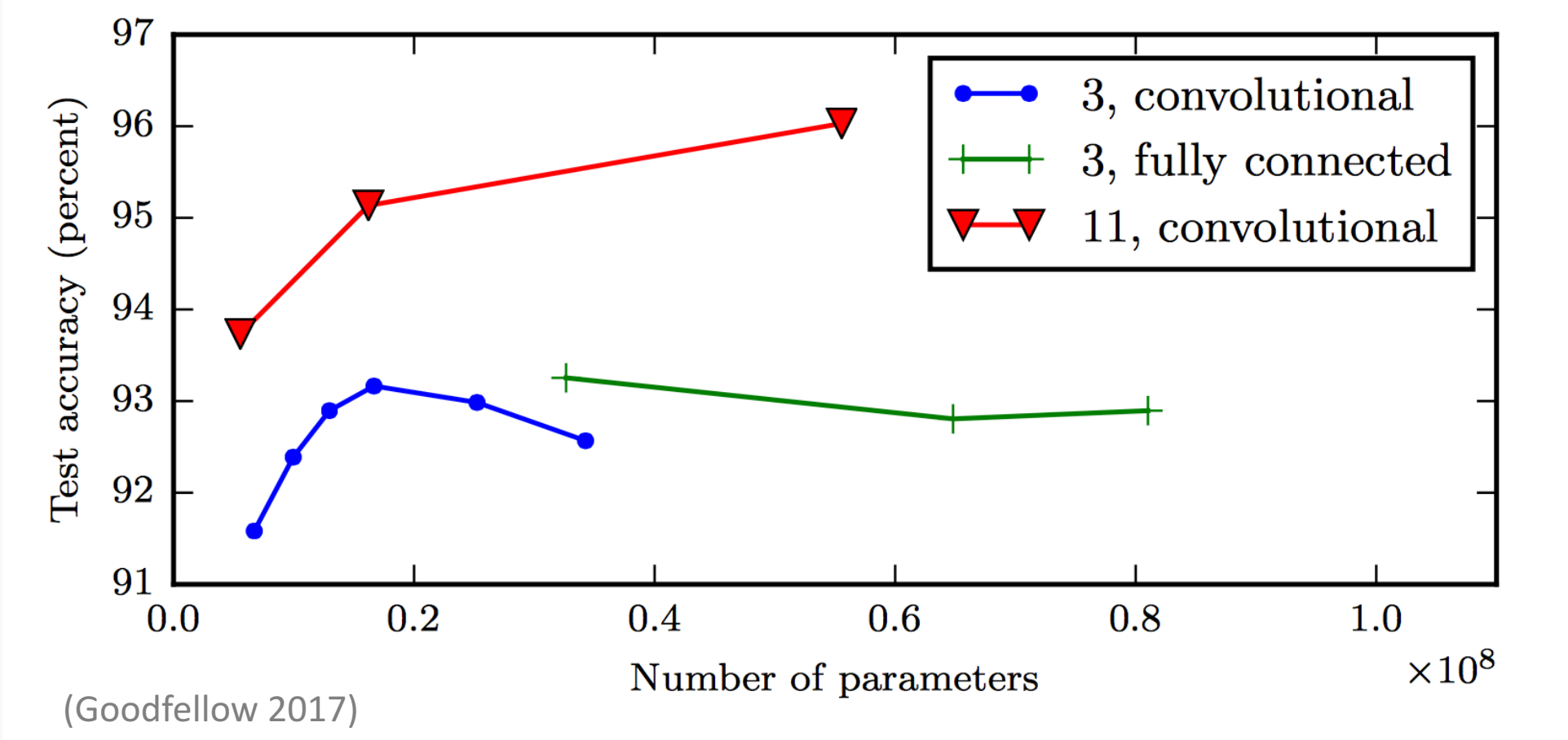


Better Generalization with Depth



(Goodfellow 2017)

Large, Shallow Nets Overfit More



(Goodfellow 2017)