Anatomy of NN

CS109B Data Science 2

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Outline

Anatomy of a NN

Design choices

- Activation function
- Loss function
- Output units
- Architecture

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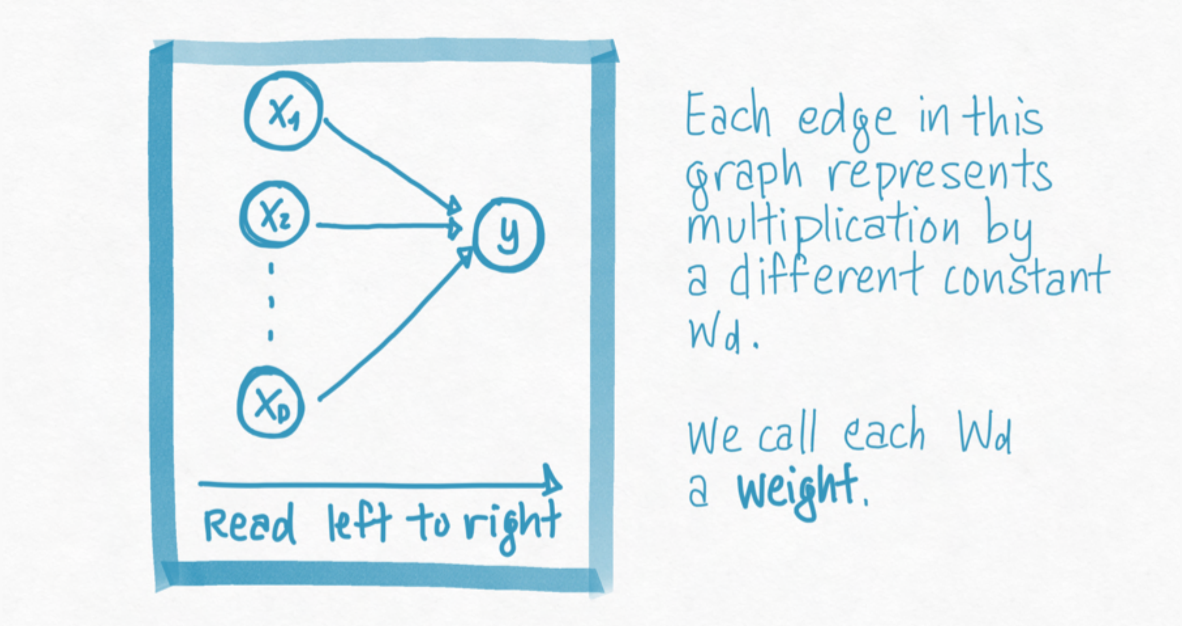
Graphical representation of simple functions

We build complex functions by composing simple functions of the form:

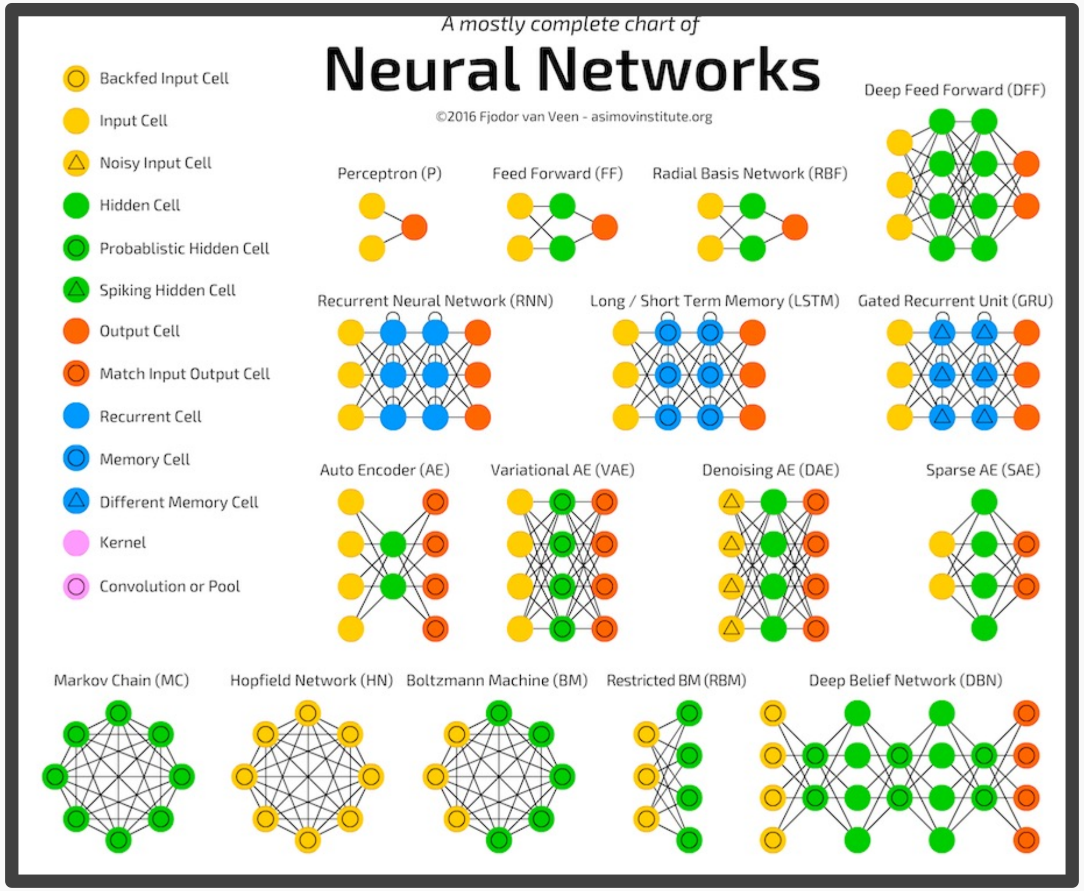
$$h_w(x) = f(XW + b)$$

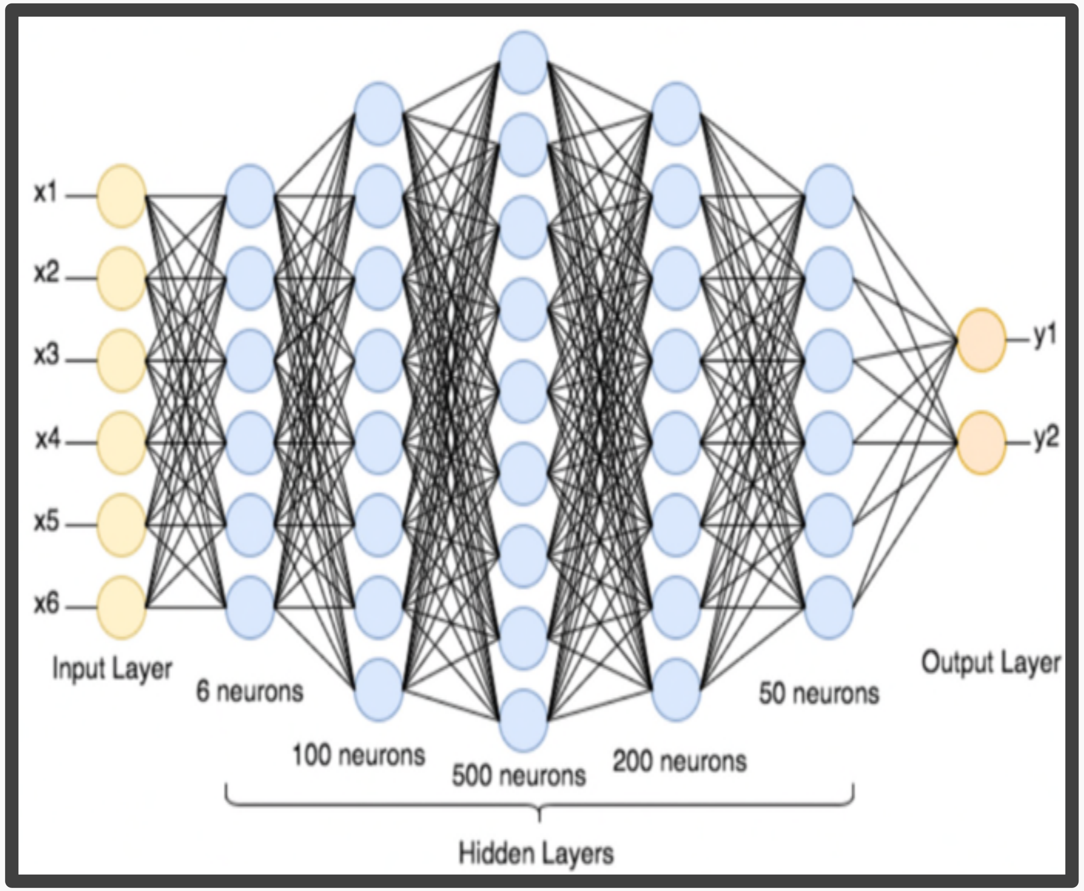
where f is the activation function.

We represent our simple function as a **graph**



The zoo of neural network architectures

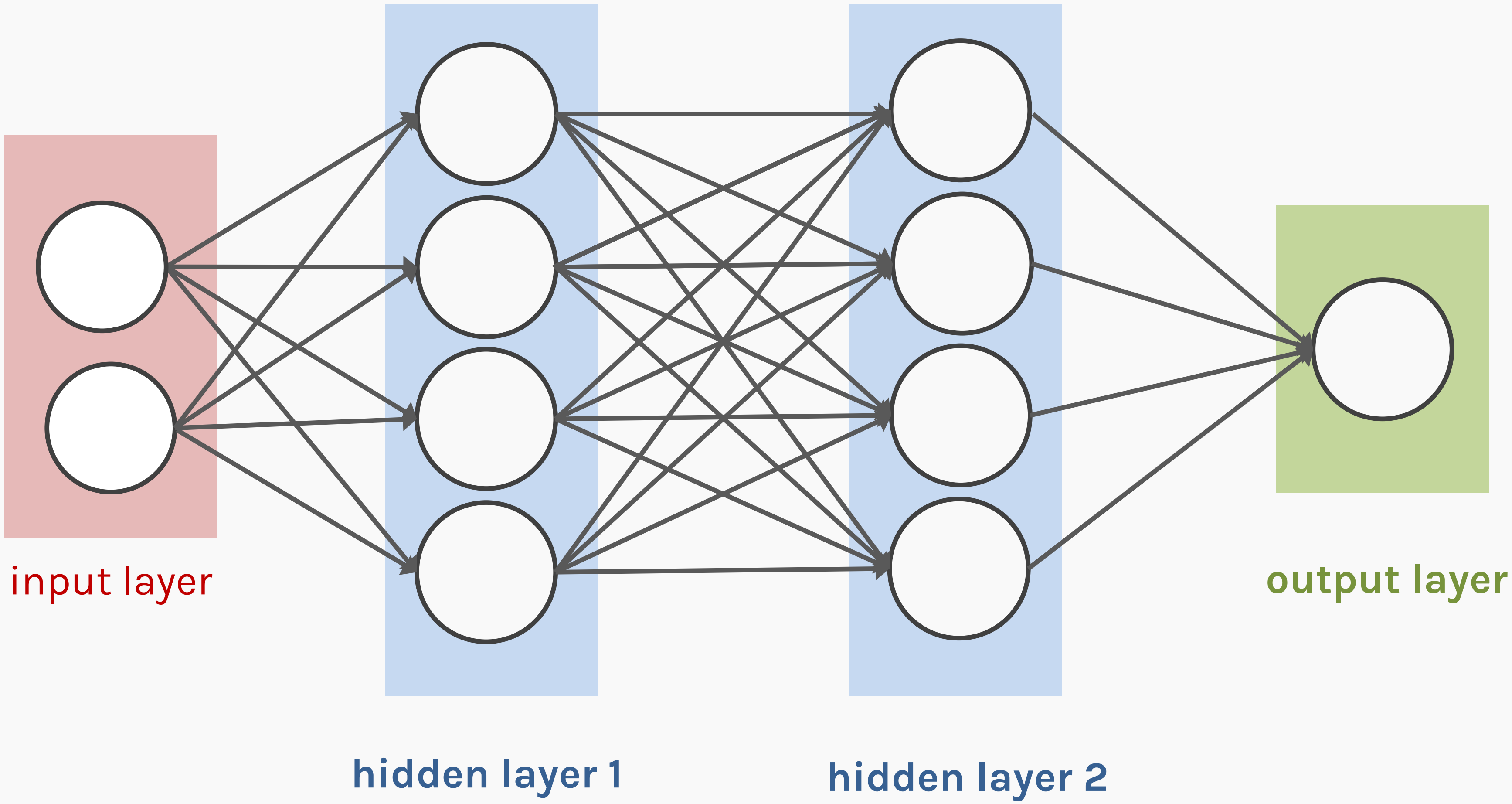




Different architectures result into functions with very different properties.

Larger networks can express more complex functions

Anatomy of artificial neural network (ANN)



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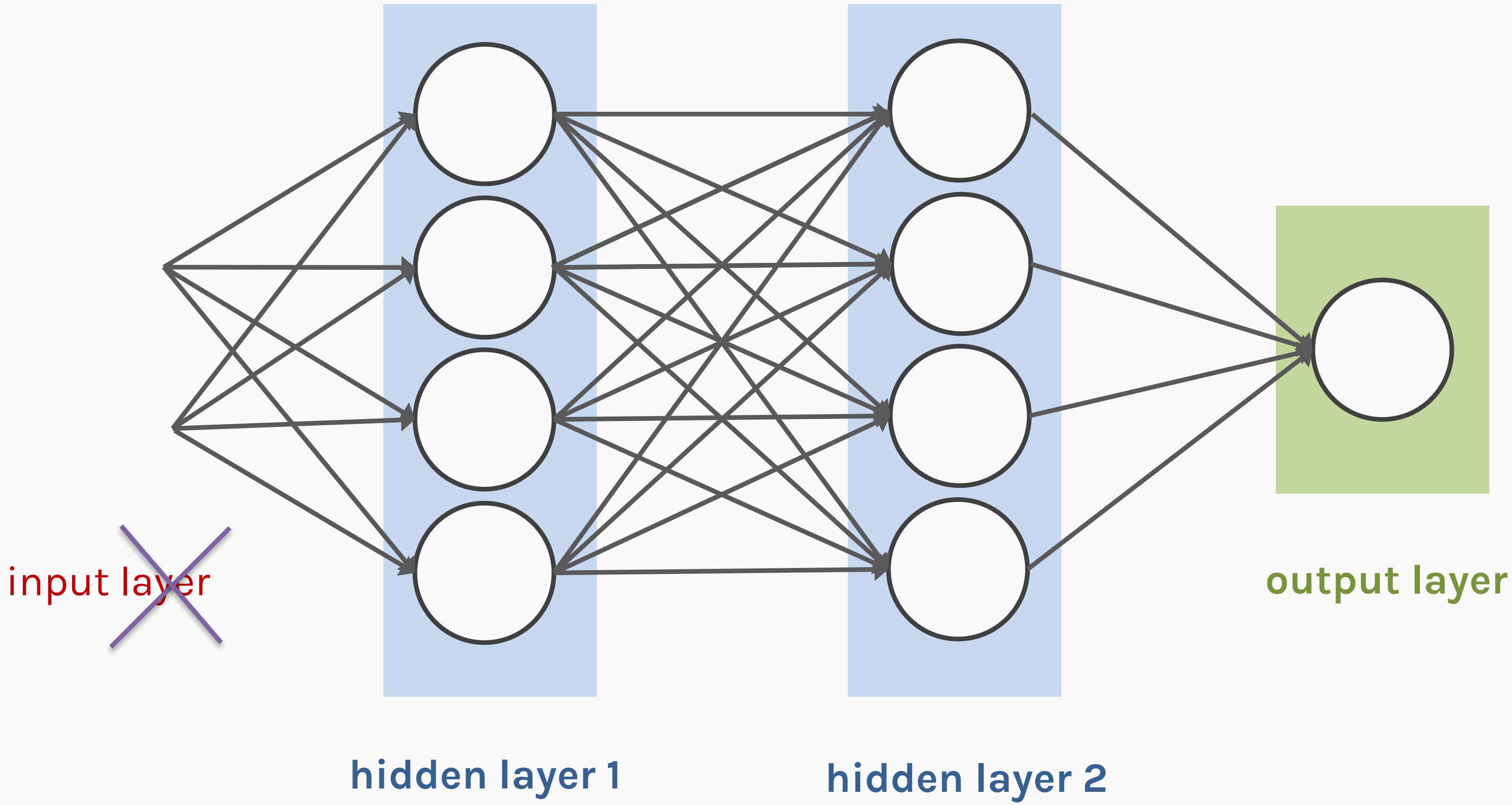

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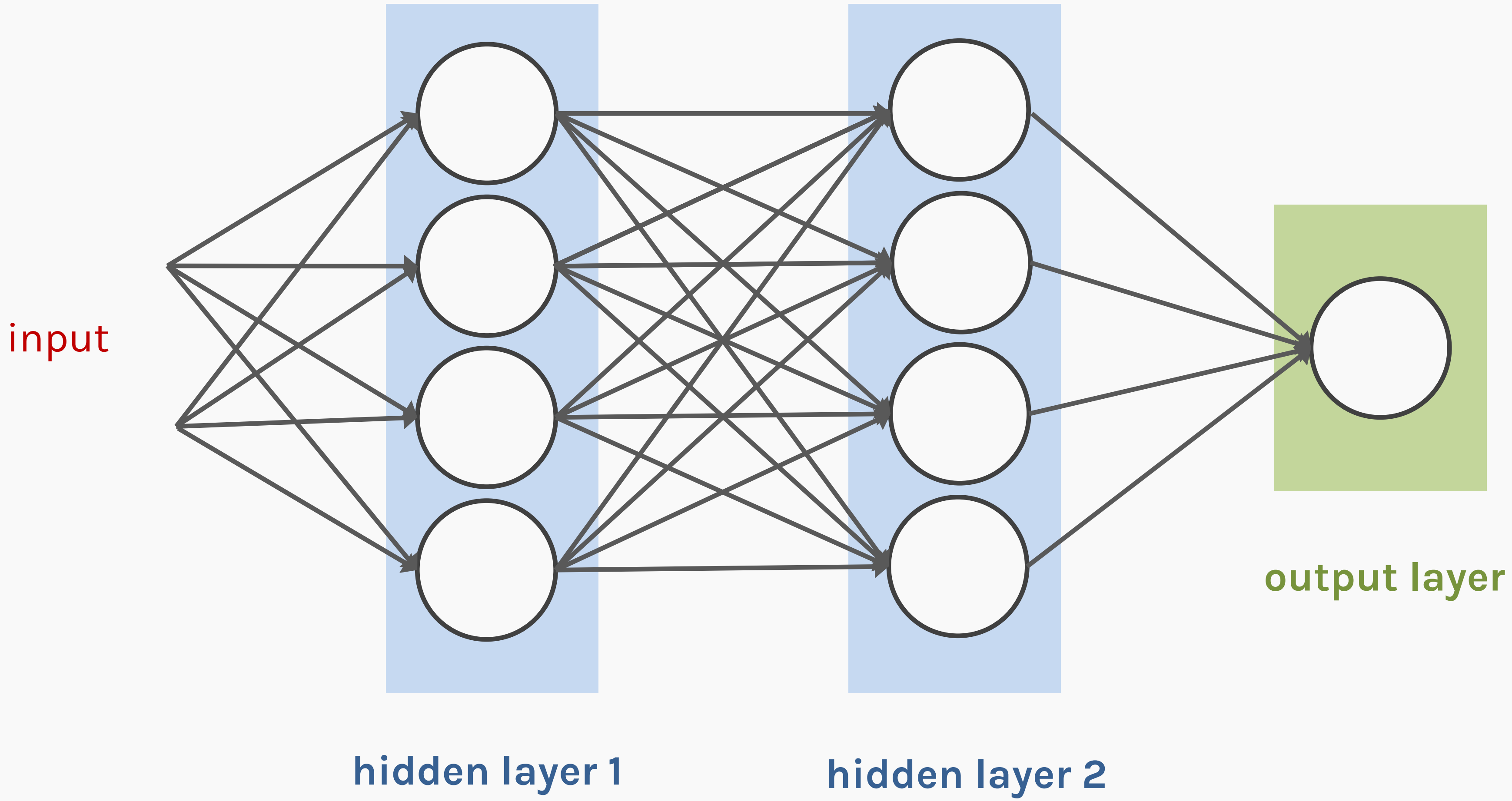

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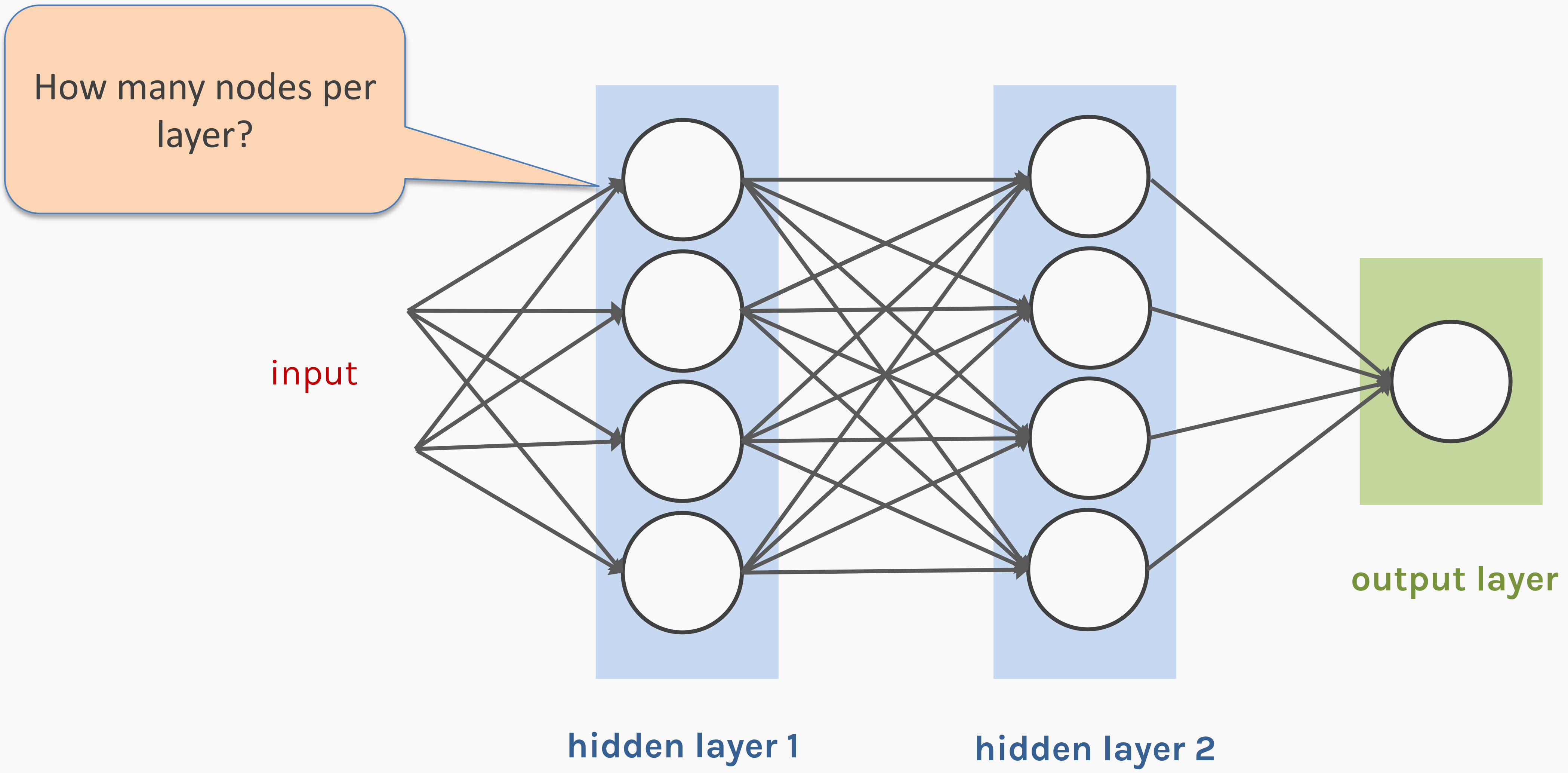

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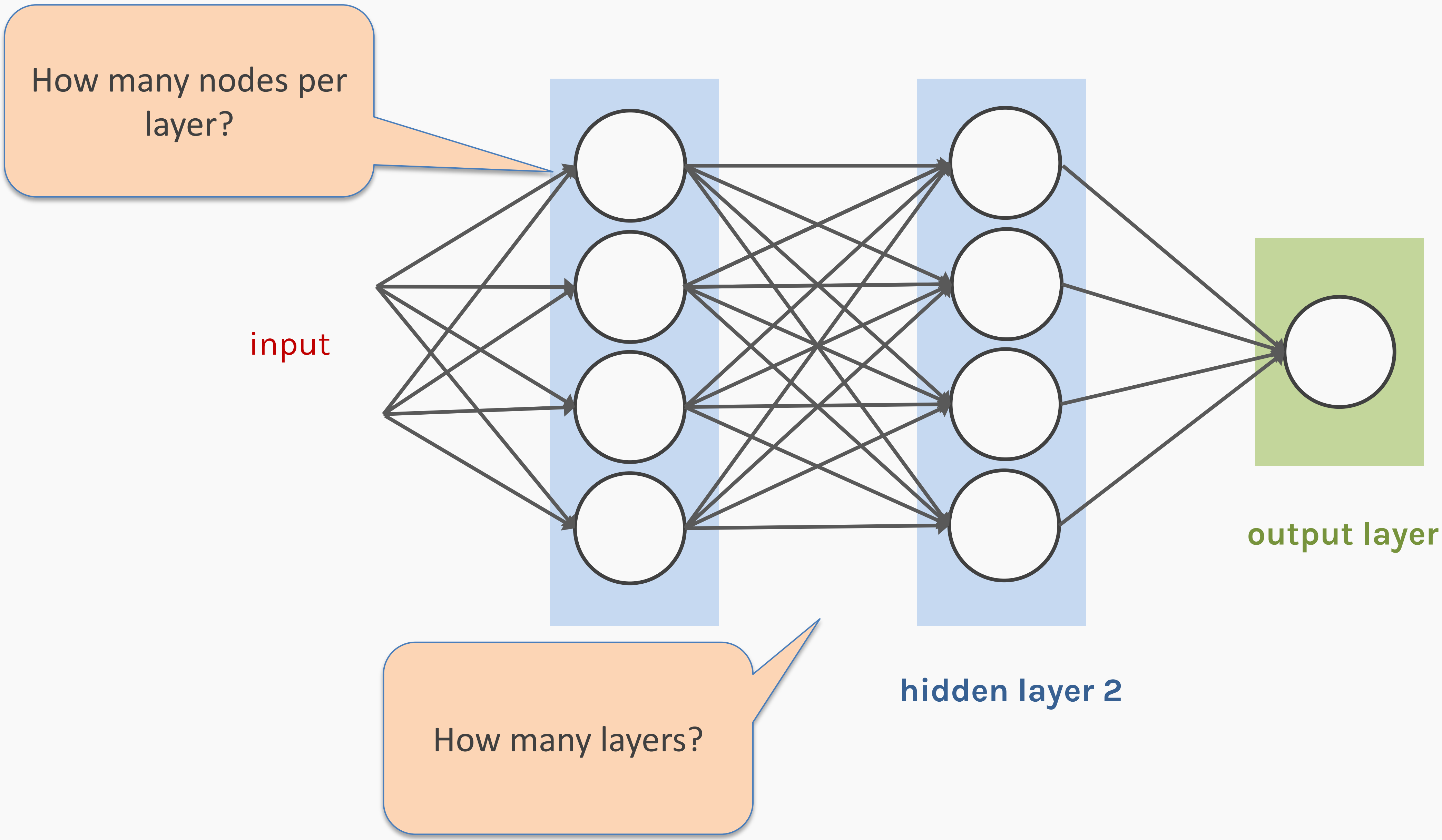

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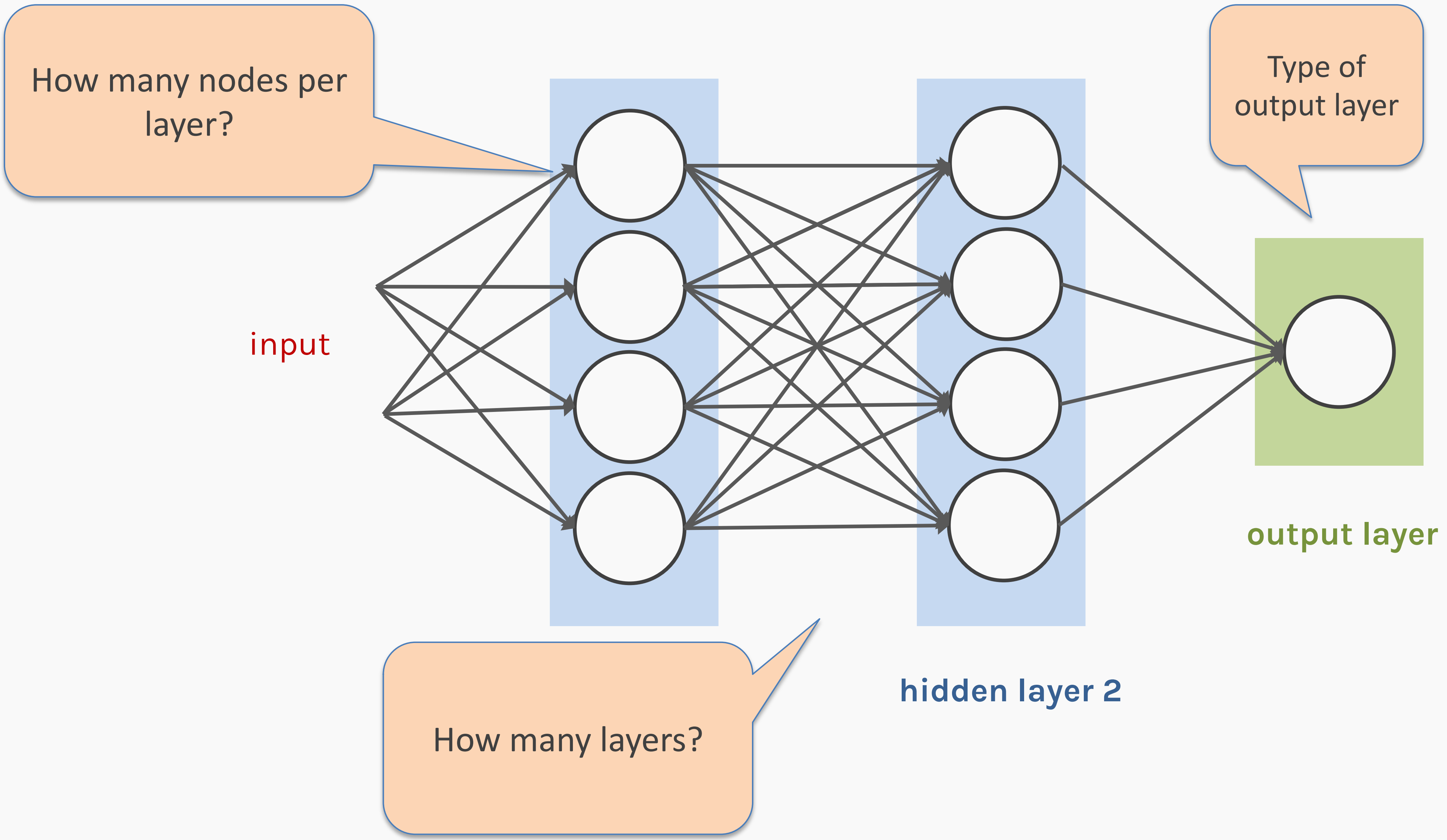

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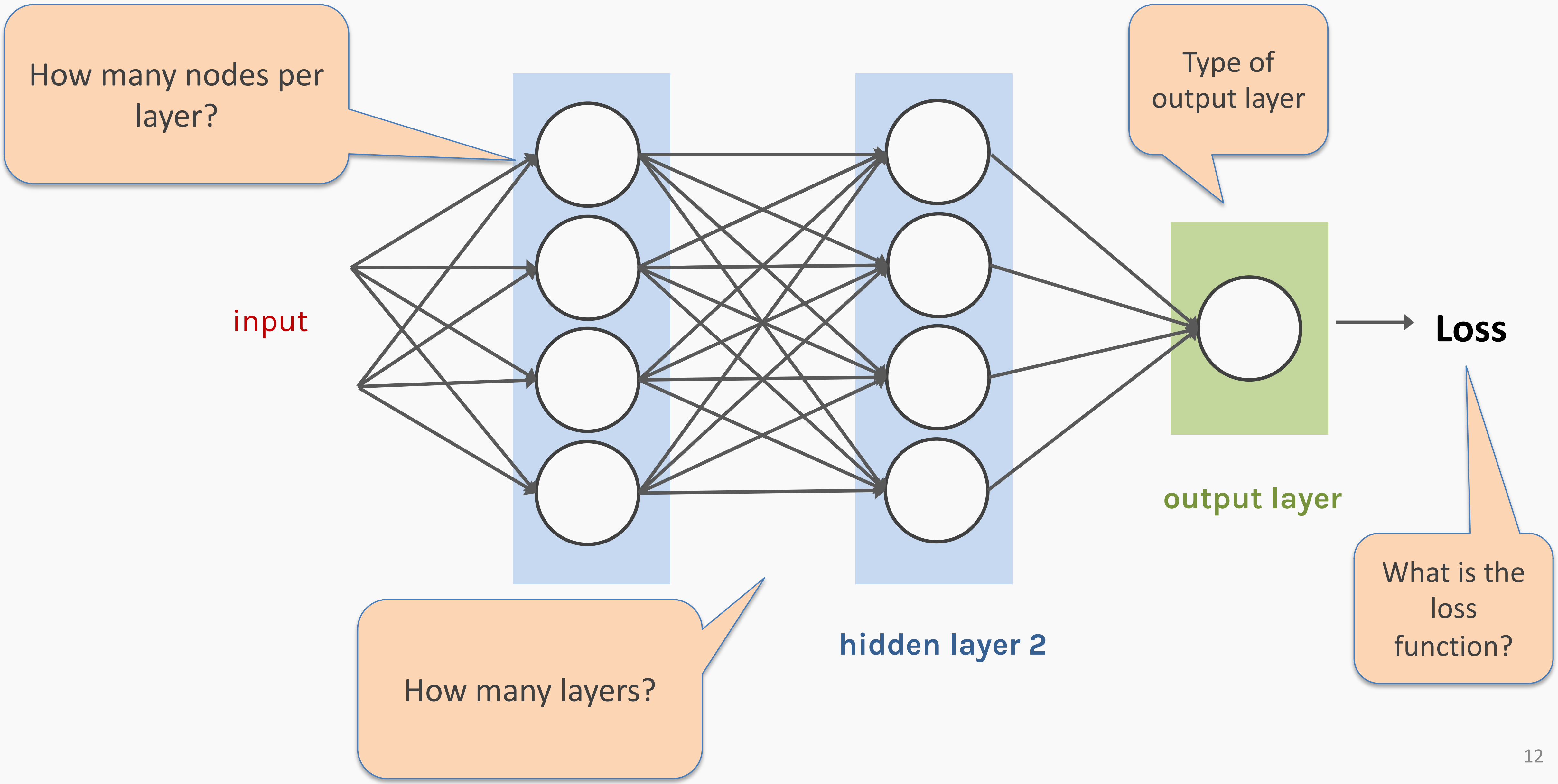

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- **Activation function**
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Activation function

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

The activation function should:

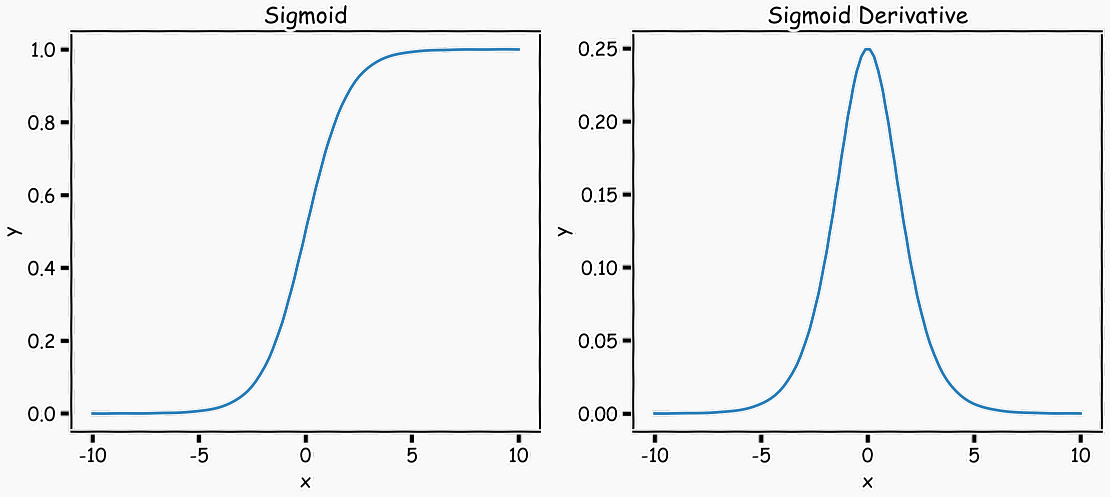
- Provide non-linearity
- Ensure gradients remain large through hidden unit

Common choices are

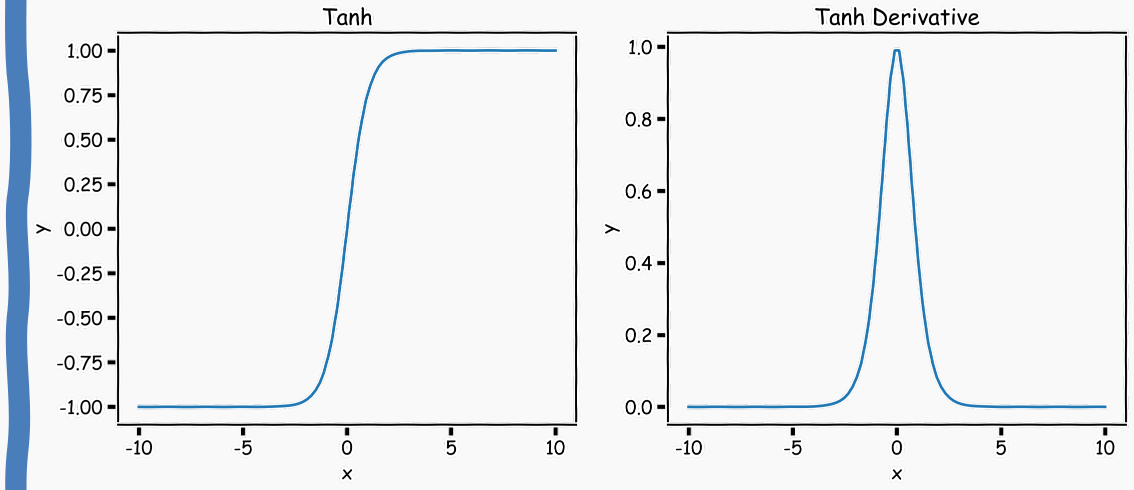
- sigmoid, tanh
- ReLU, leaky ReLU, Generalized ReLU
- softplus
- swish

Sigmoid, $\sigma()$ (aka logistic) and tanh

$$y = \frac{1}{1 + e^{-x}}$$



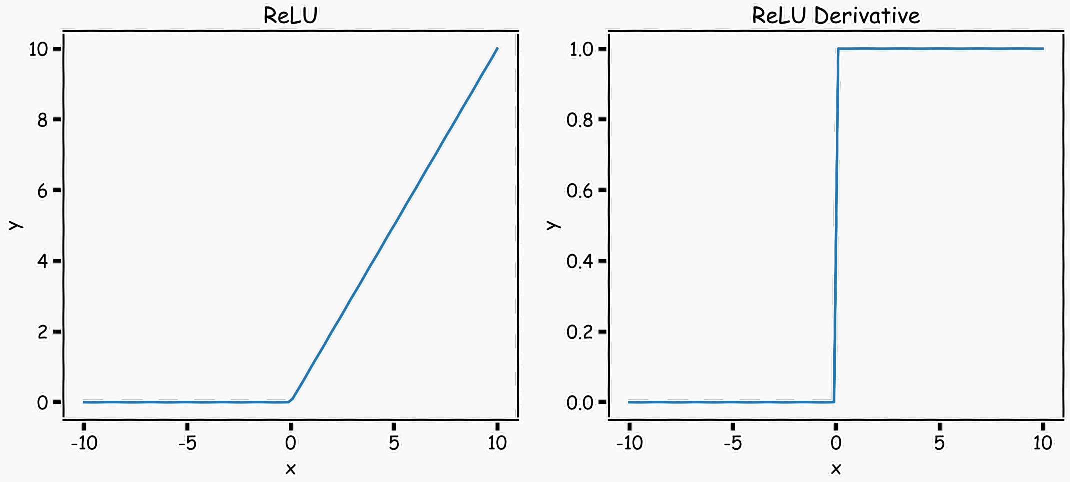
$$y = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$



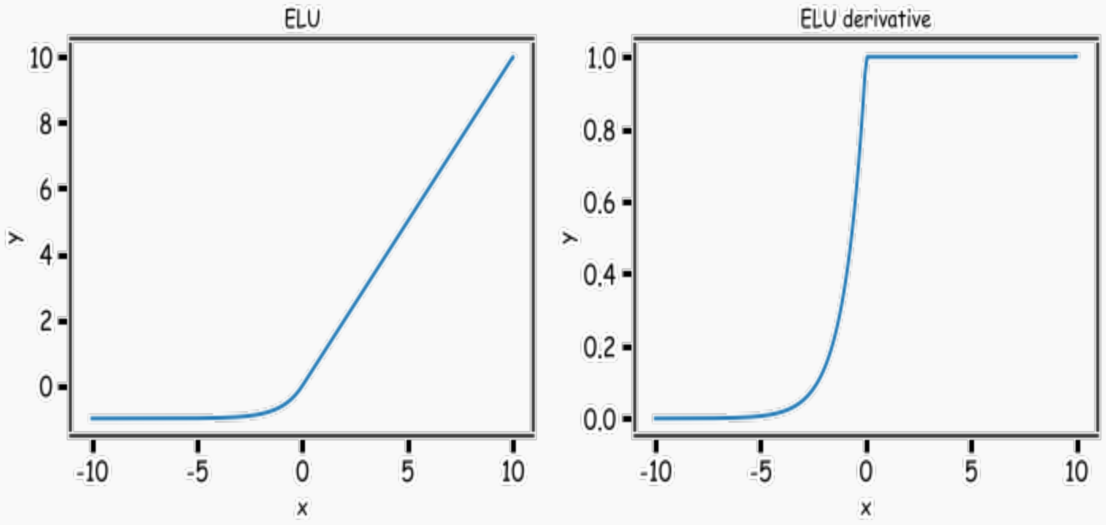
Derivative is **zero** for much of the domain. This leads to “vanishing gradients” in backpropagation.

Rectified Linear Unit, `ReLU()`, Exponential ReLU (ELU)

$$y = \max(0, x)$$



$$y = \max(0, x) + \alpha \min(0, e^{x} - 1)$$
where α takes a small value



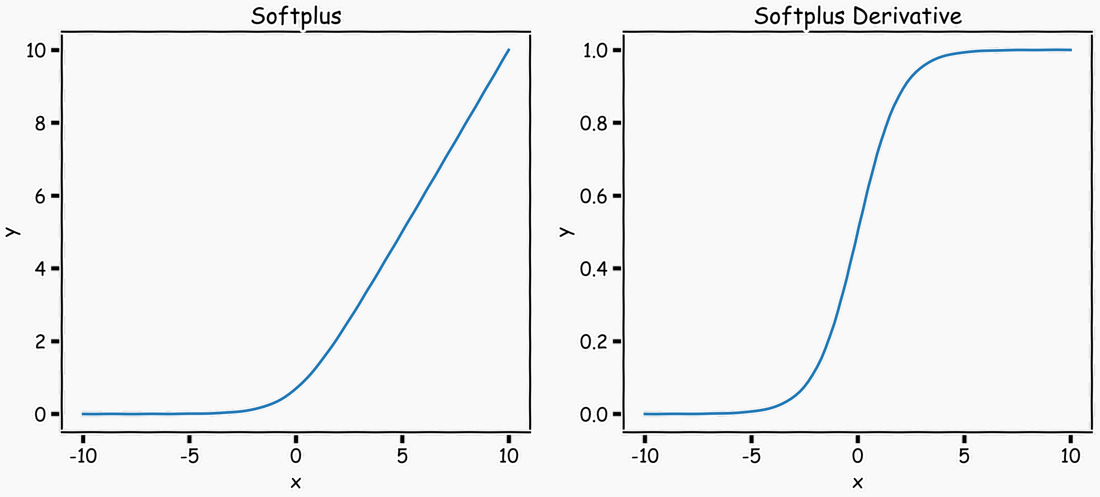
Two major advantages:

1. No vanishing gradient when x > 0
2. Provides sparsity (regularization) since y = 0 when x < 0

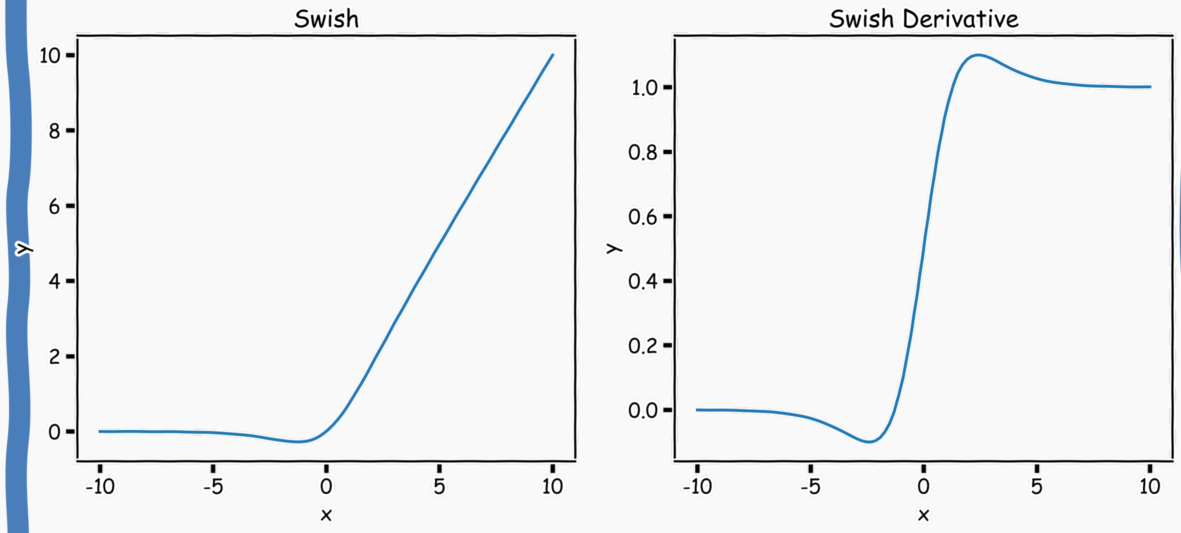
No vanishing gradients and easy to calculate.

Softplus and Swish

$$y = \log(1 + e^x)$$



$$g(x) = x\,\sigma(x)$$



The derivative of the softplus is the sigmoid logistic function, which is a smooth approximation of the derivative of the rectifier. So the derivative of the softplus is continuous.

Swish tends to work better than ReLU on deeper models across a number of challenging datasets.

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- **Loss function**
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Loss Function

Probabilistic modeling

Likelihood for a given measurement:

$$p(y_i|W;x_i)$$

Assume **independency**, likelihood for all measurements:

$$L(W;X,Y) = p(Y|W;X) = \prod_i p(y_i|W;x_i)$$

Maximize the likelihood, or equivalently minimizing the –ve log-likelihood:

$$\boxed{\mathcal{L}(W;X,Y) = -\log L(W;X,Y) = \sum_i \log p(y_i|W;x_i)}$$

Loss Function

Do not need to design separate loss functions if we follow the probabilistic modeling approach, i.e. minimize the –ve likelihood function.

Examples:

- Distribution is **Normal** then –ve log-likelihood is **MSE** :

$$p(y_i|W;x_i) = \frac{1}{\sqrt{\{2\pi^2\sigma\}}} e^{-\frac{(y_i - \hat{y}_i)^2}{2\sigma^2}}$$

$$\mathcal{L}(W;X,Y) = \sum_i (y_i - \hat{y}_i)^2$$

- Distribution is **Bernouli** then –ve log-likelihood is **Binary Cross-Entropy**:

$$p(y_i|W;x_i) = p_i^{y_i}(1 - p_i)^{1-y_i}$$

$$\mathcal{L}(W;X,Y) = -\sum_i [y_i \log p_i + (1 - y_i) \log(1 - p_i)]$$

Design Choices

Activation function

Loss function

Output units

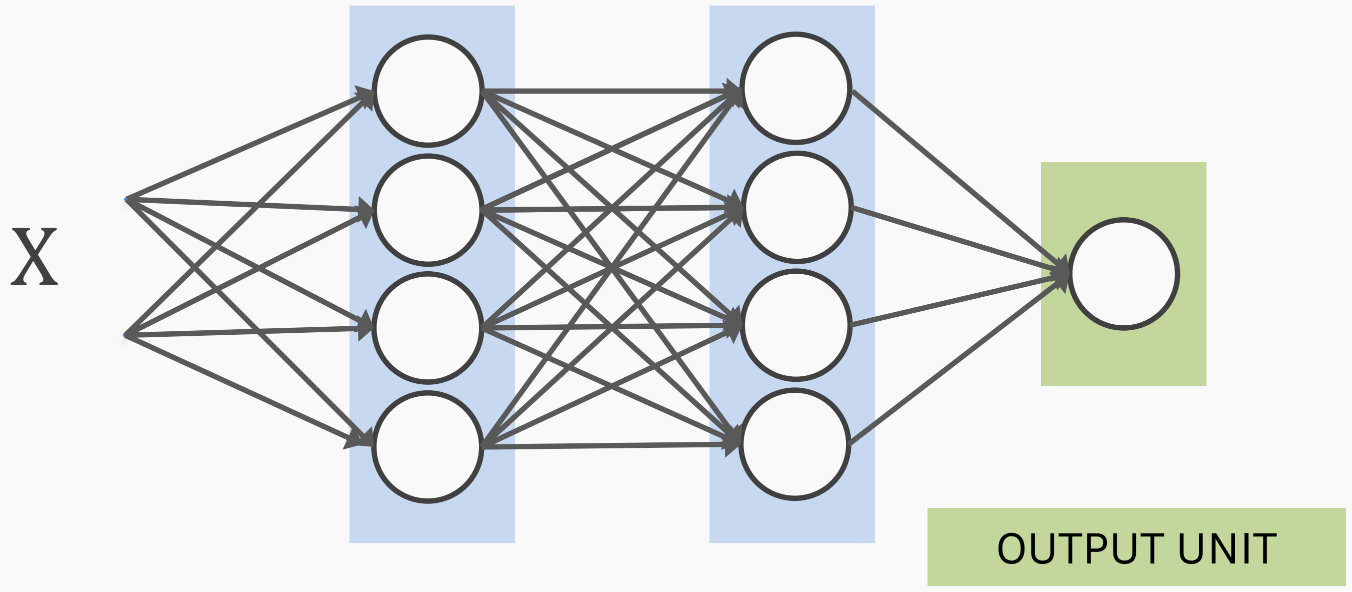
Architecture

Optimizer

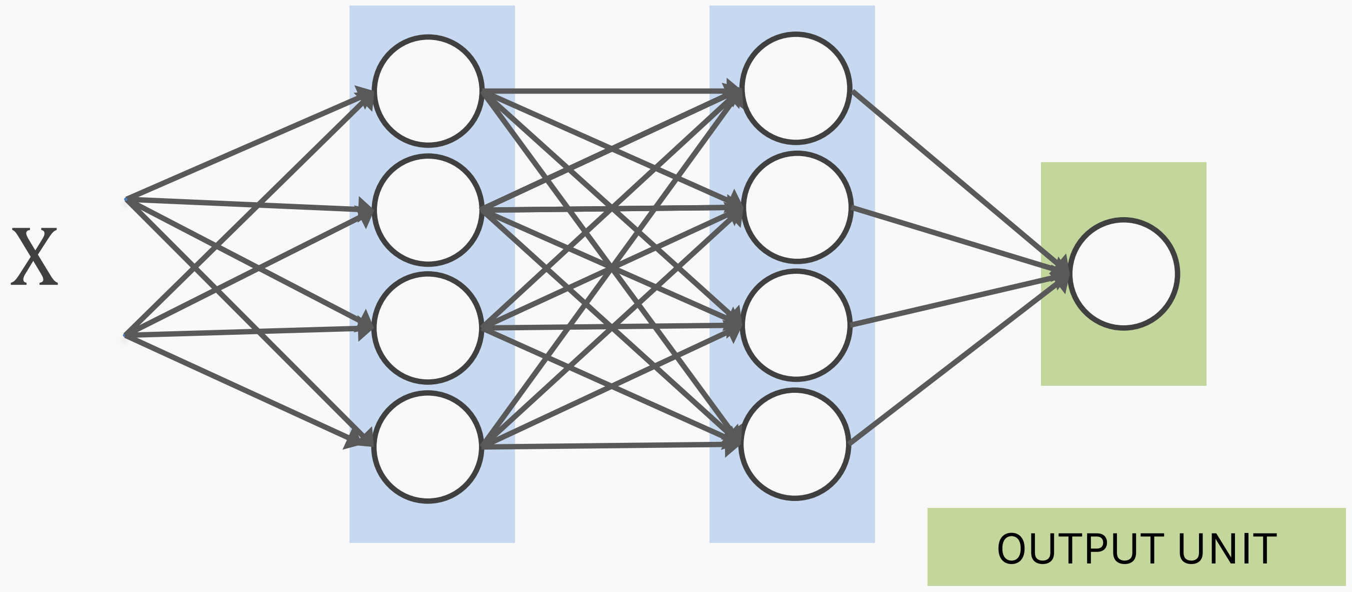
Output Units

Output Type	Output Distribution	Output layer	Loss Function
Binary	Bernoulli	?	Binary Cross Entropy

Output unit for binary classification

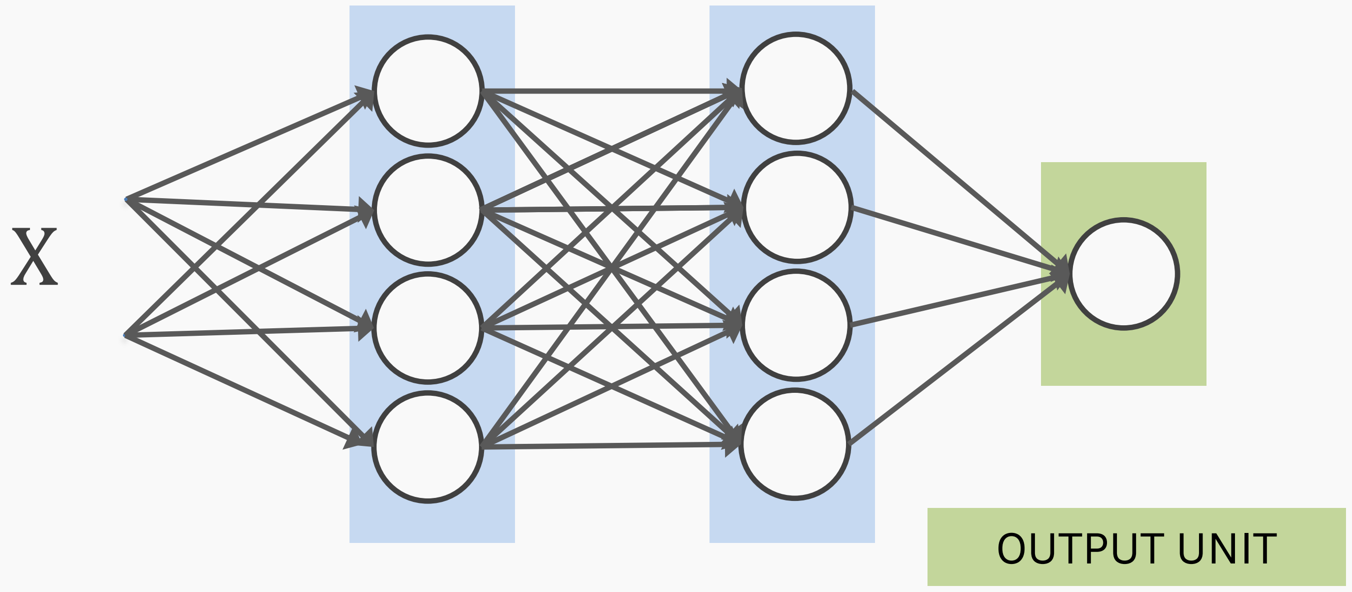


Output unit for binary classification



$$\hat{Y} = \mathrm{P}(\mathrm{y} = 1)$$

Output unit for binary classification



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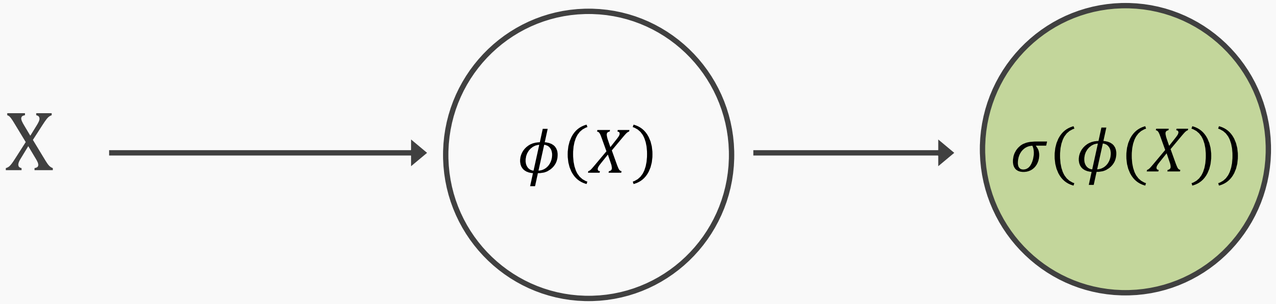


$\hat{Y} = \mathrm{P}(\mathrm{y} = 1)$

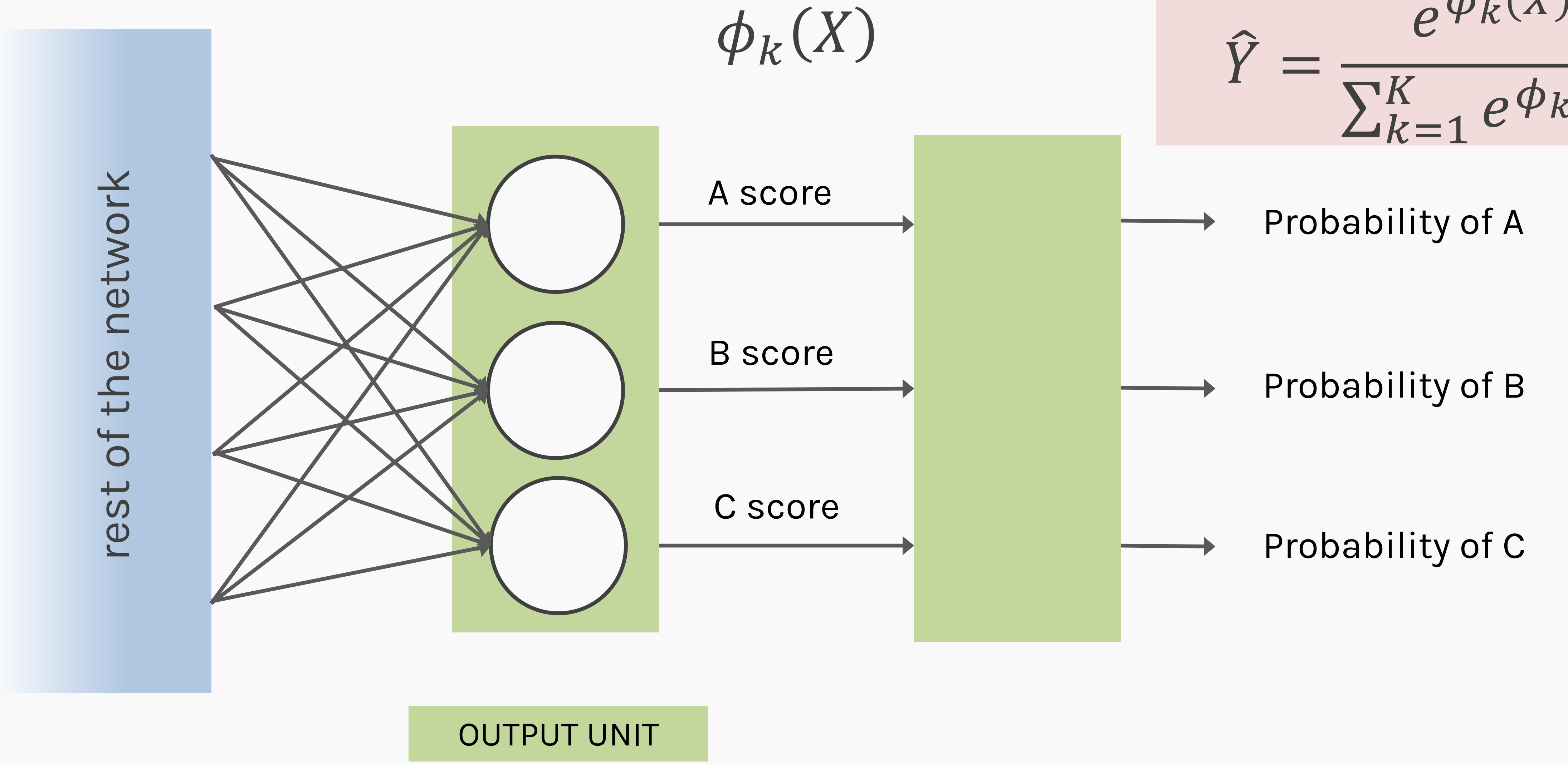
$$X \Longrightarrow \phi(X) \Longrightarrow P(y = 1) = \frac{1}{1 + e^{-\phi(X)}}$$

Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary Cross Entropy
Discrete	Multinouli	?	Cross Entropy

SoftMax

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



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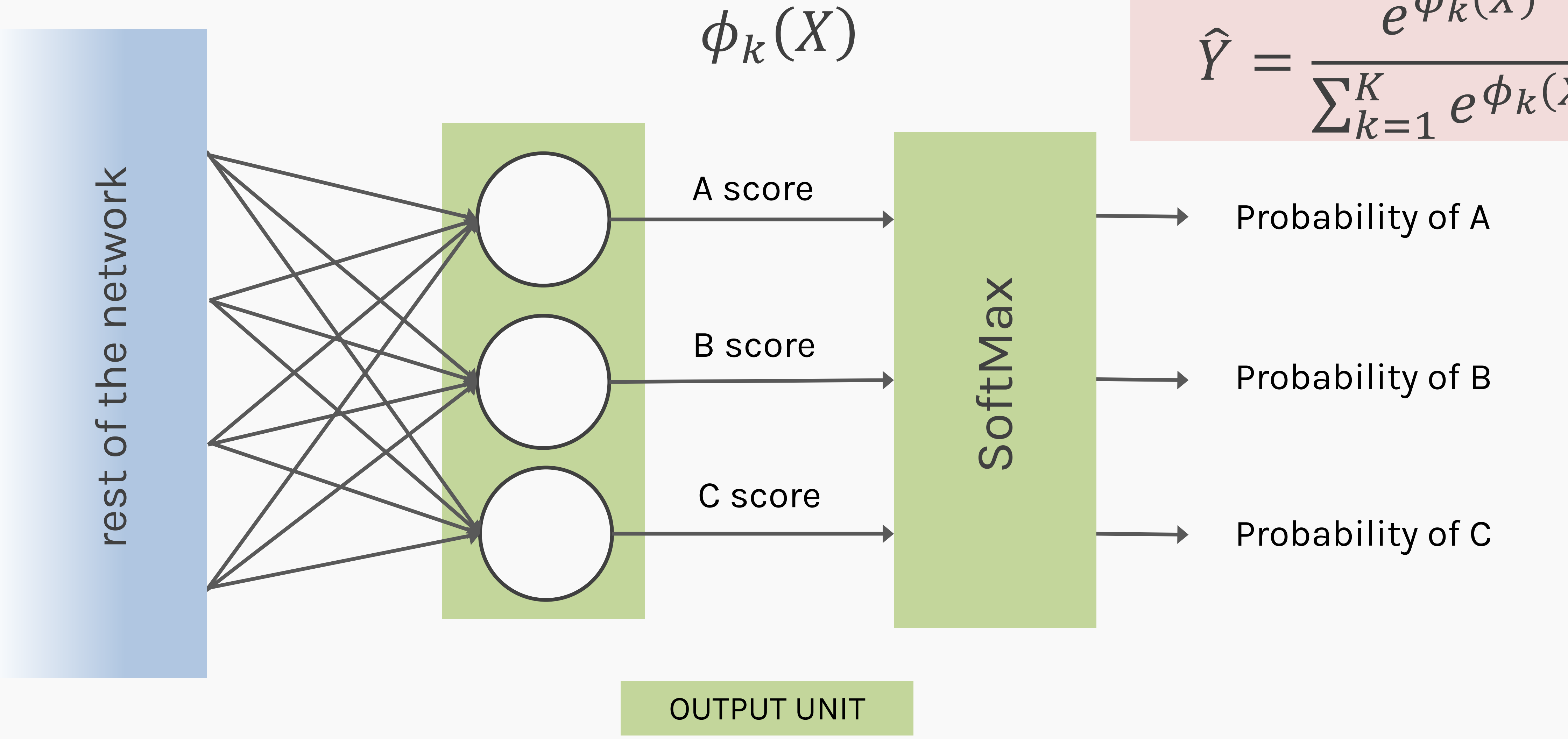
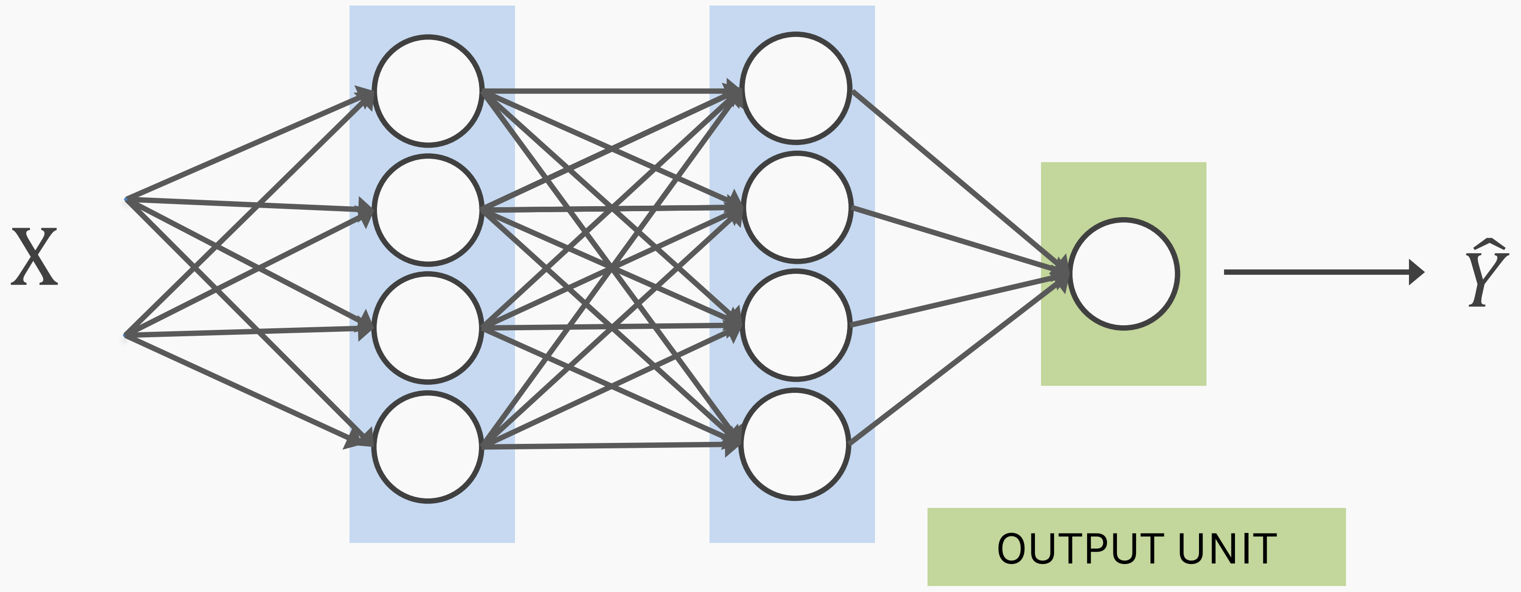
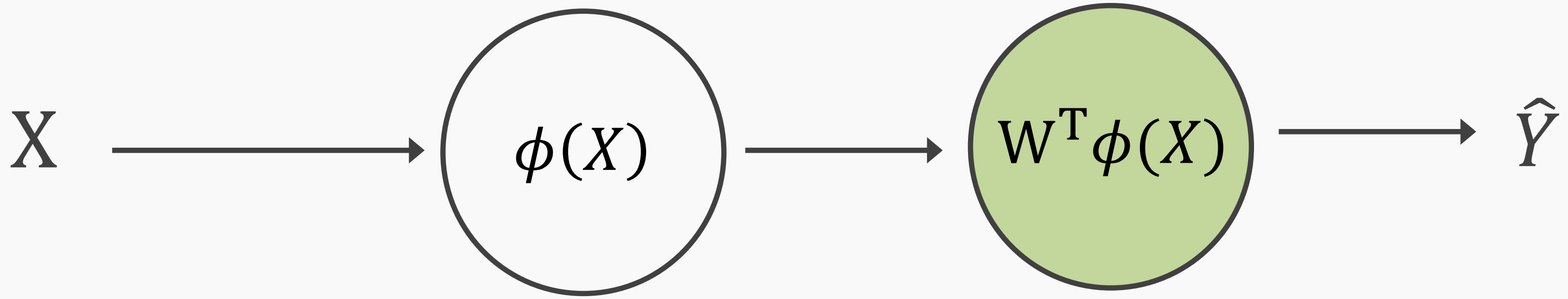


Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary Cross Entropy
Discrete	Multinoulli	Softmax	Cross Entropy
Continuous	Gaussian	?	MSE

Output unit for regression





$$X \Longrightarrow \phi(X) \Longrightarrow \hat{Y} = W^T \phi(X)$$

Output Units

Output Type	Output Distribution	Output layer	Cost Function
Binary	Bernoulli	Sigmoid	Binary Cross Entropy
Discrete	Multinoulli	Softmax	Cross Entropy
Continuous	Gaussian	Linear	MSE
Continuous	Arbitrary	-	GANS

Design Choices

Activation function

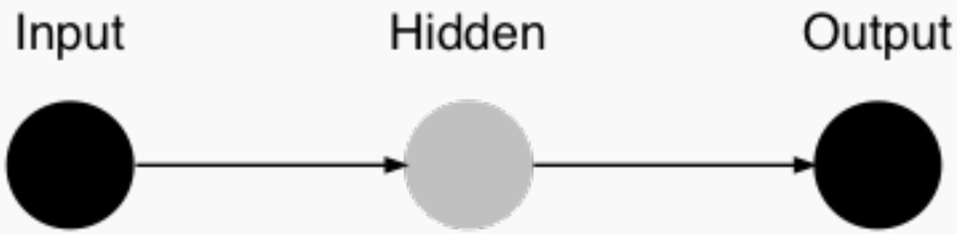
Loss function

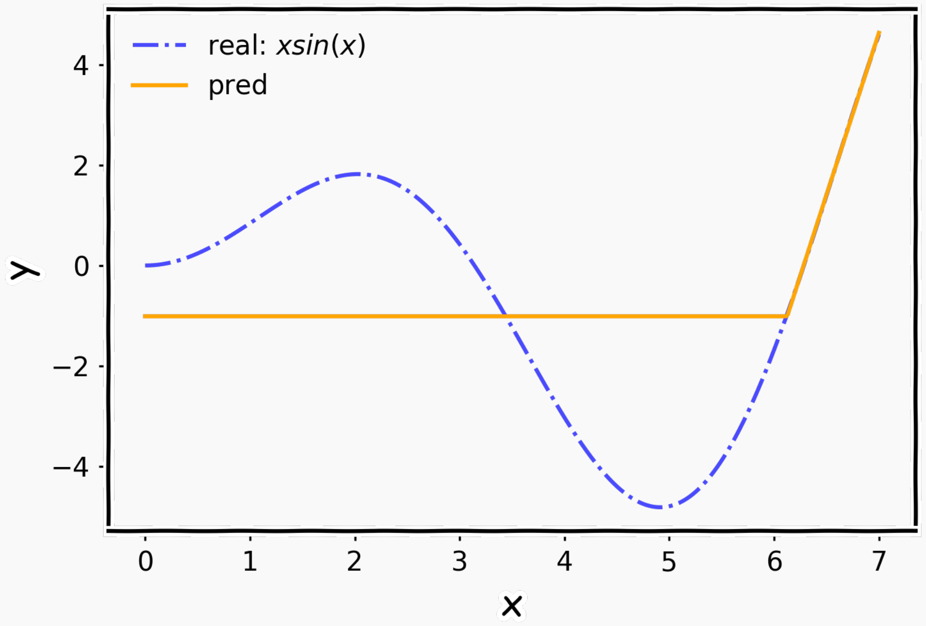
Output units

Architecture

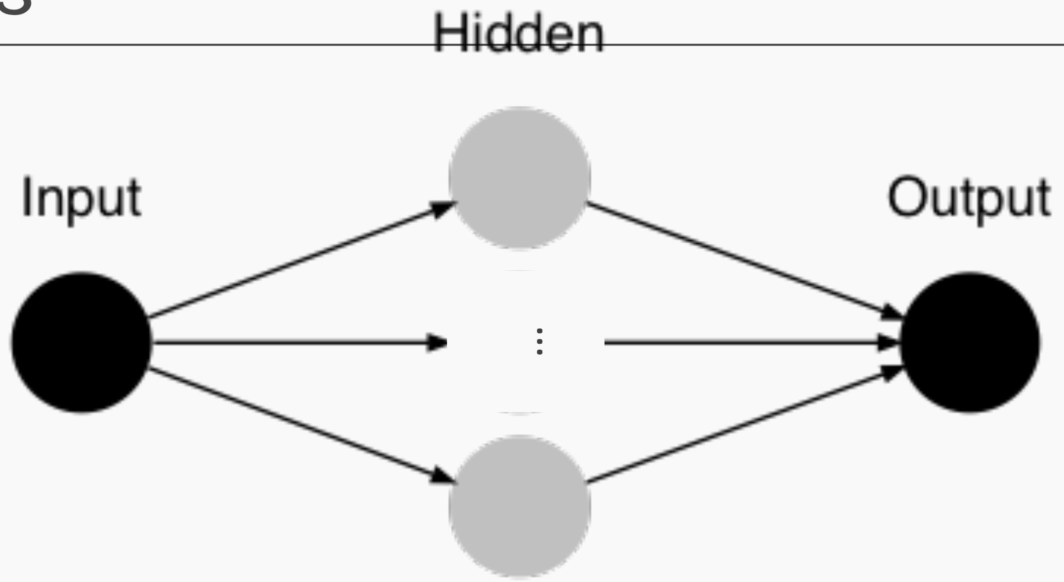
Optimizer

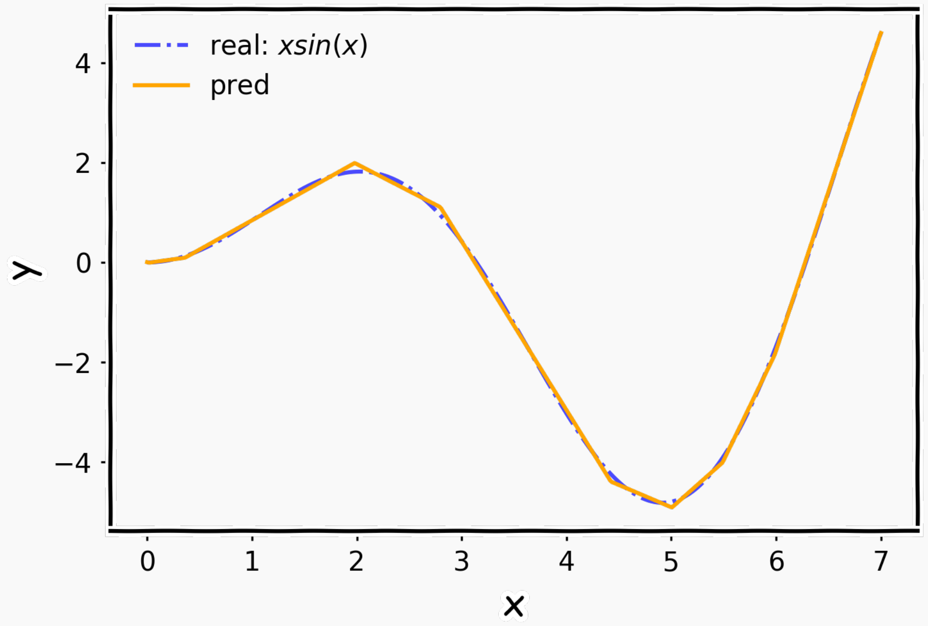
Number of nodes



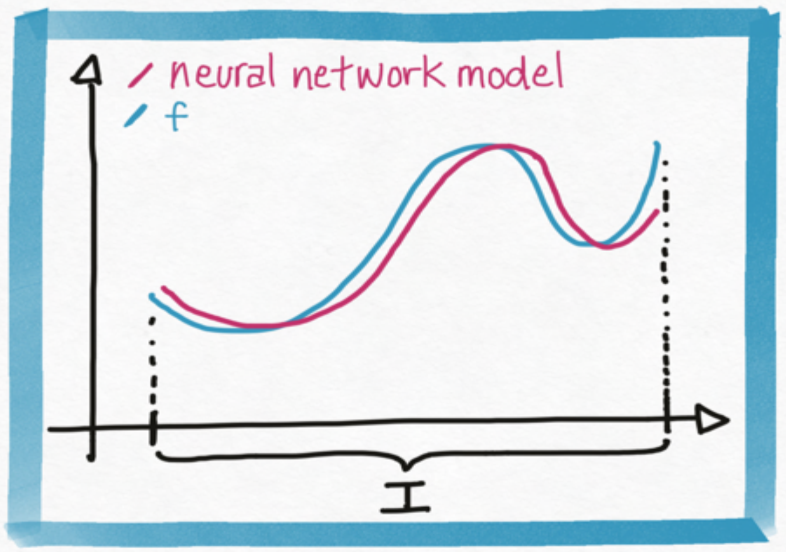


Number of nodes





Neural Networks as Universal Approximators

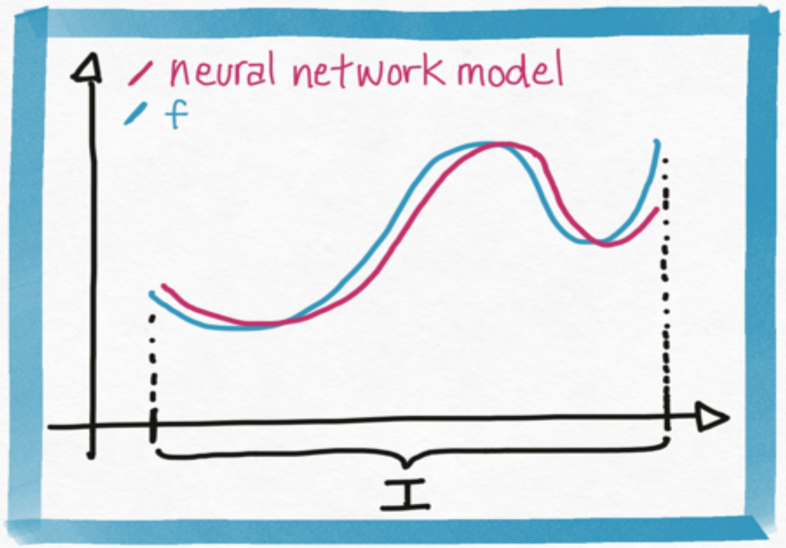


We have seen that neural networks can represent complex functions, but are there limitations on what a neural network can express?

Theorem:

For any continuous function f defined on a bounded domain, we can find a neural network that approximates f with an arbitrary degree of accuracy.

Neural Networks as Universal Approximators



We have seen that neural networks can represent complex functions, but are there limitations on what a neural network can express?

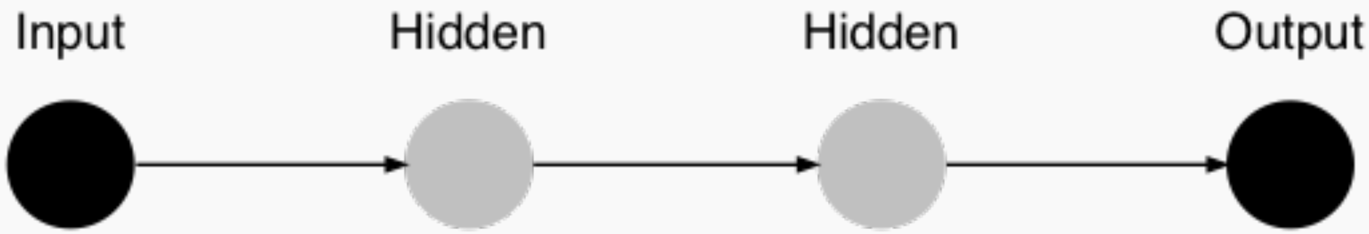
Theorem:

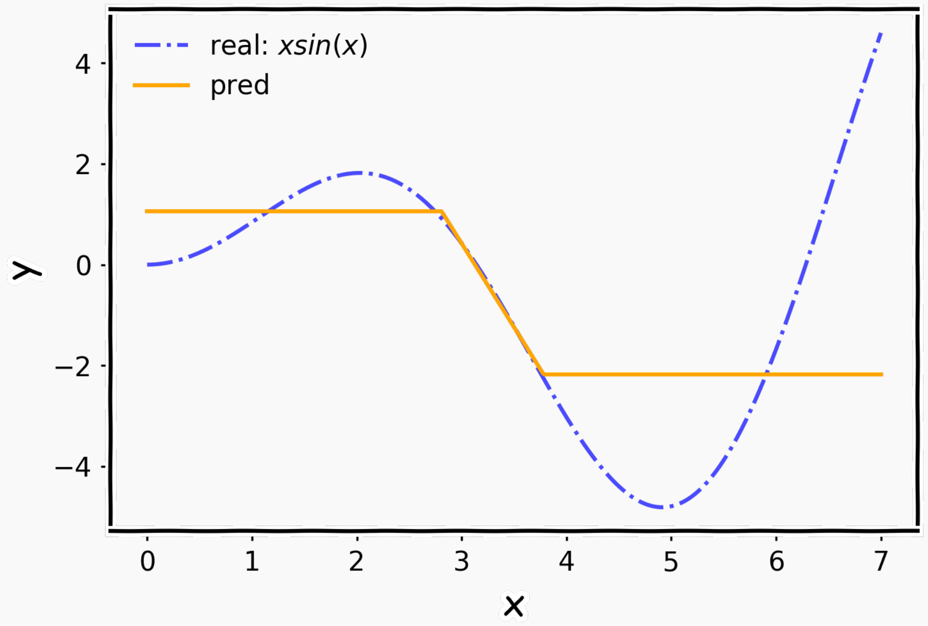
For any continuous function f defined on a bounded domain, we can find a neural network that approximates f with an arbitrary degree of accuracy.

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

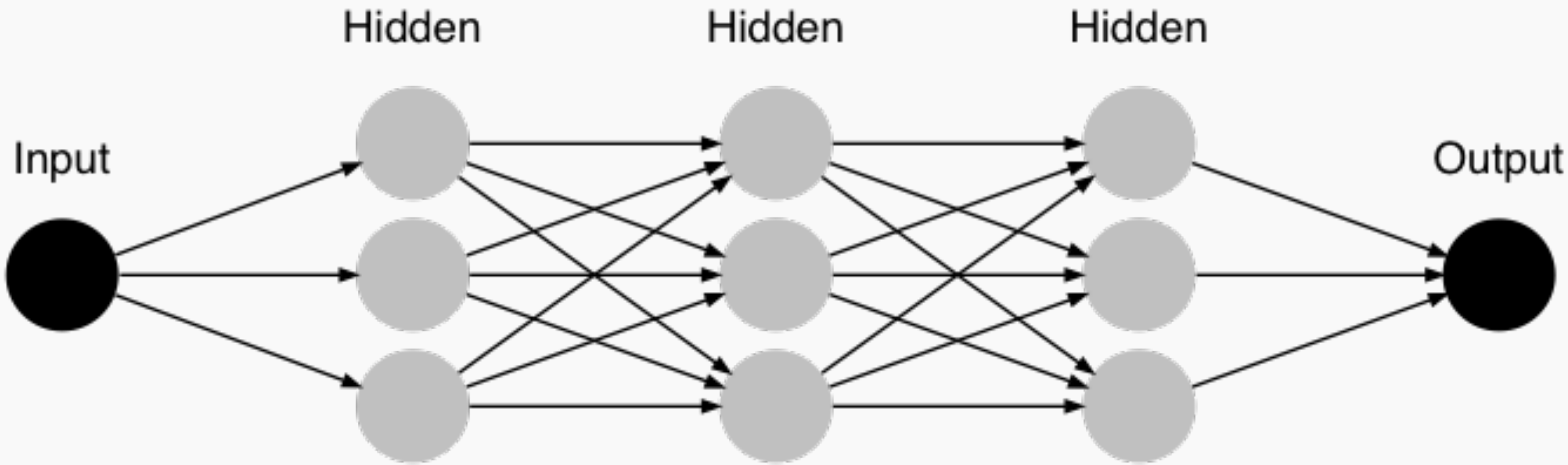
So why deeper?

Layers

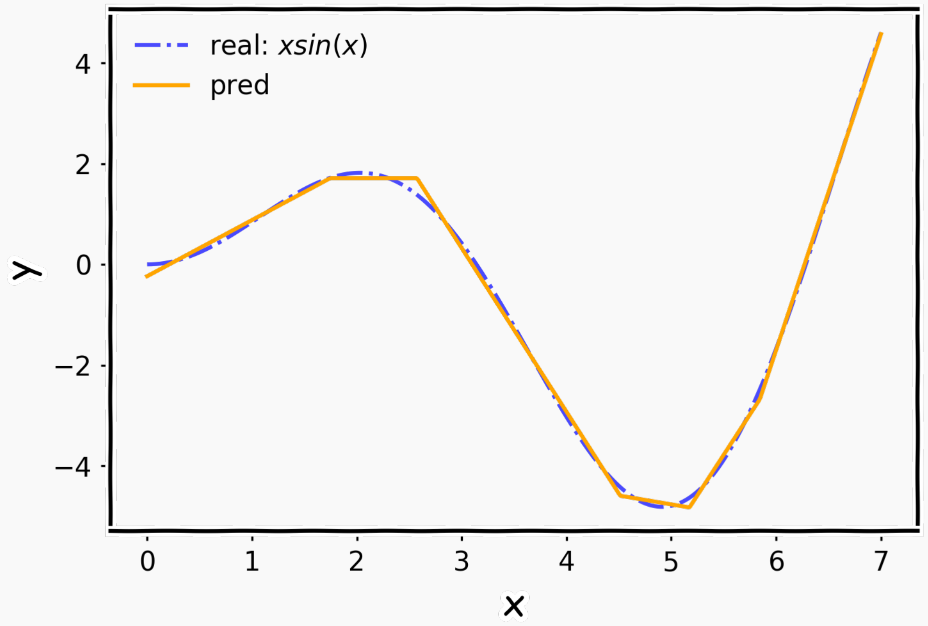

Input
Hidden
Hidden
Output


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

Layers



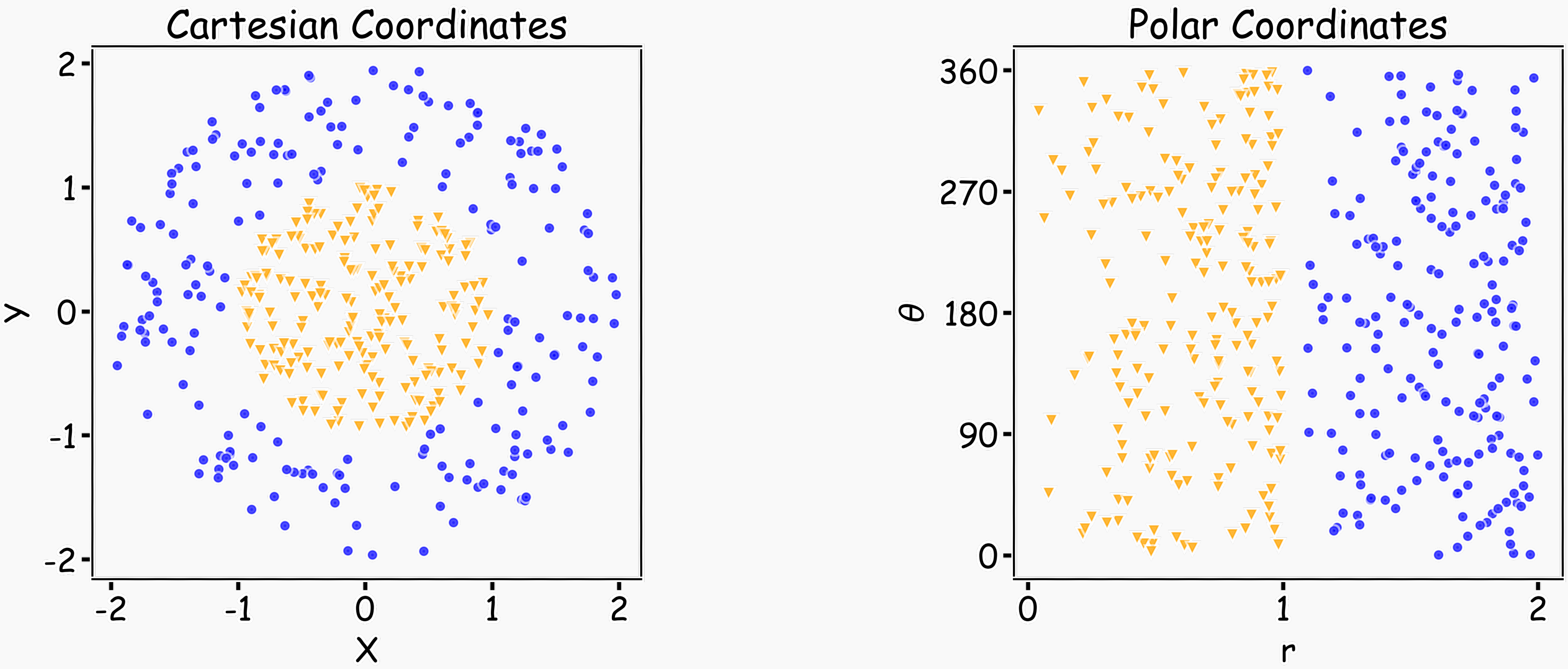
Hidden
Hidden
Hidden
Input
Output



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

Why layers?

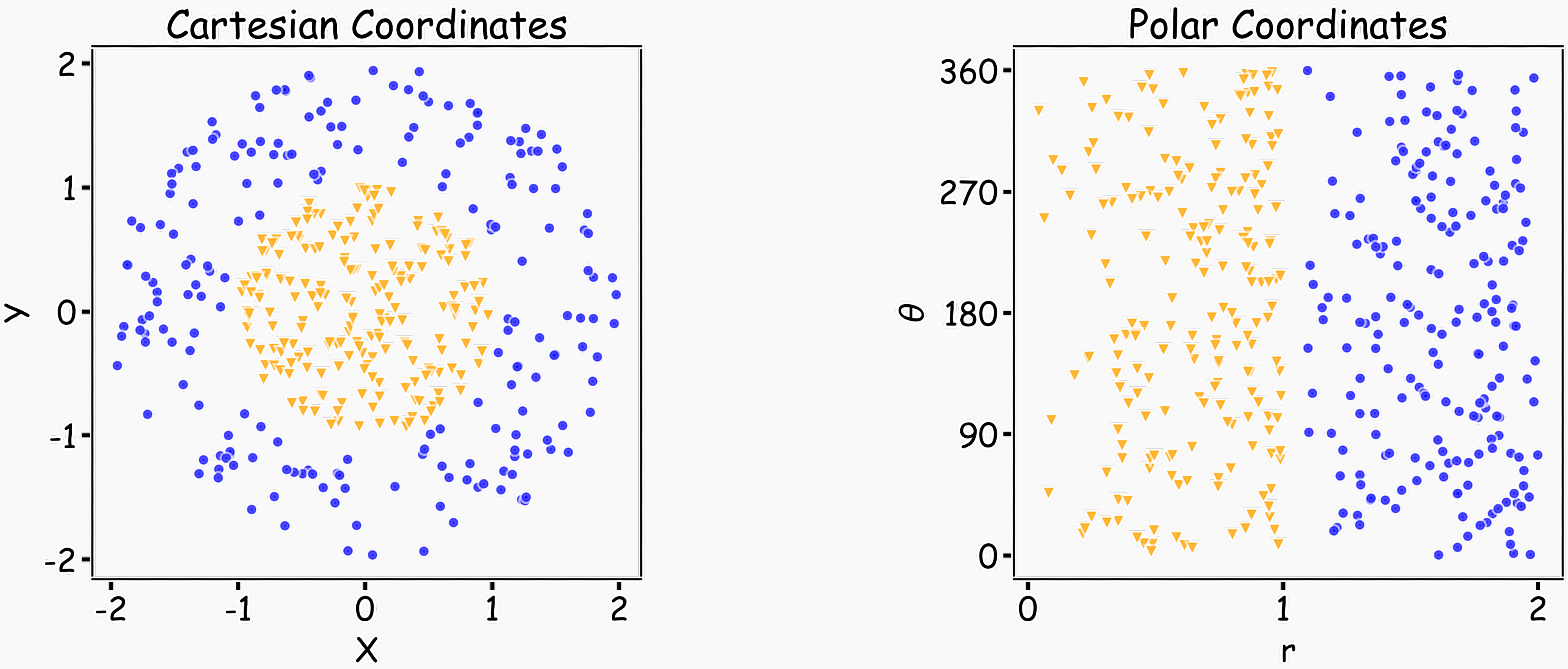
Representation matters!



Neural networks can **learn useful representations** for the problem. This is another reason why they can be so powerful!

Why layers?

Representation matters!



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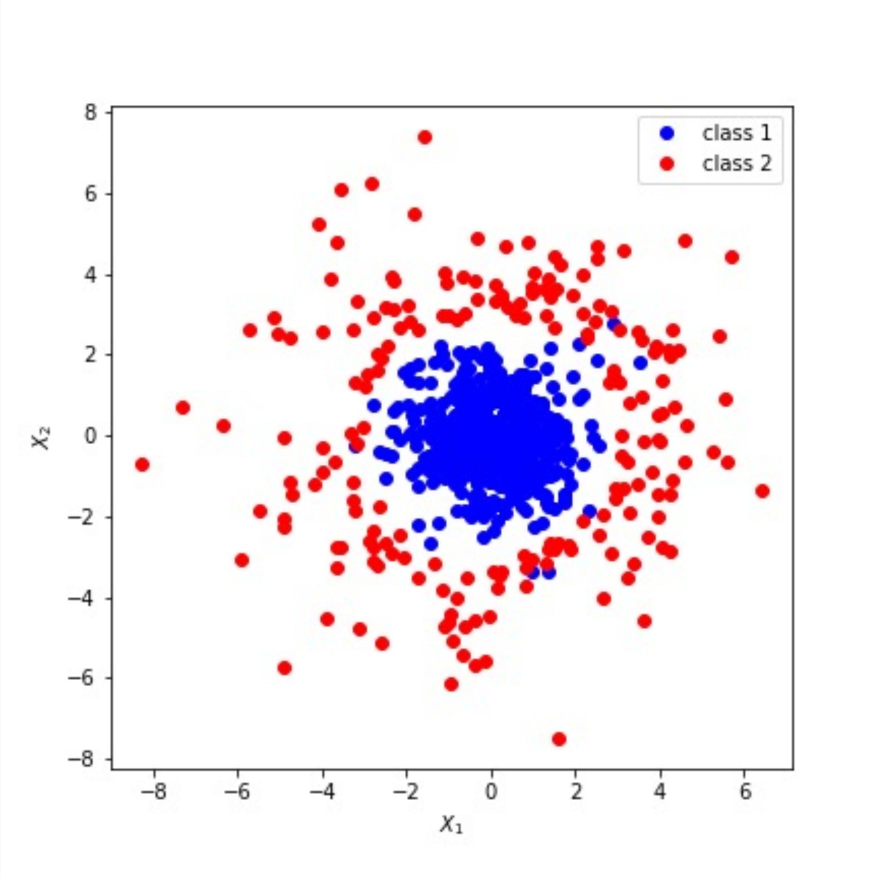
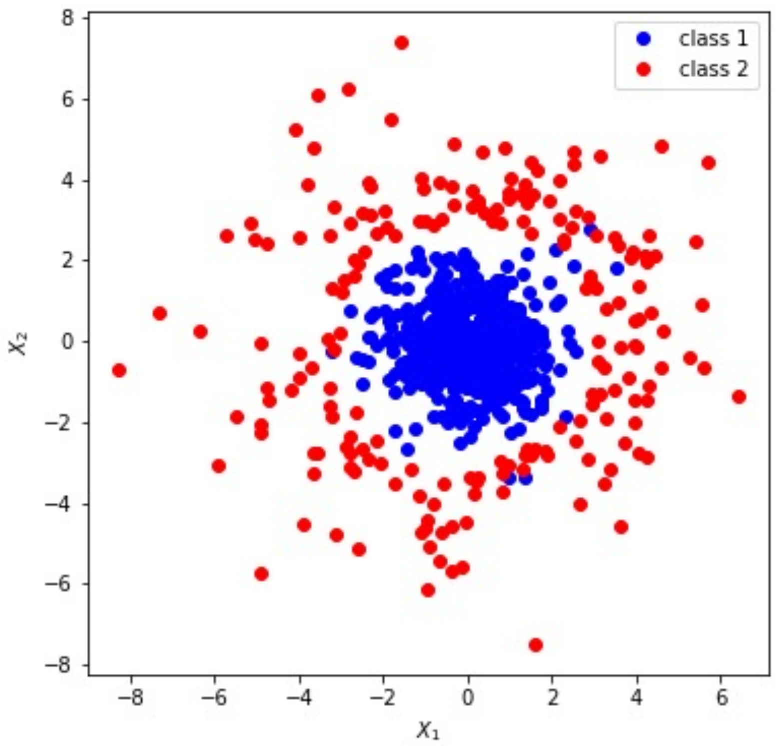
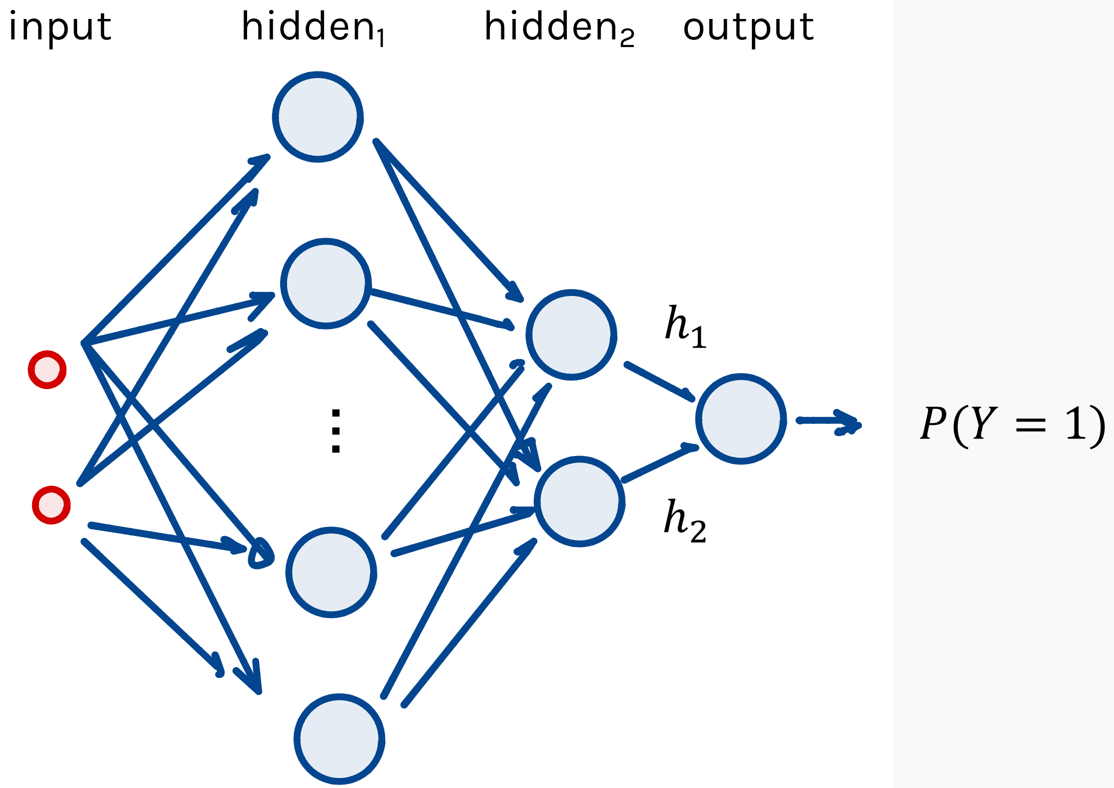
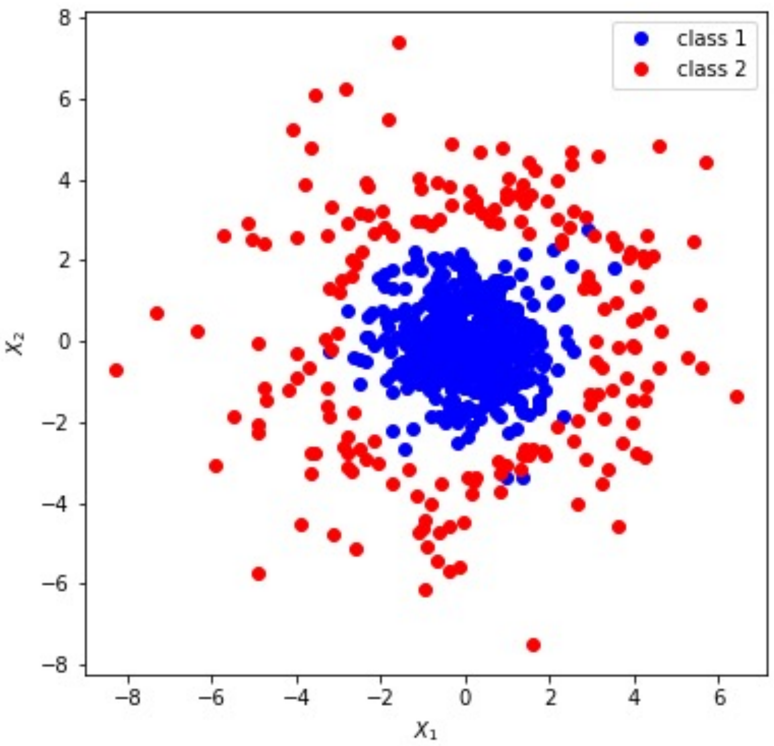


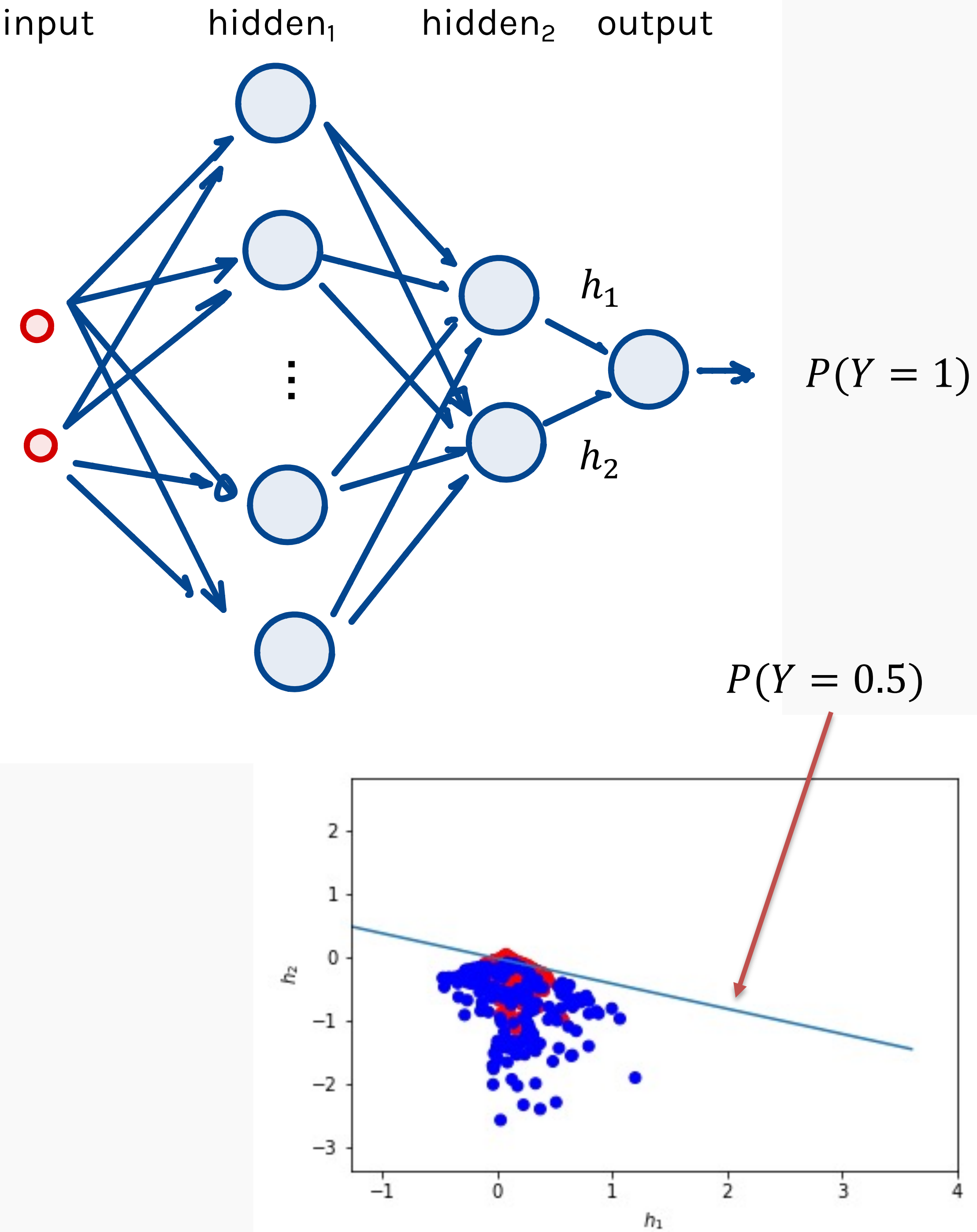
class 1
class 2
X_1
X_2
8
6
4
2
0
−2
−4
−6
−8
−8
−6
−4
−2
0
2
4
6


class 1
class 2
X_1
X_2
−8 −6 −4 −2 0 2 4 6
8 6 4 2 0 −2 −4 −6 −8


input
hidden$_1$
hidden$_2$
output
h_1
h_2
$P(Y = 1)$

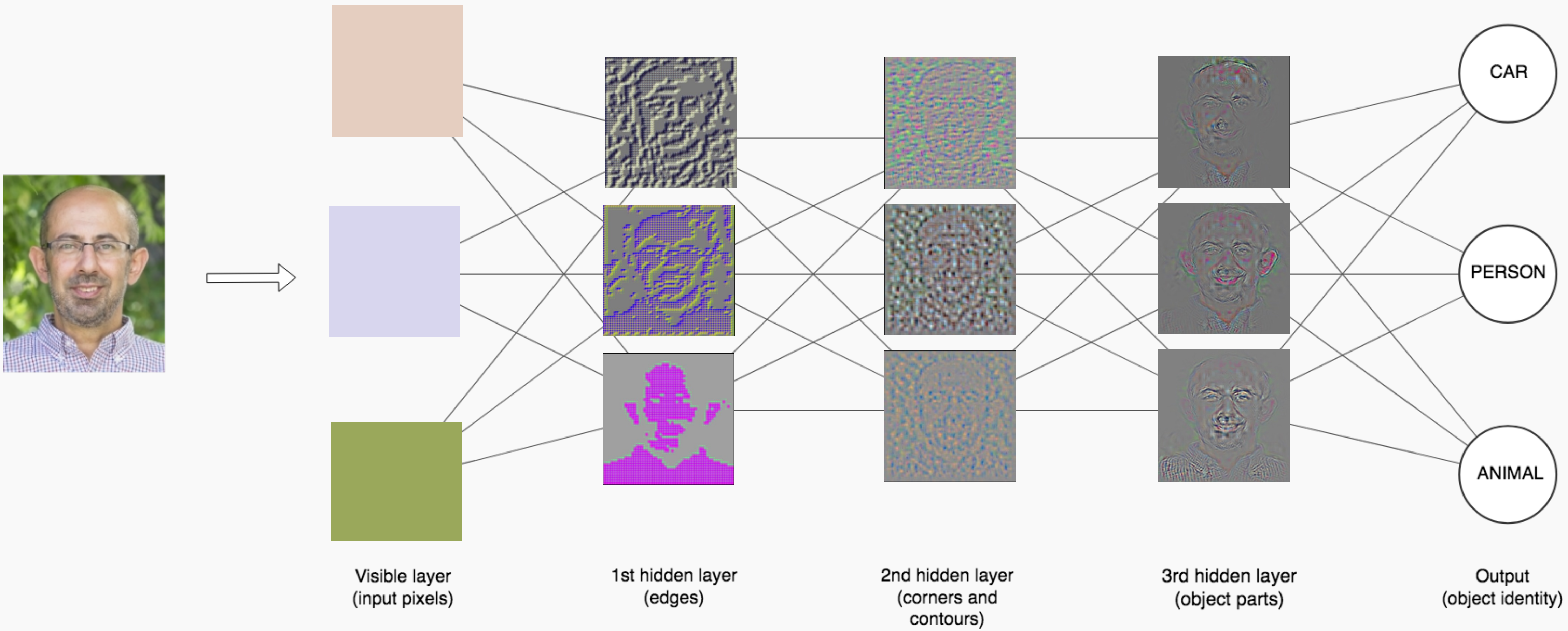


class 1
class 2
X_1
X_2



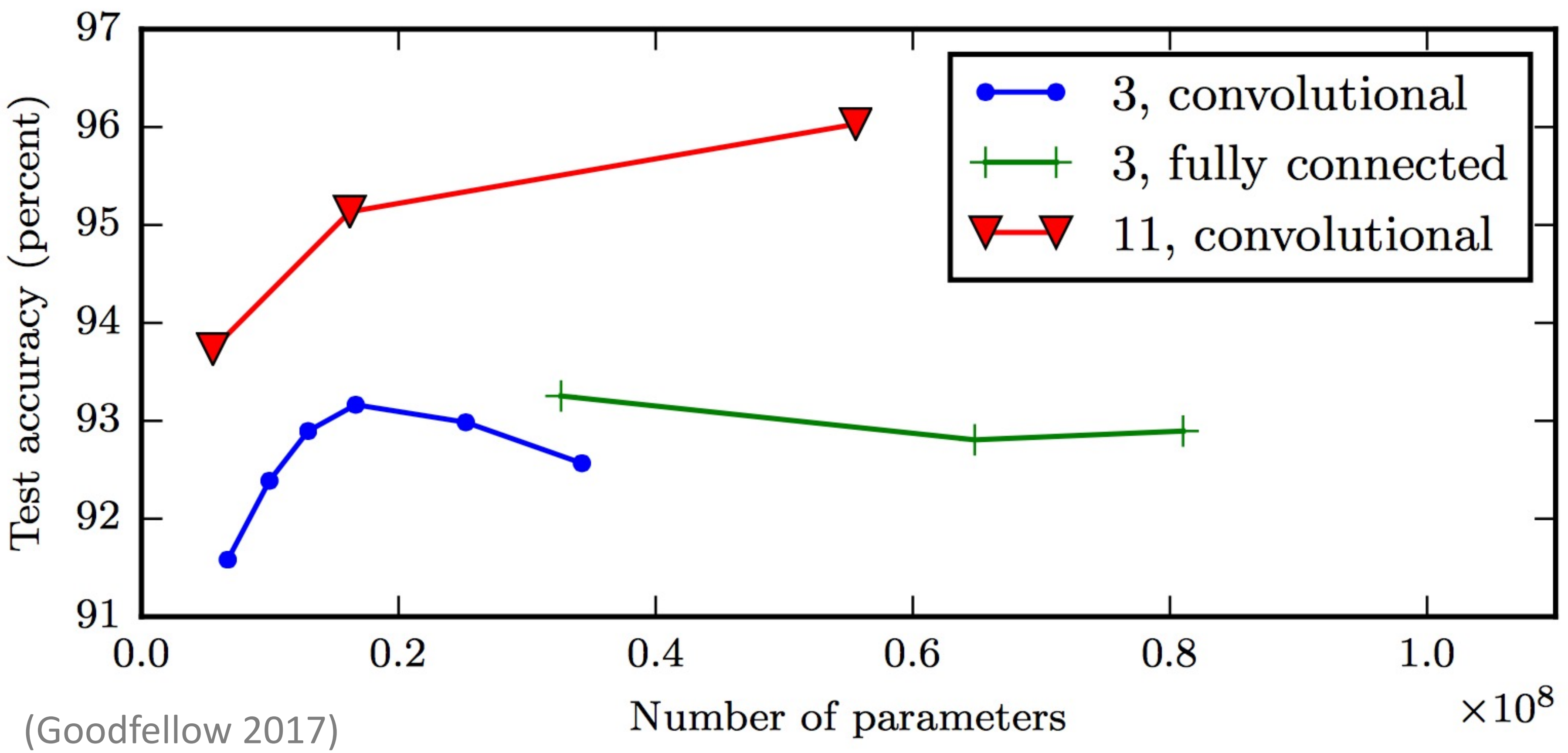
input
hidden$_1$
hidden$_2$
output
h_1
h_2
$P(Y = 1)$
$P(Y = 0.5)$
h_1
h_2

Depth = Repeated Compositions



Shallow Nets Overfit More

Depth helps, and it's not just because of more parameters



(Goodfellow 2017)

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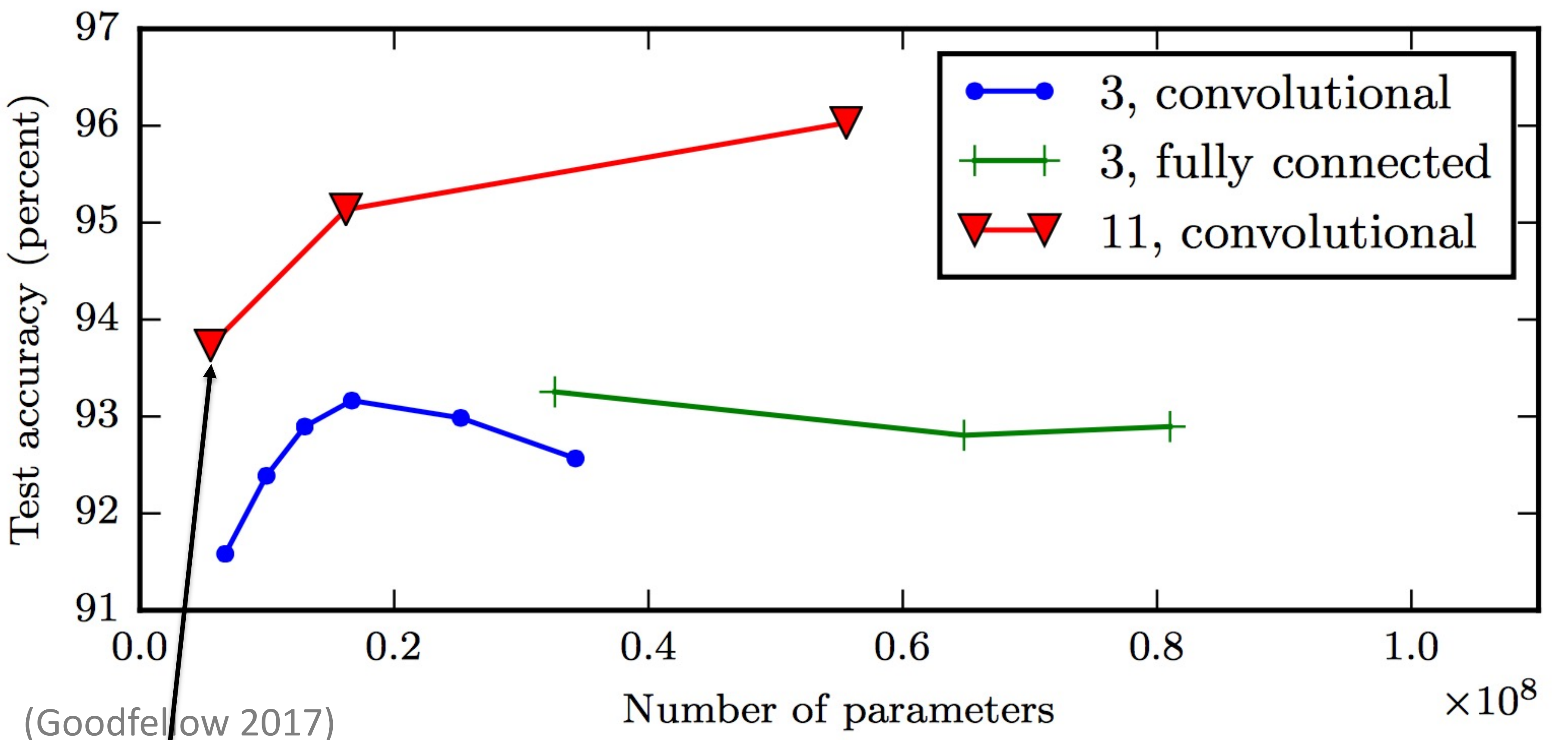

(Goodfellow 2017)

The **11-layer net** generalizes better on the test set when controlling for number of parameters.

Shallow Nets Overfit More

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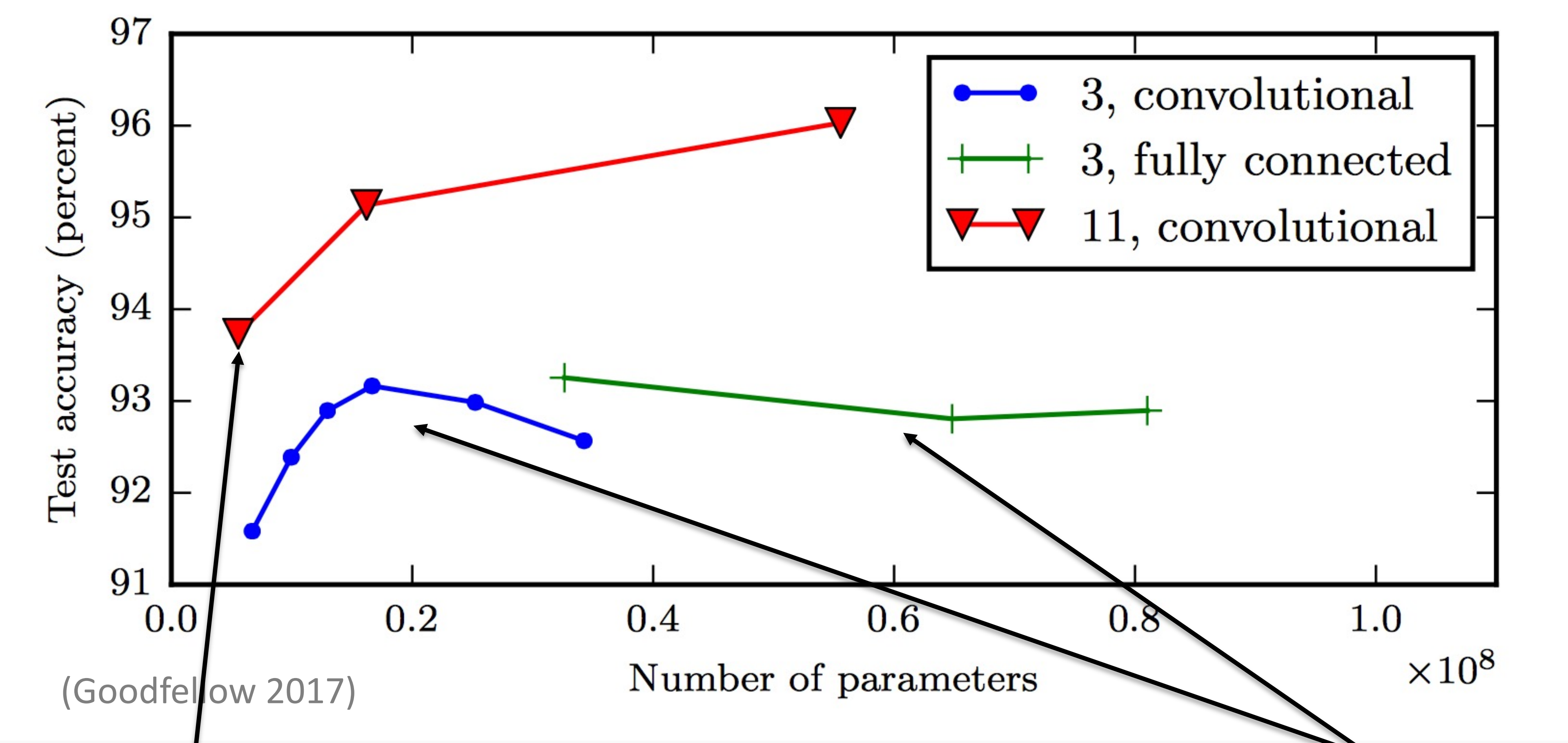


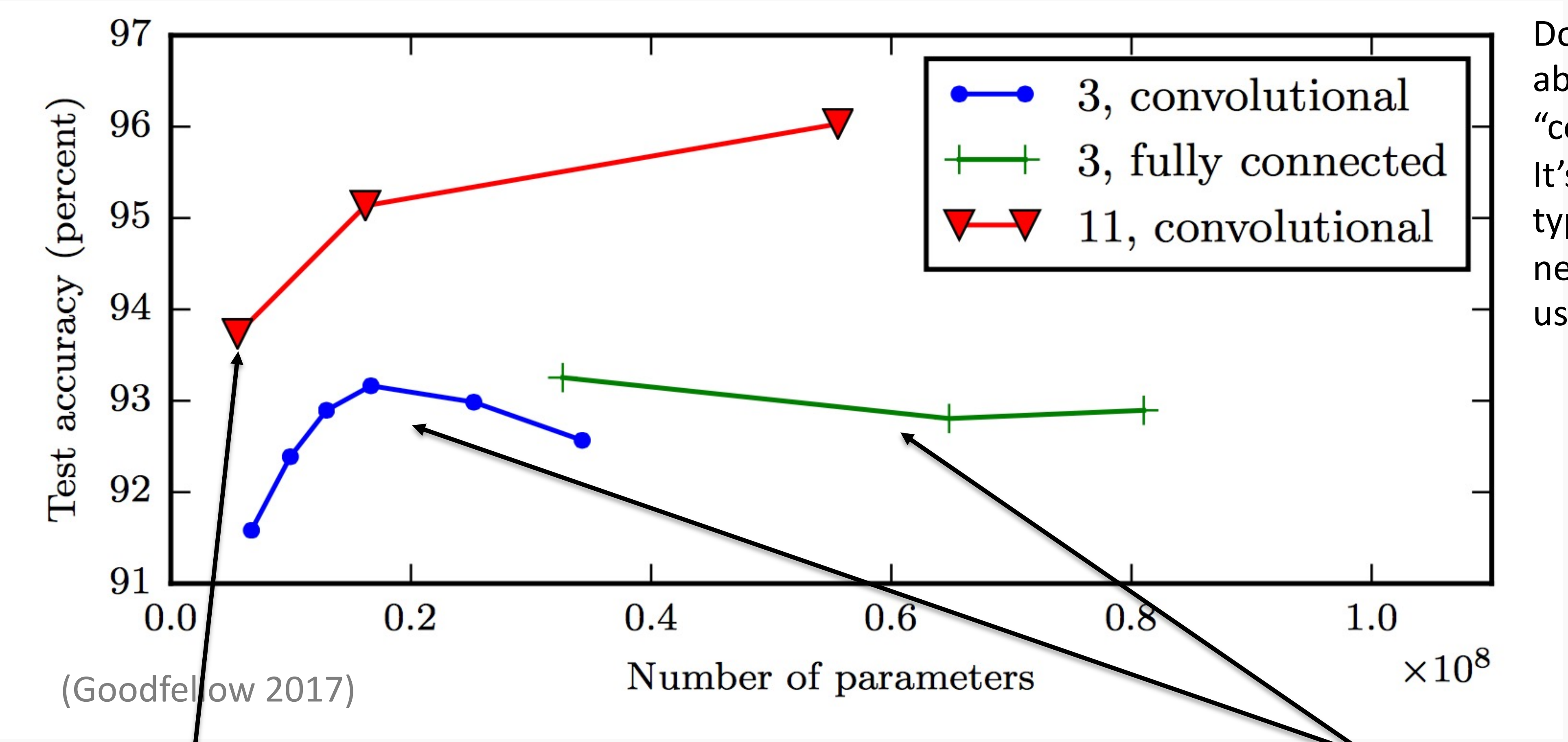
(Goodfellow 2017)

The **11-layer net** generalizes better on the test set when controlling for number of parameters.

The 3-layer nets perform worse on the test set, even with similar number of total parameters.

Shallow Nets Overfit More

Depth helps, and it's not just because of more parameters



Don't worry about this word "convolutional". It's just a special type of neural network, often used for images.

The **11-layer net** generalizes better on the test set when controlling for number of parameters.

The 3-layer nets perform worse on the test set, even with similar number of total parameters.