

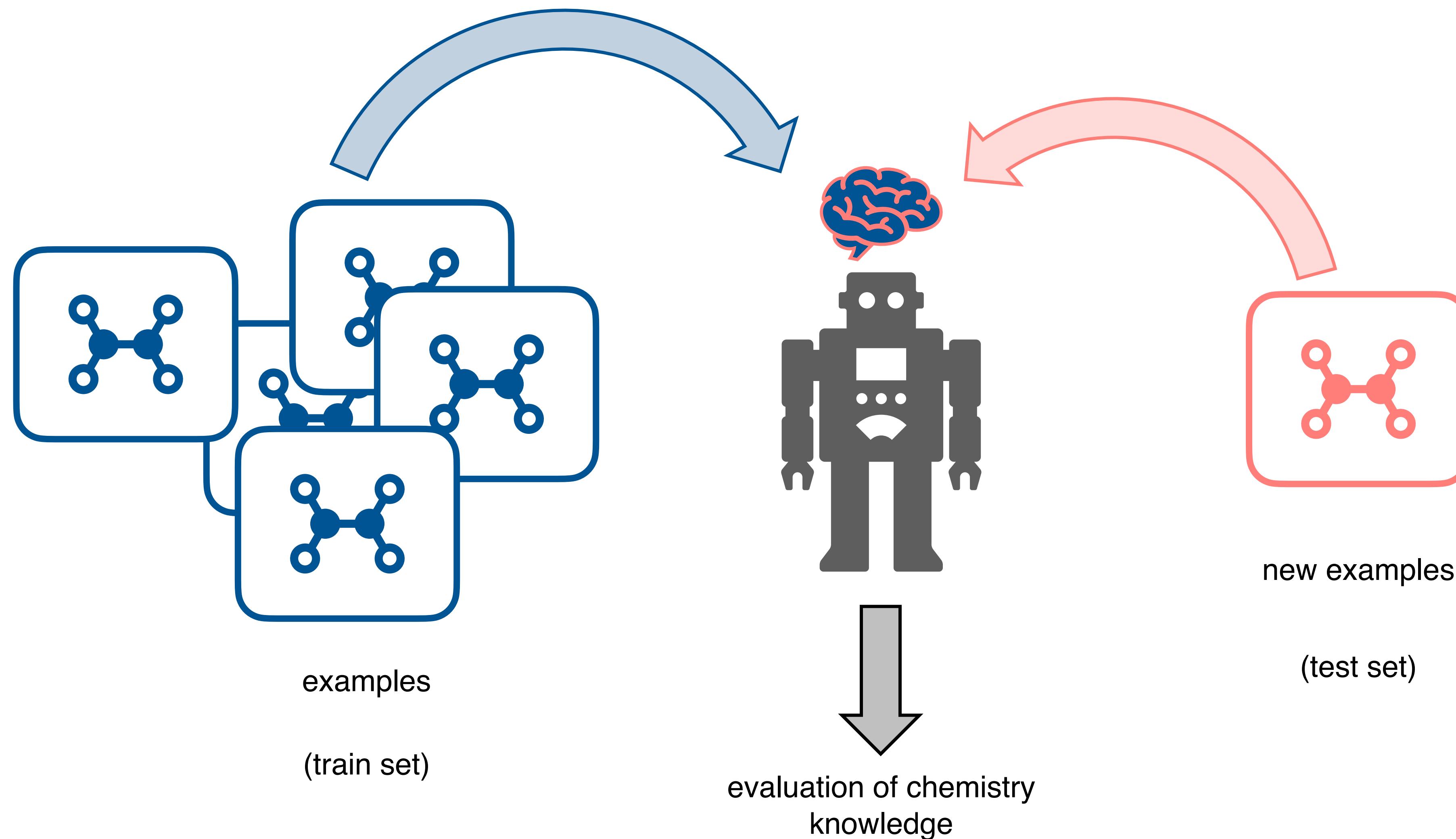
# *Machine Learning for Chemists*

## *– Feed Forward Neural Networks –*

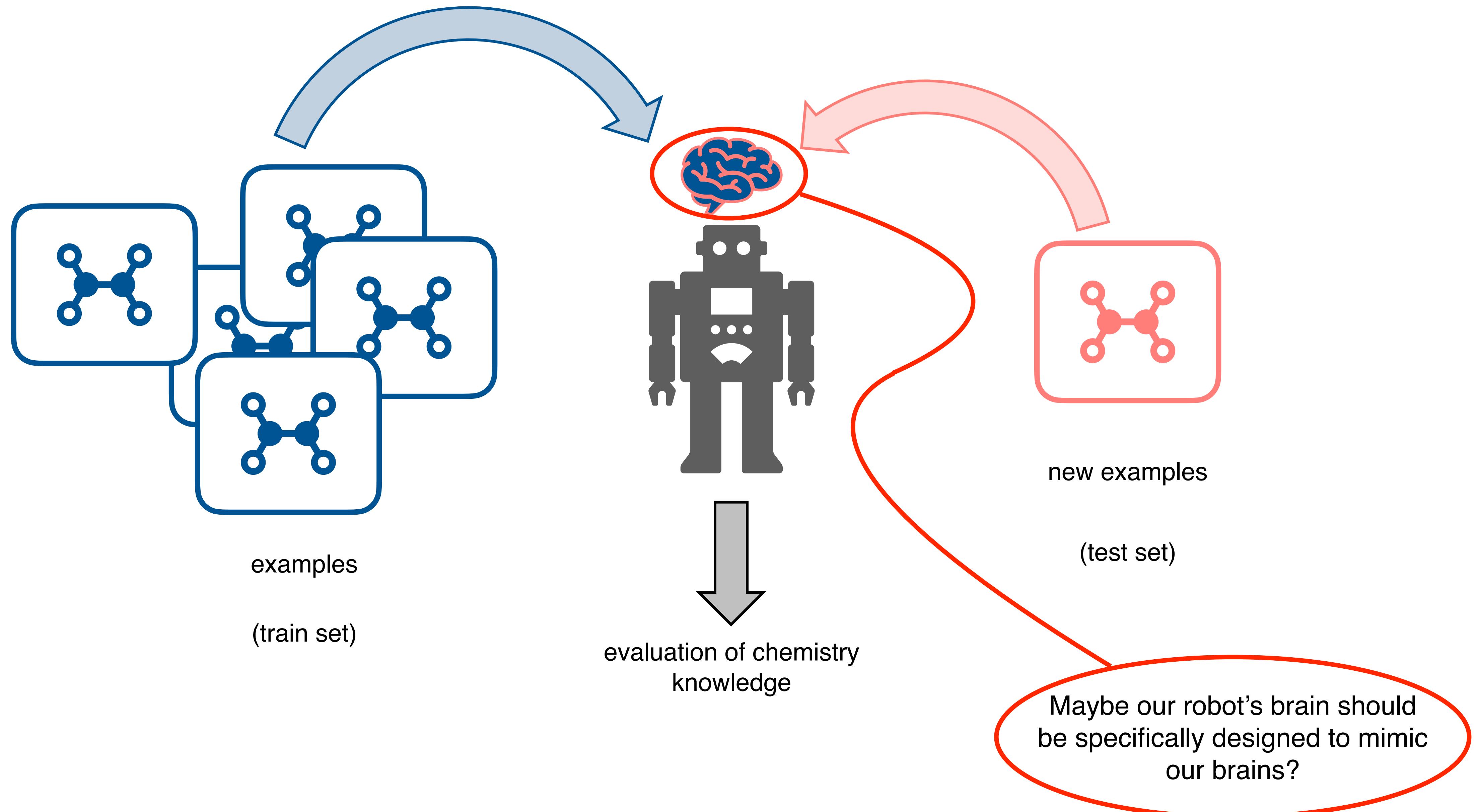
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4 March 2024

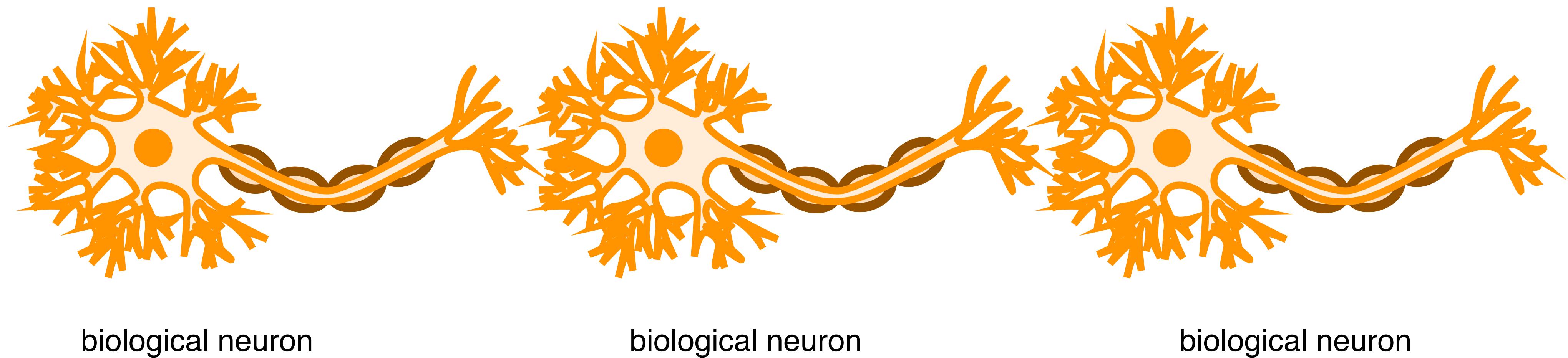
# What Is Deep Learning?



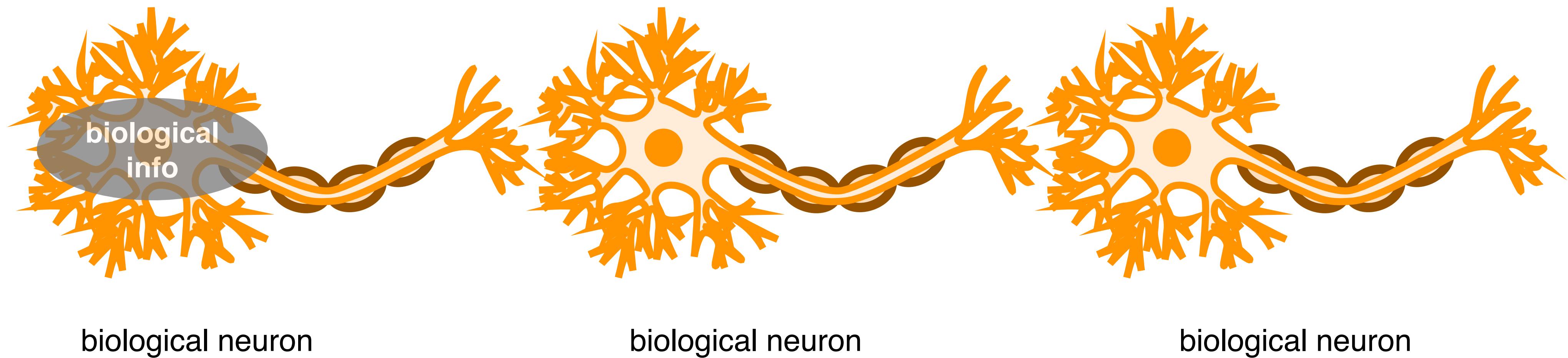
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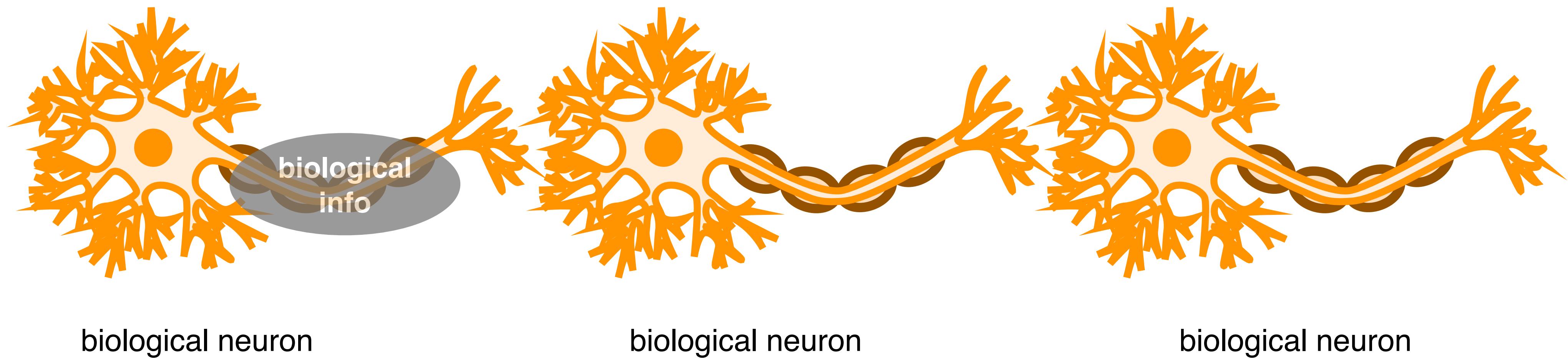
Our neurons receive (biological) information, process the information, and send it to other neurons.



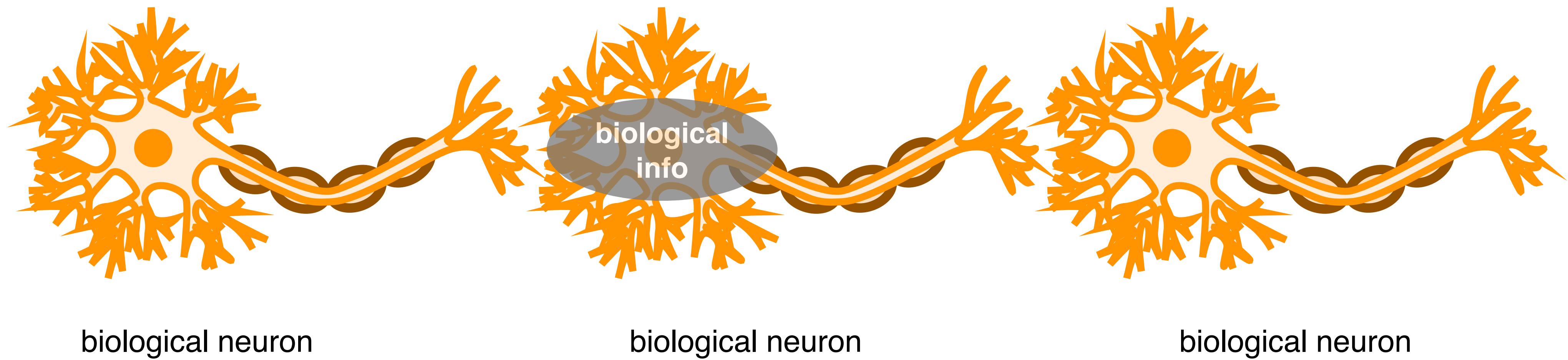
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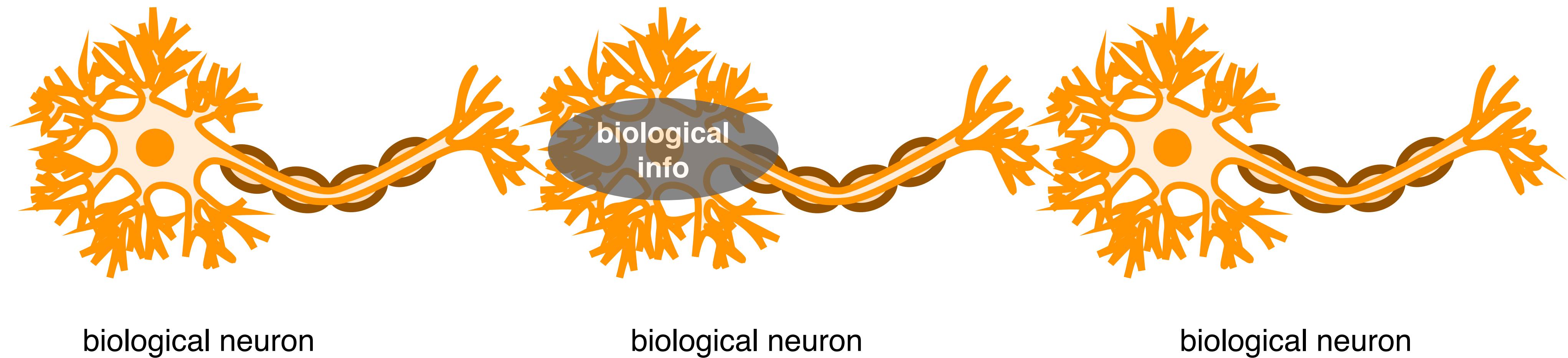
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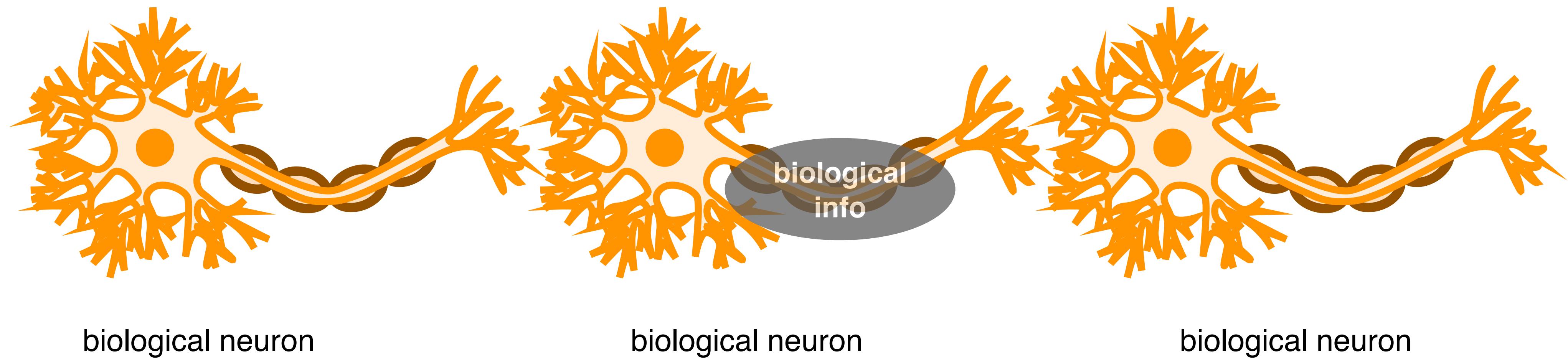
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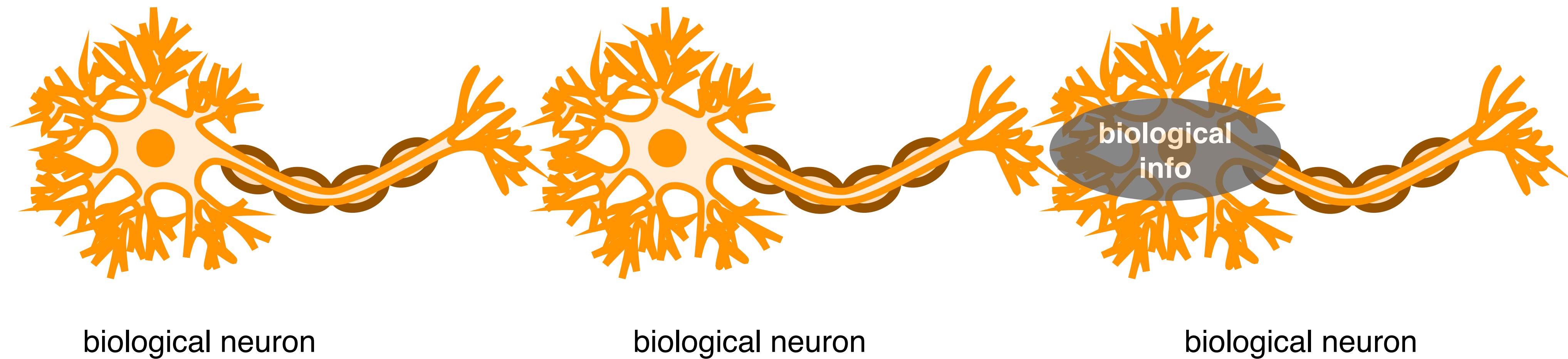
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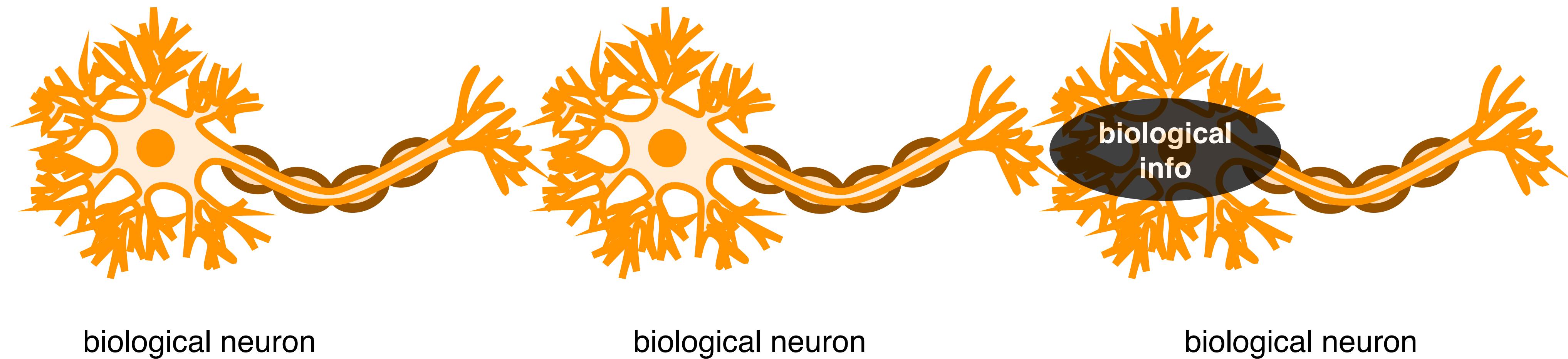
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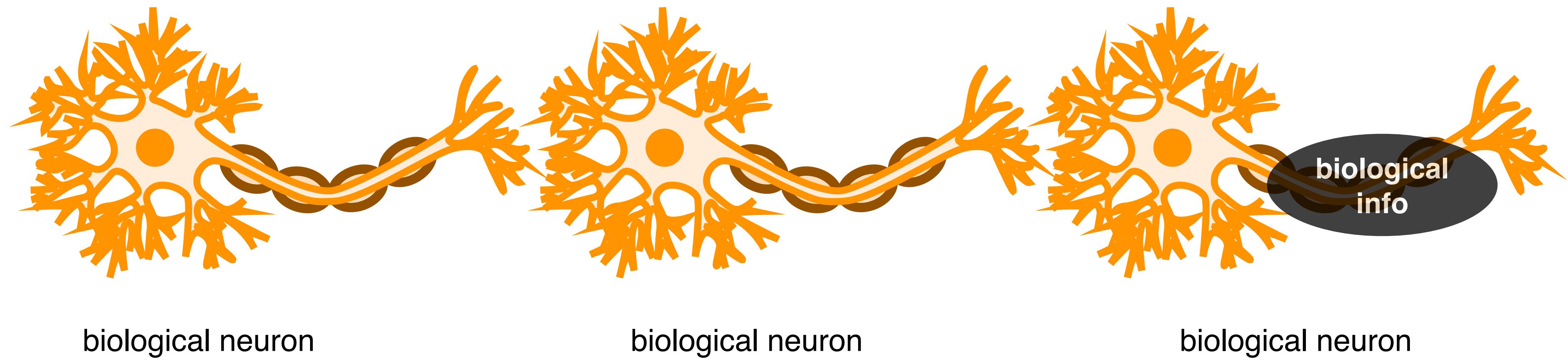
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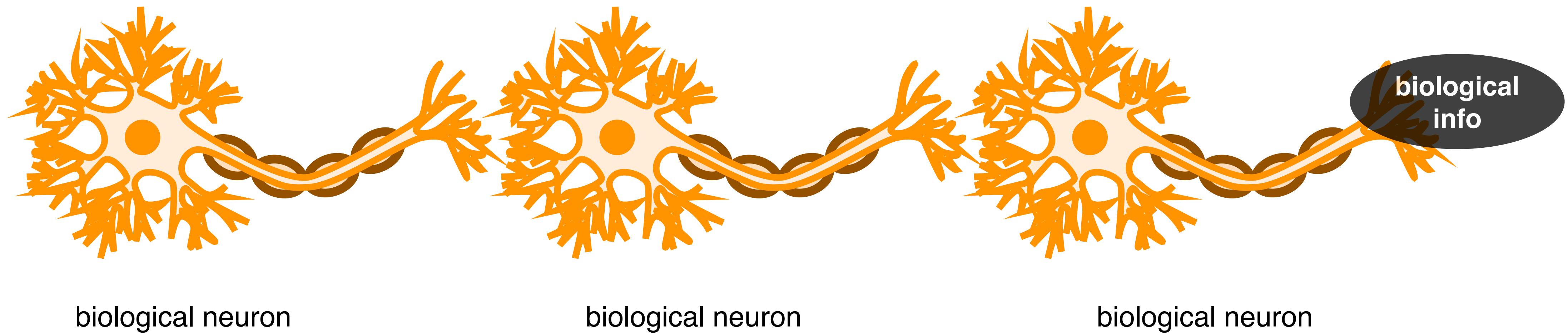
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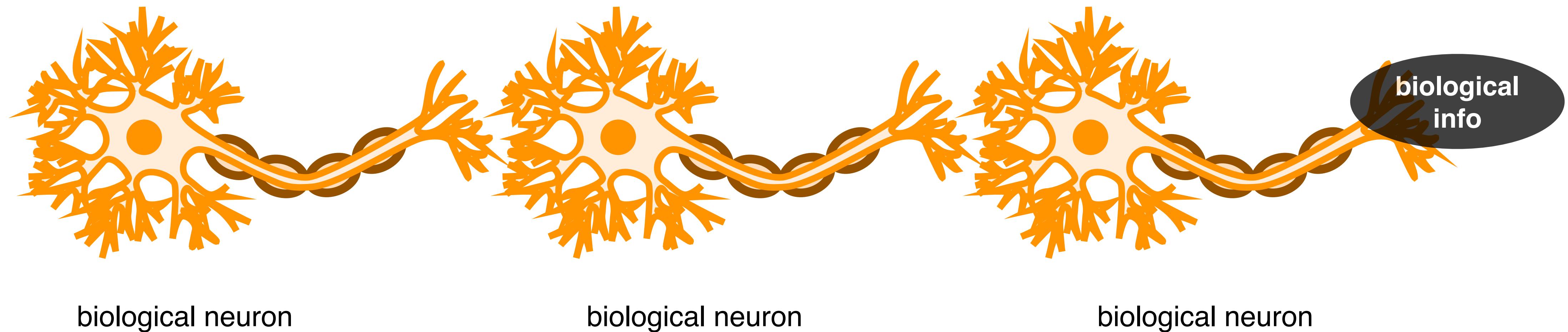
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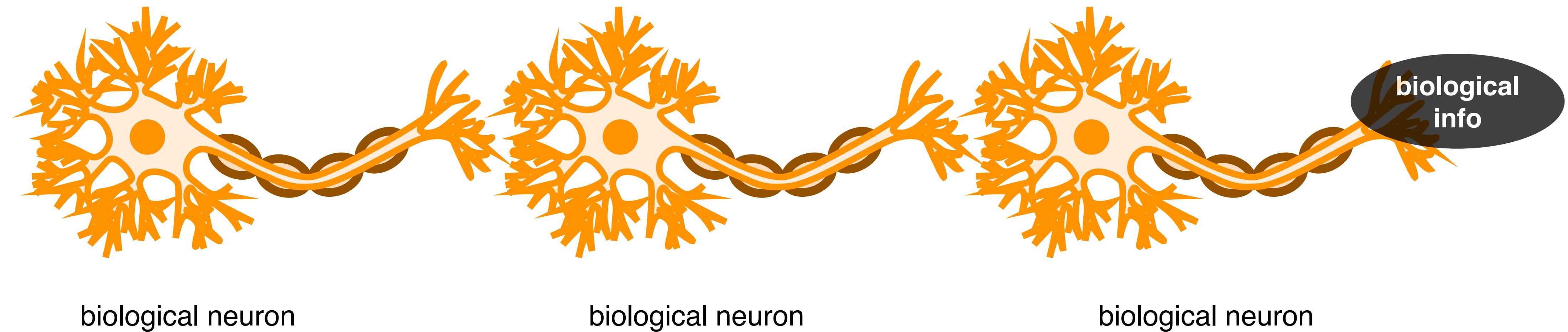
biological neuron

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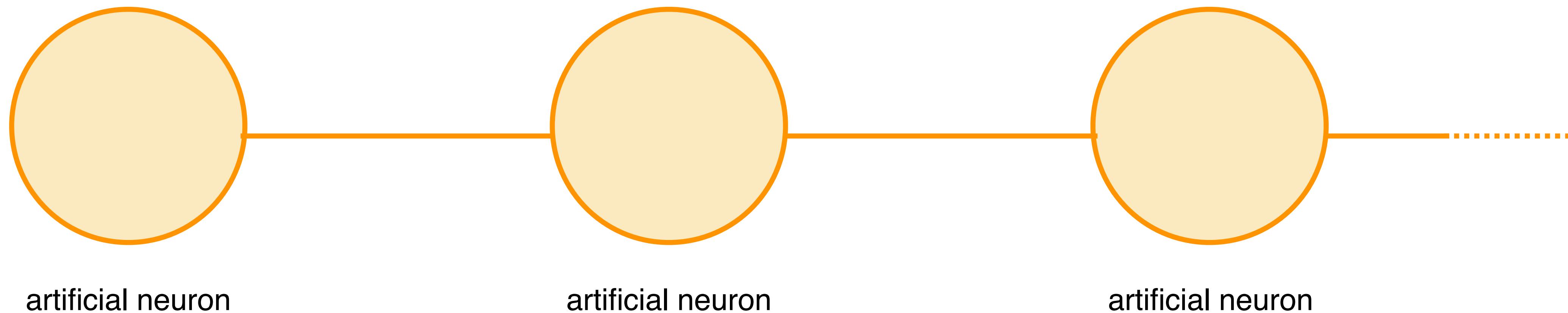
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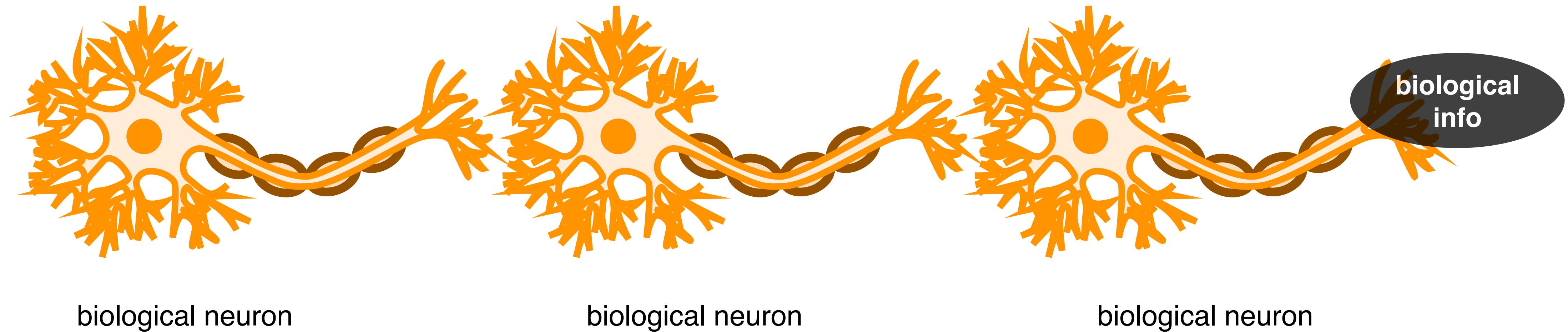


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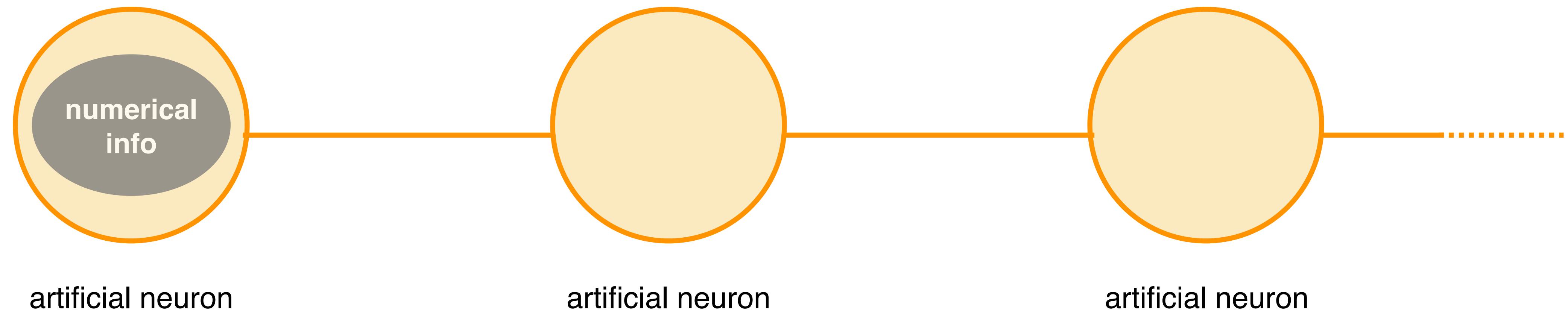




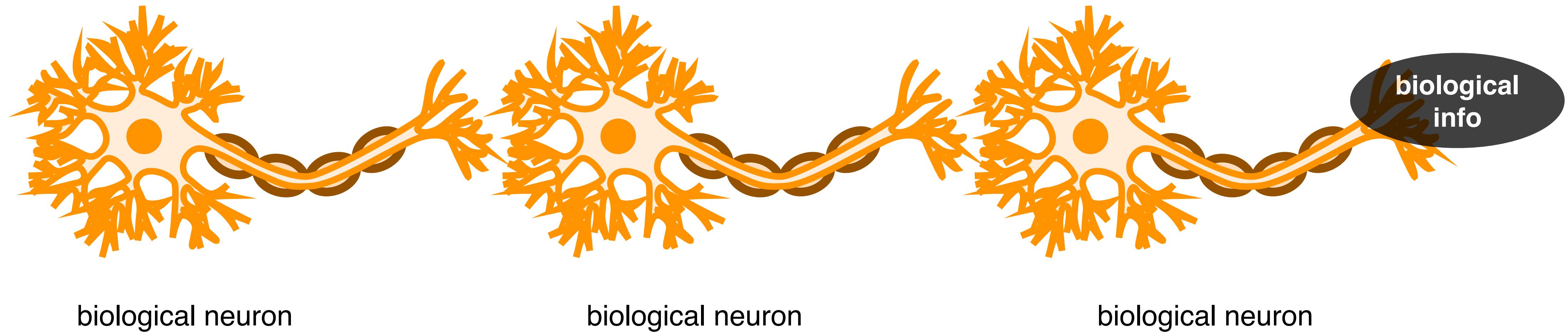
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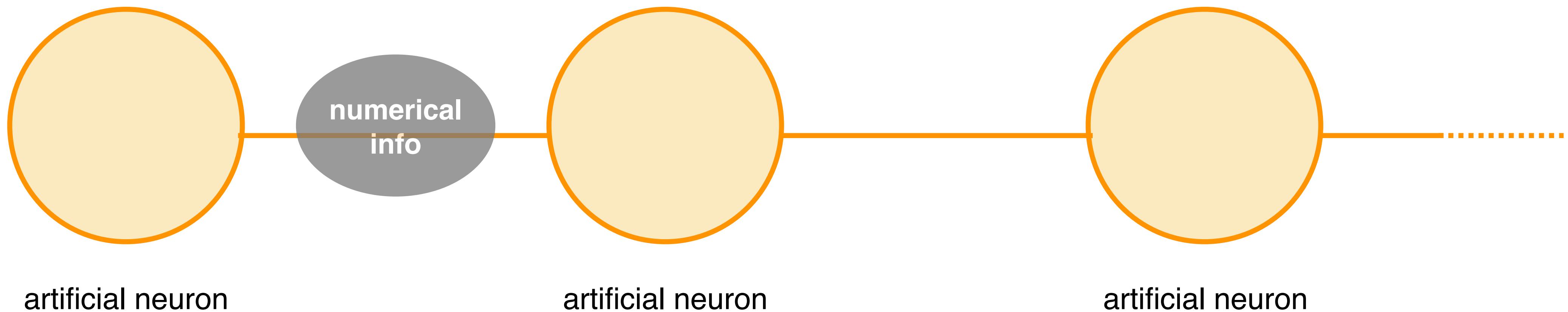
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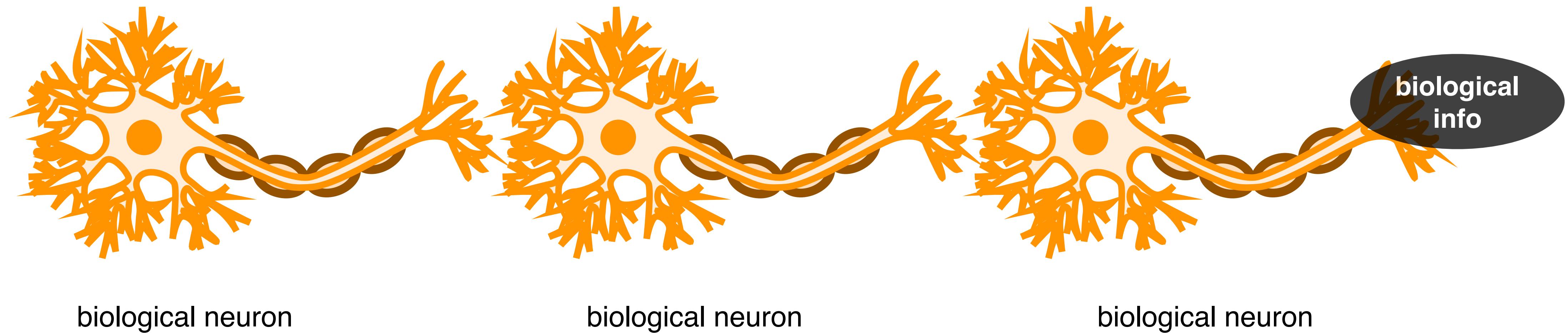
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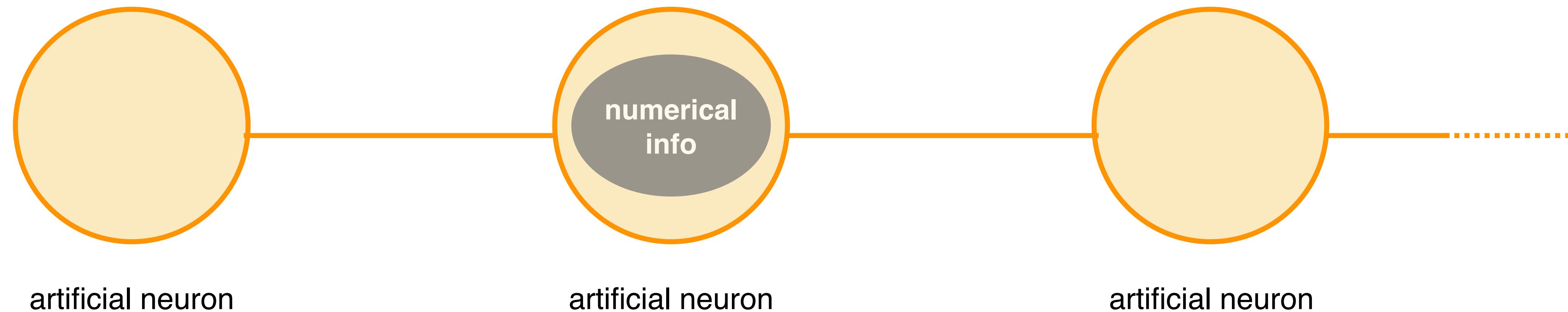
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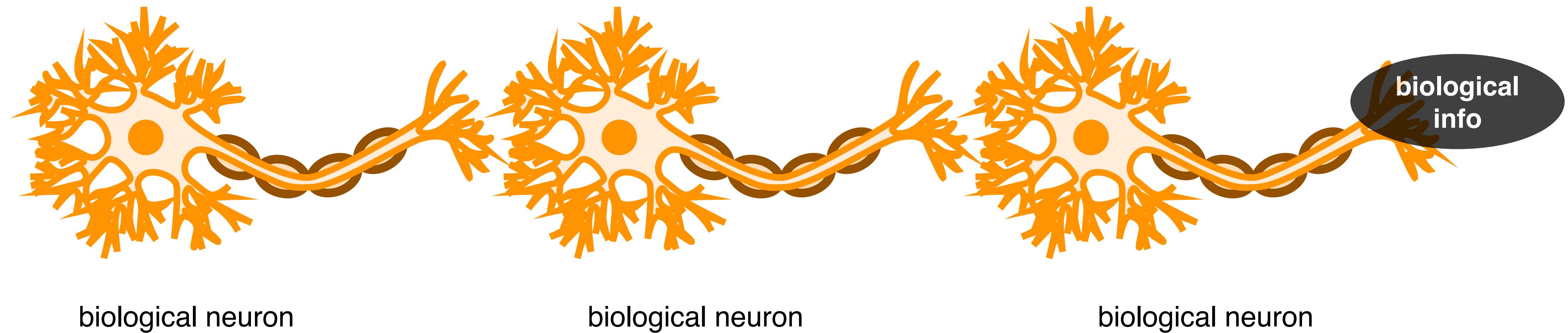
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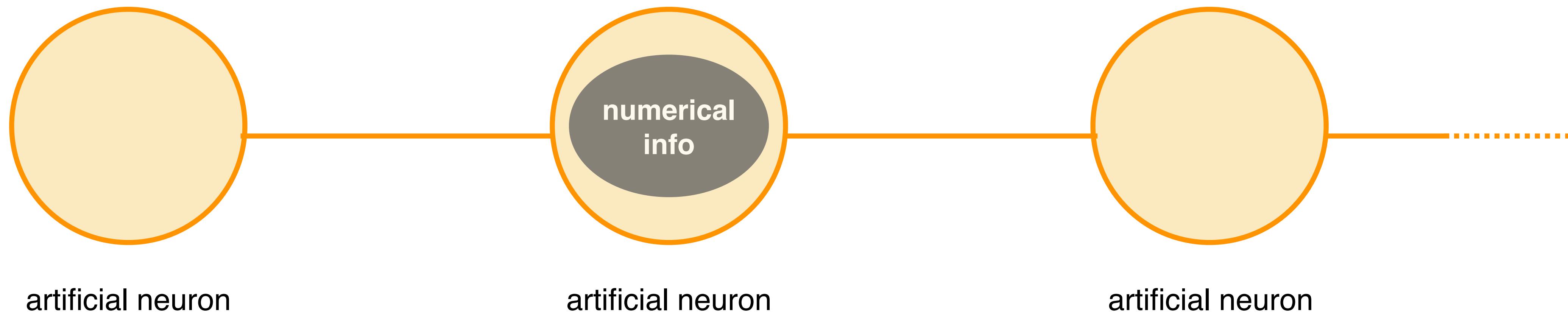
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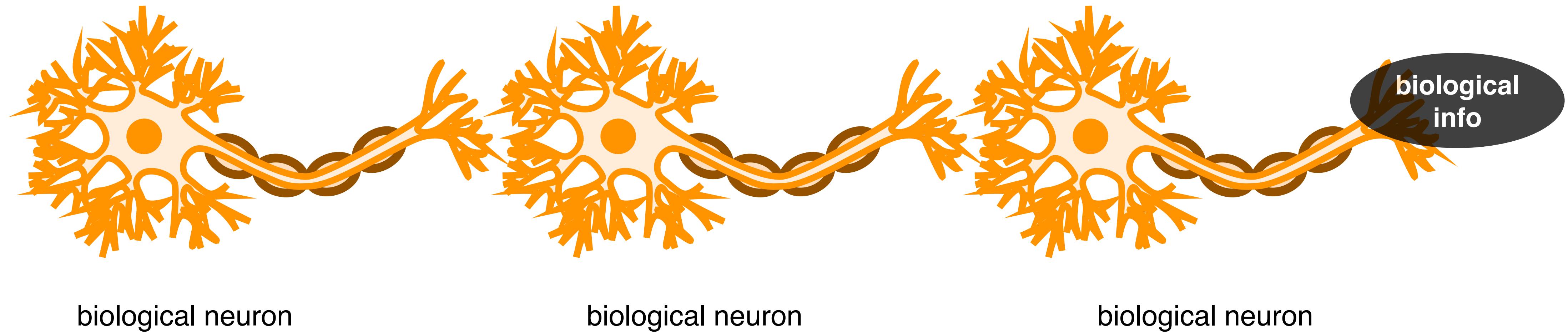
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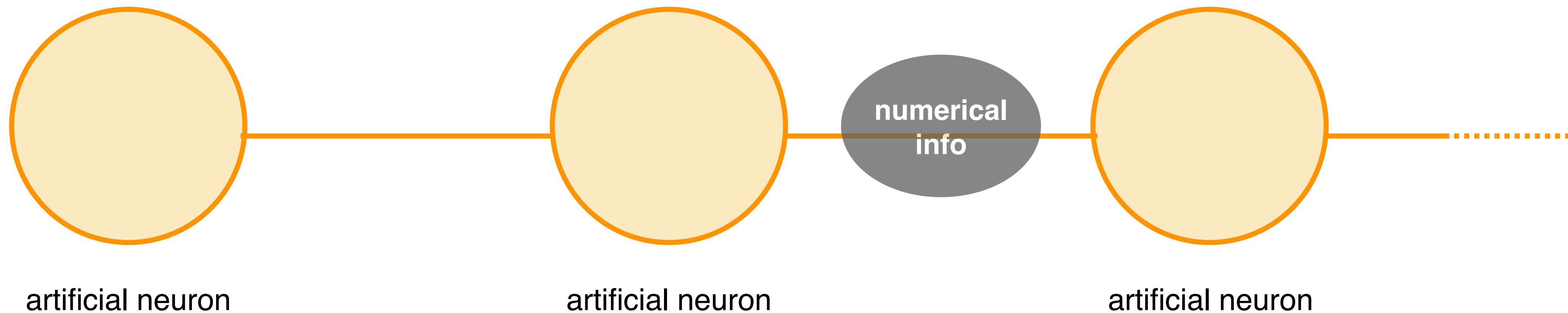
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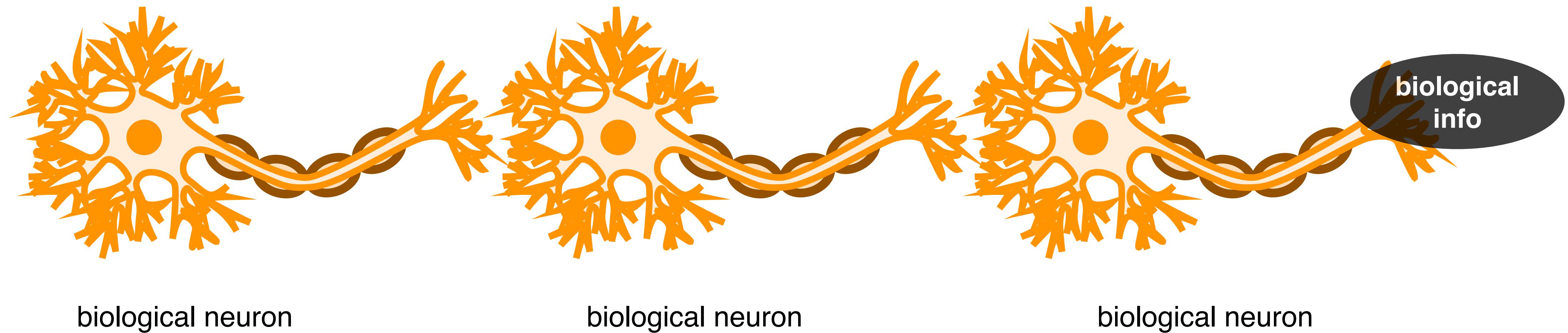
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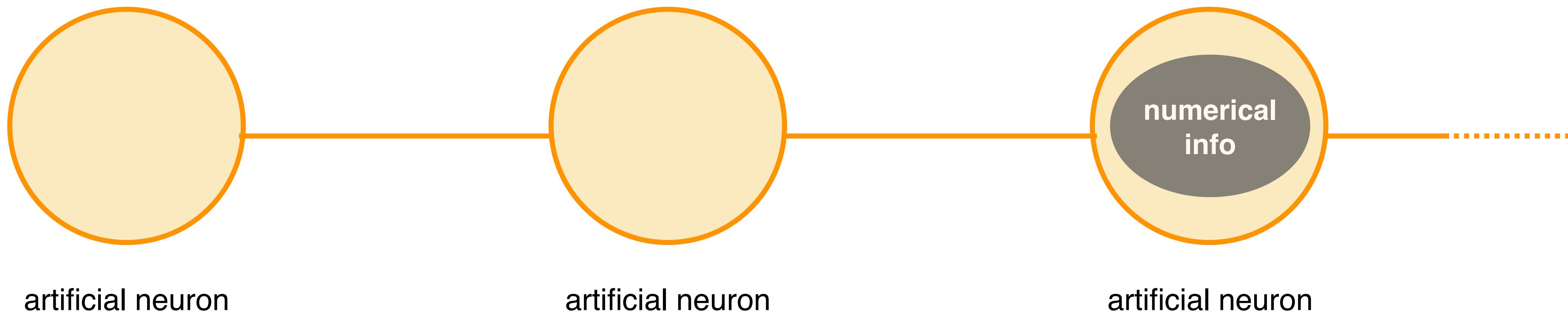
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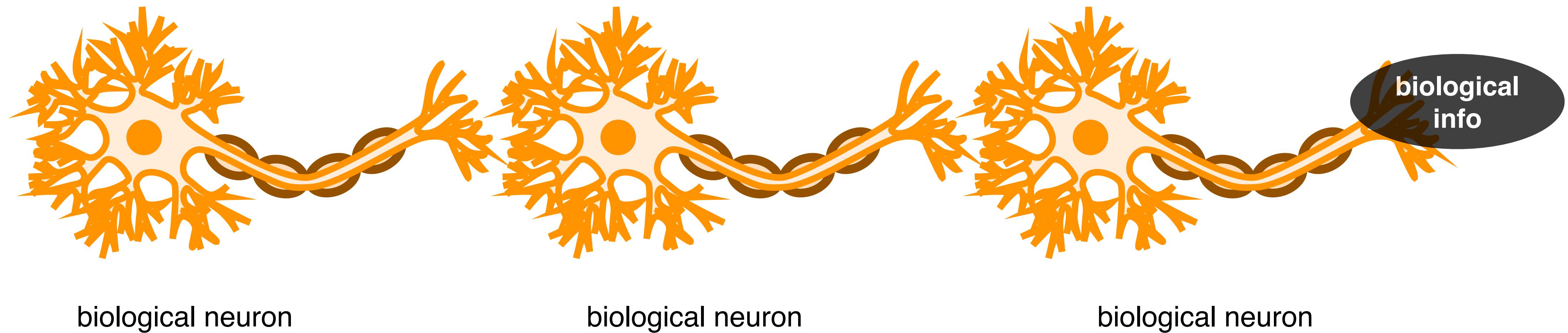
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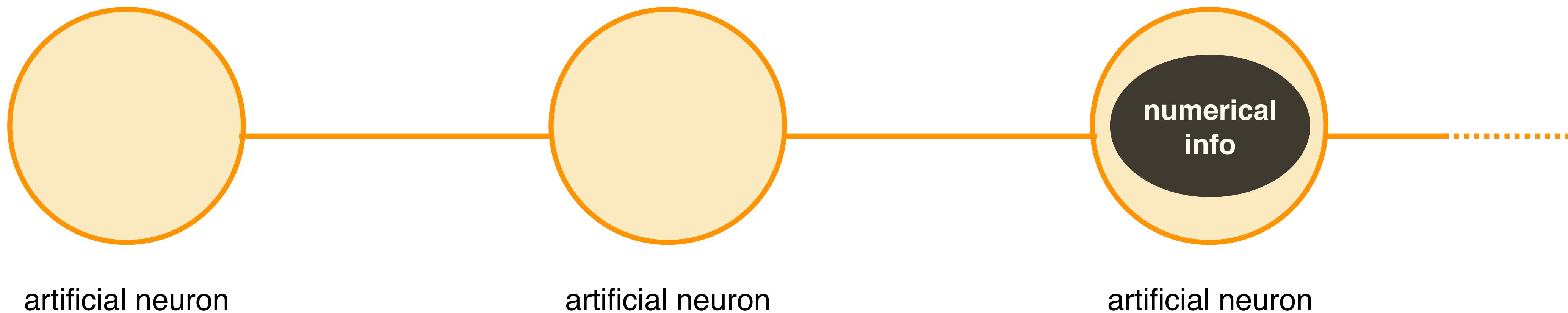
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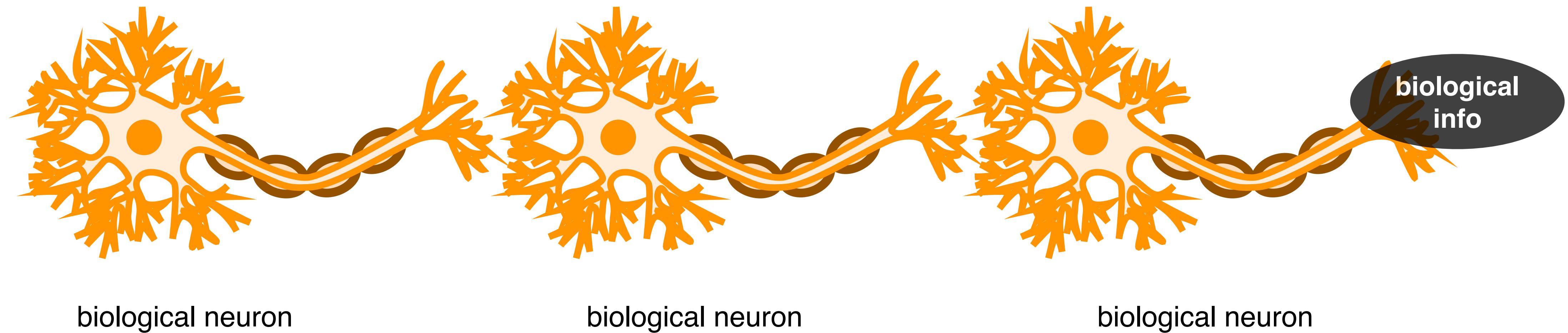
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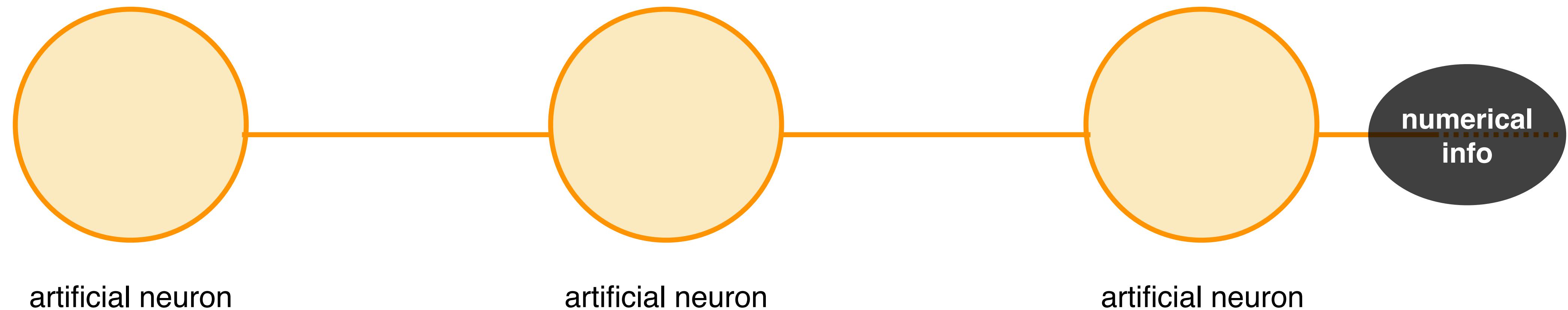
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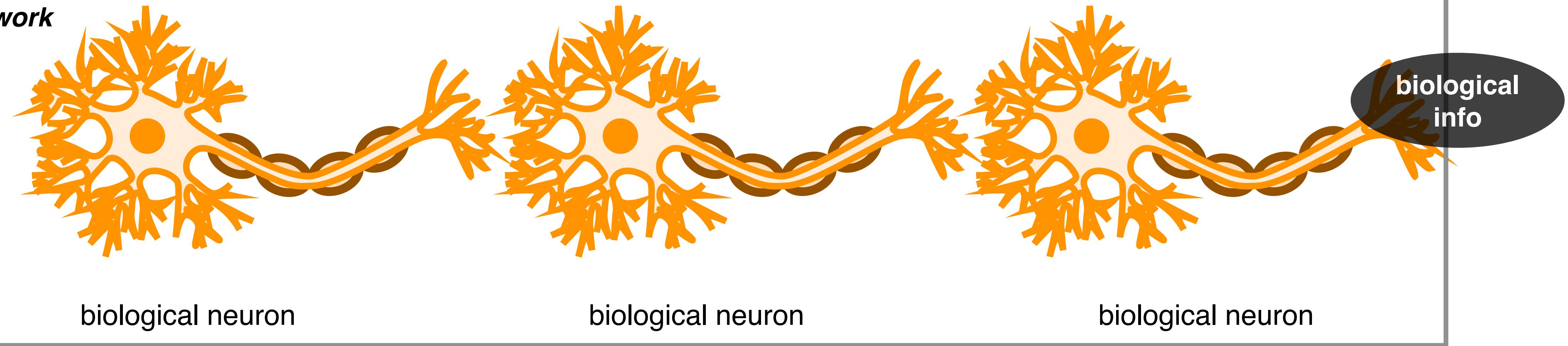


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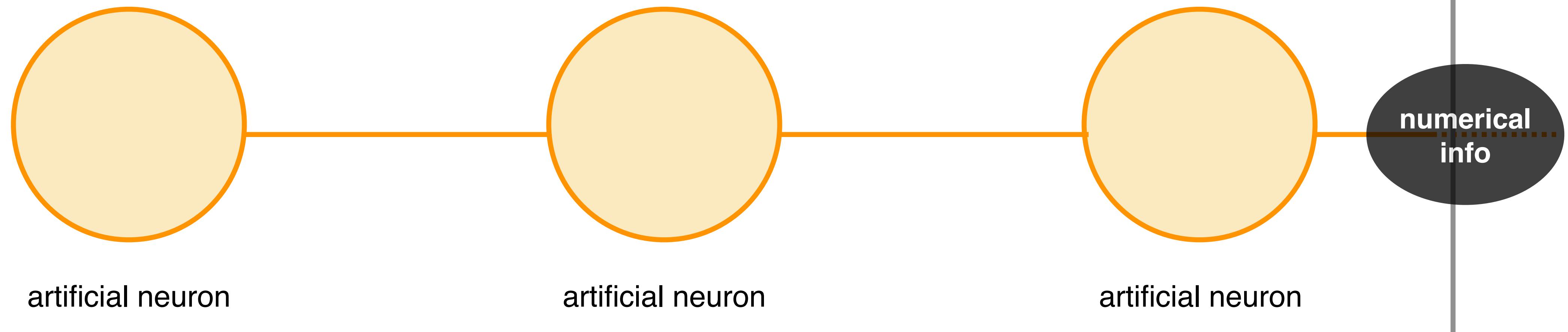
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**Neural Network**



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**Artificial Neural Network**



Occasionally abbreviated just as ANN (artificial neural network) or MLP (multi-layer perceptron).

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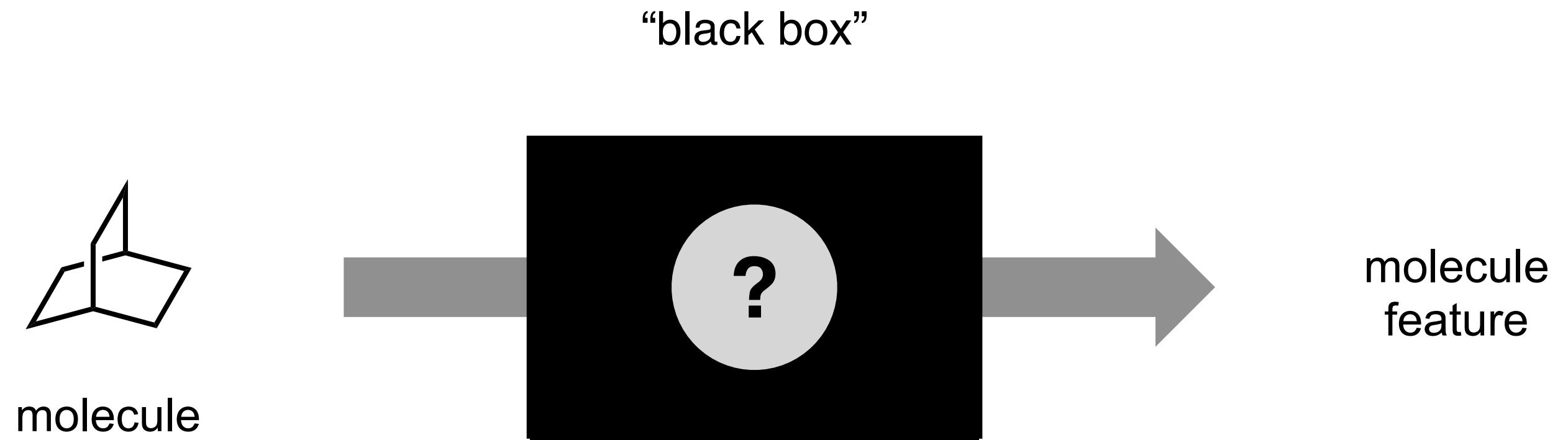
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Different methods of moving information from artificial neuron (node) to node are called “architectures”.

# The Elements of a Feed Forward Neural Network

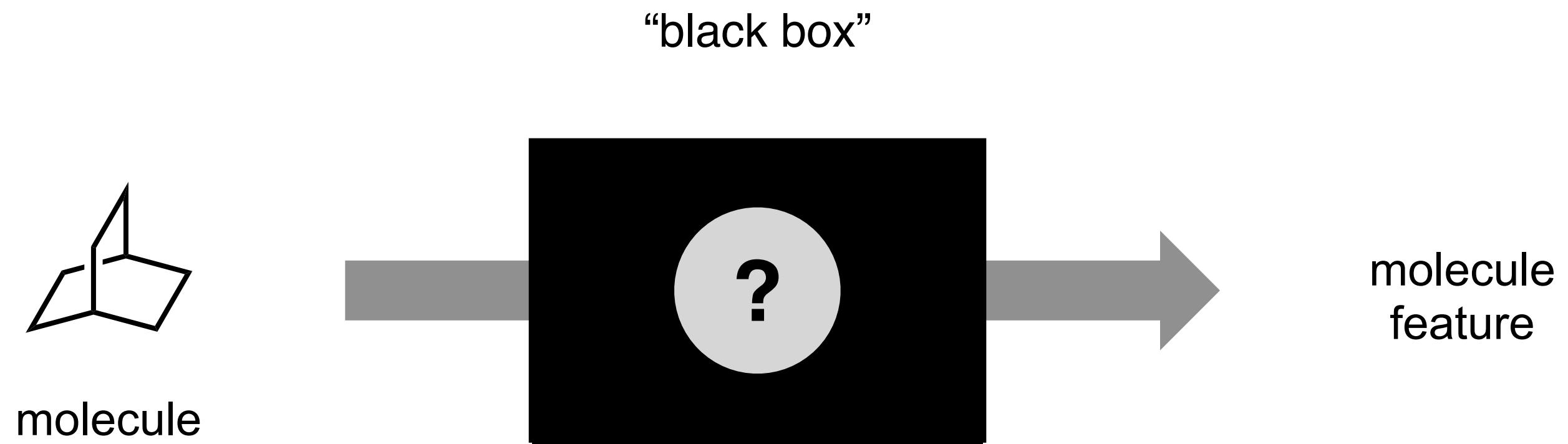


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We do not always understand **why** some bits of the molecule are deemed important

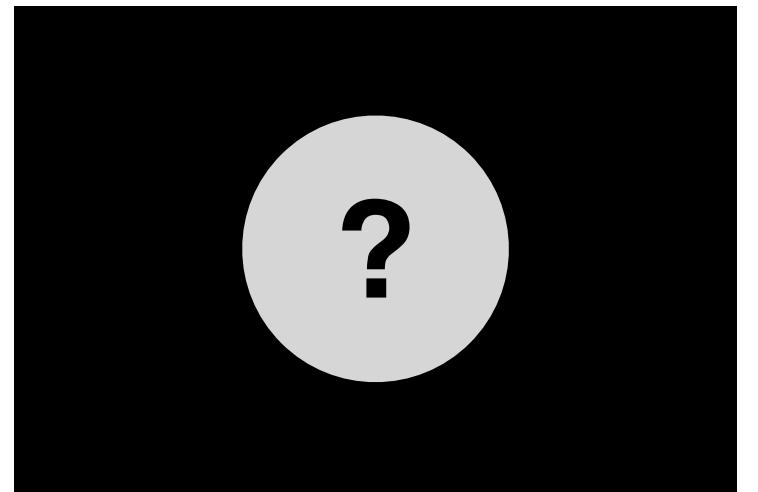
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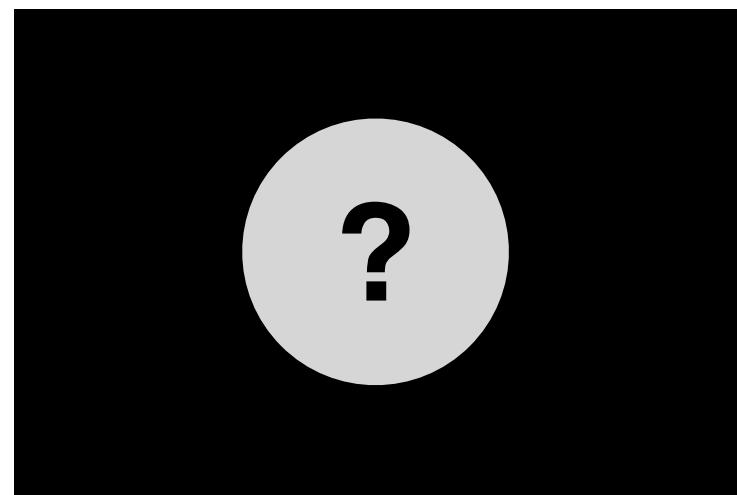
We **do** know what is happening in the black box!

# What is in the Black Box?

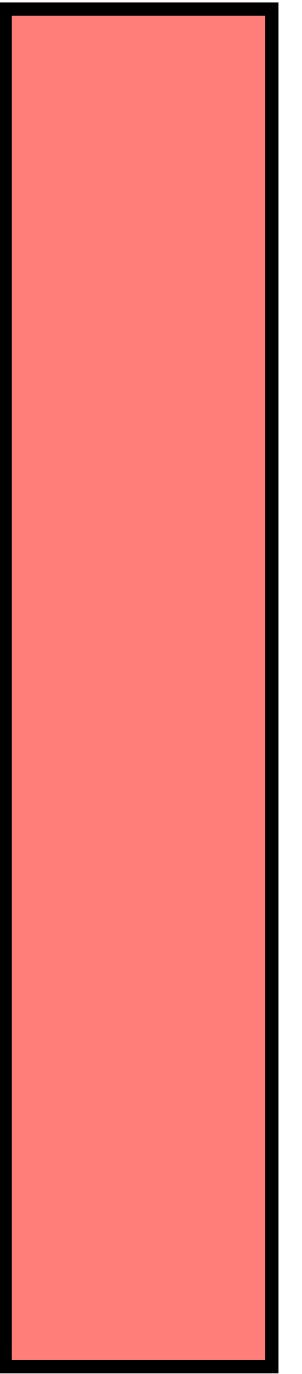


The “black box” is built up of layers

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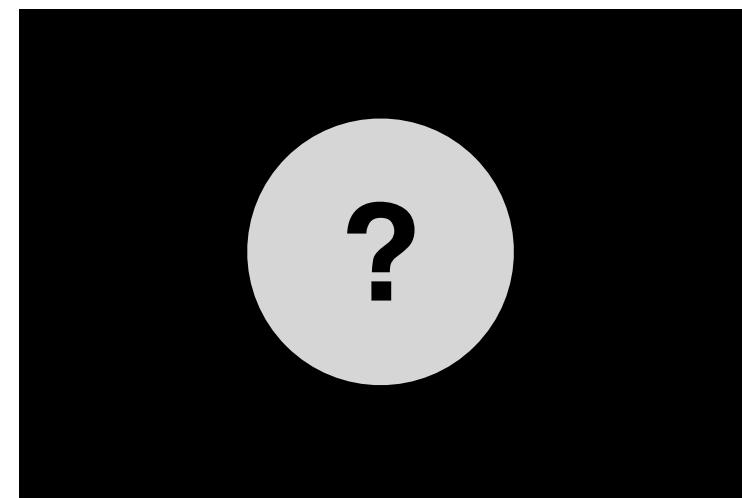


Layer 0

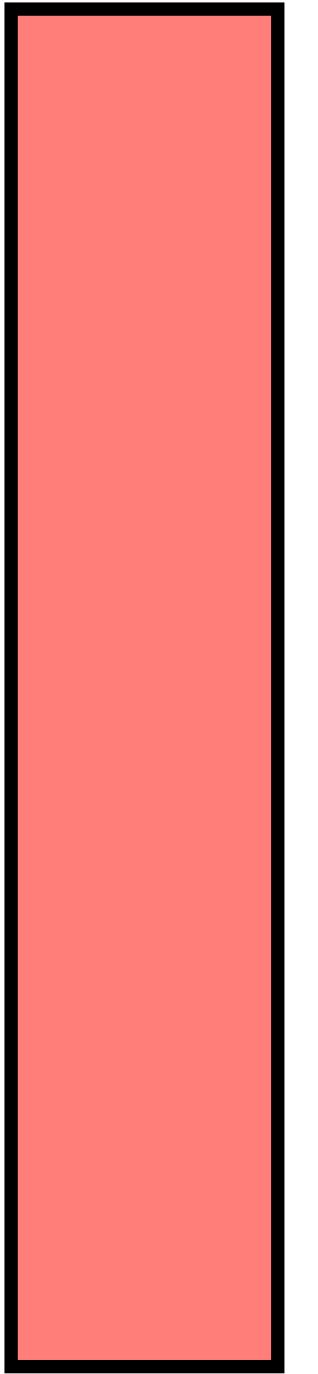


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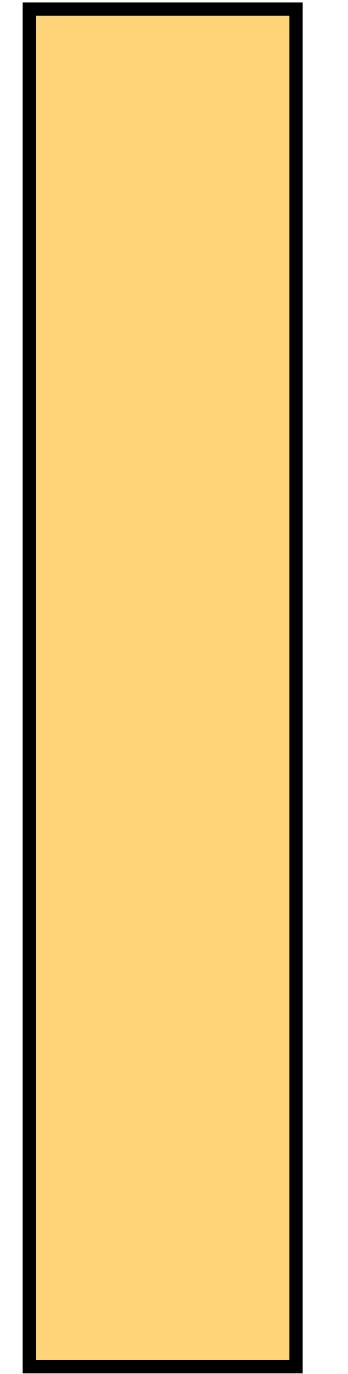
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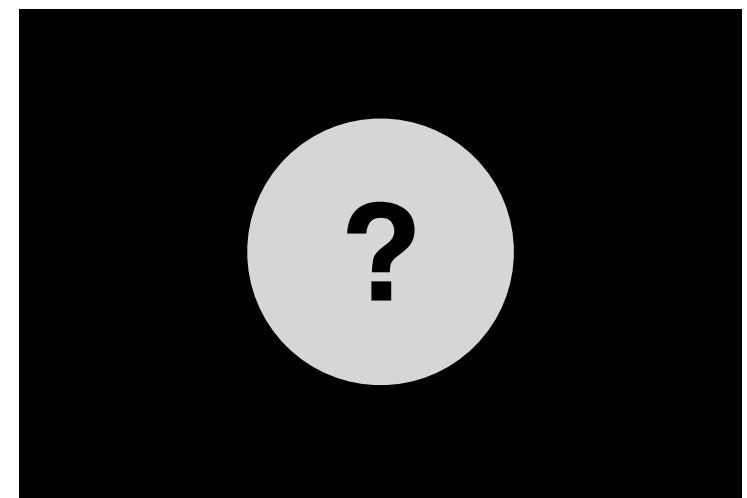
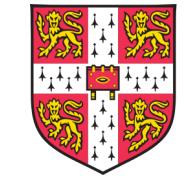


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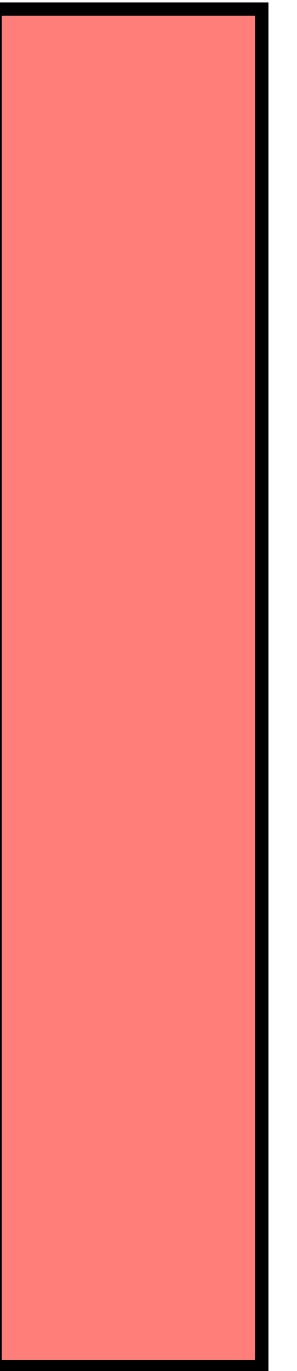
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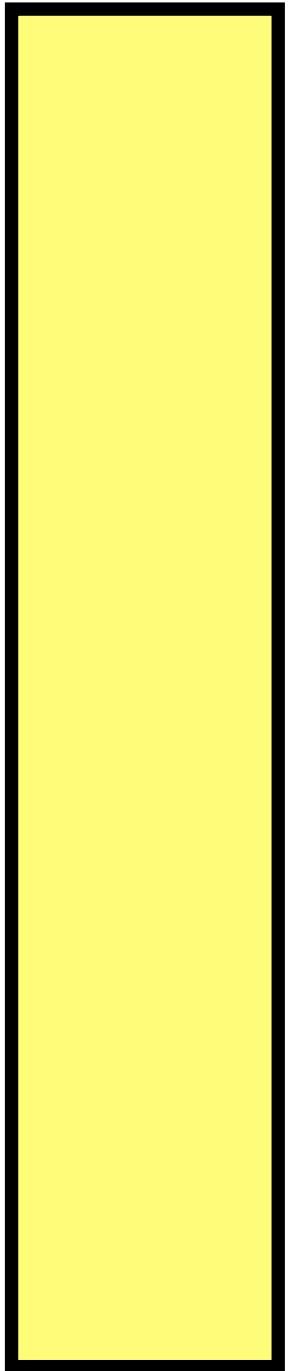
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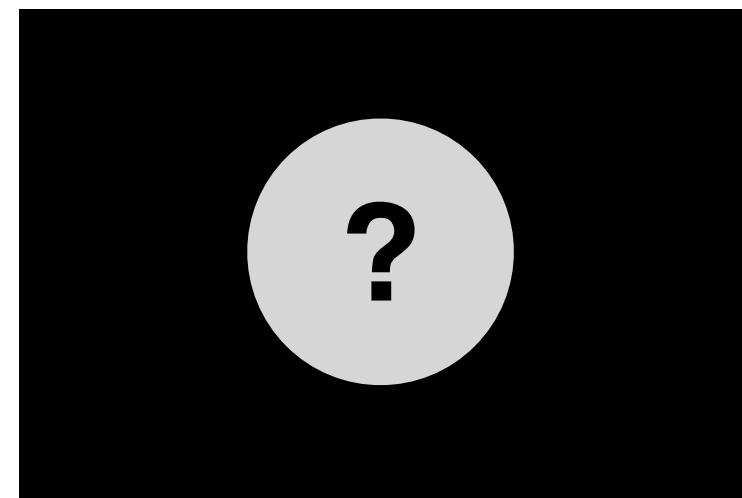
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Layer 2

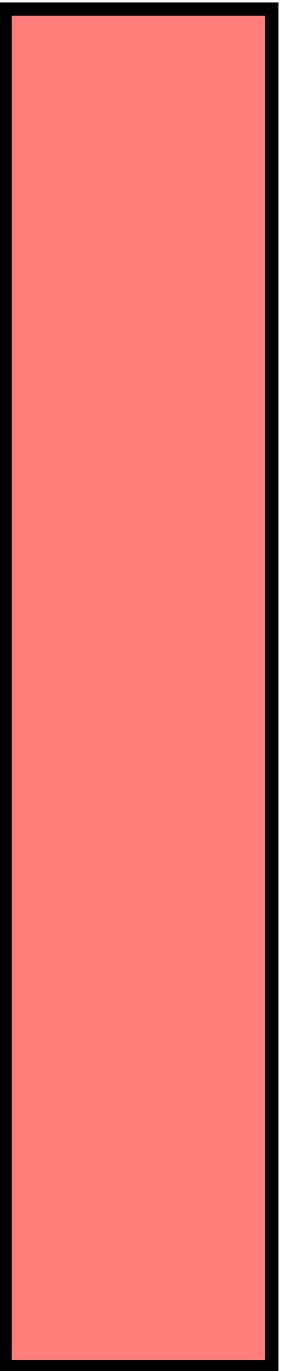


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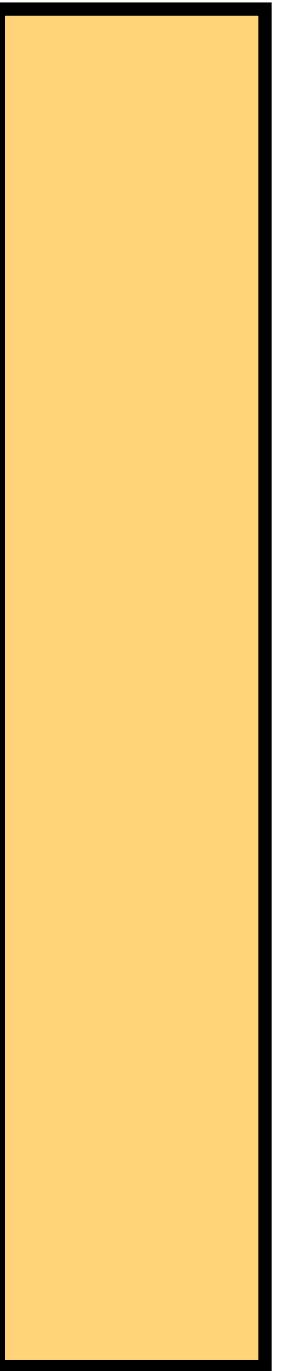


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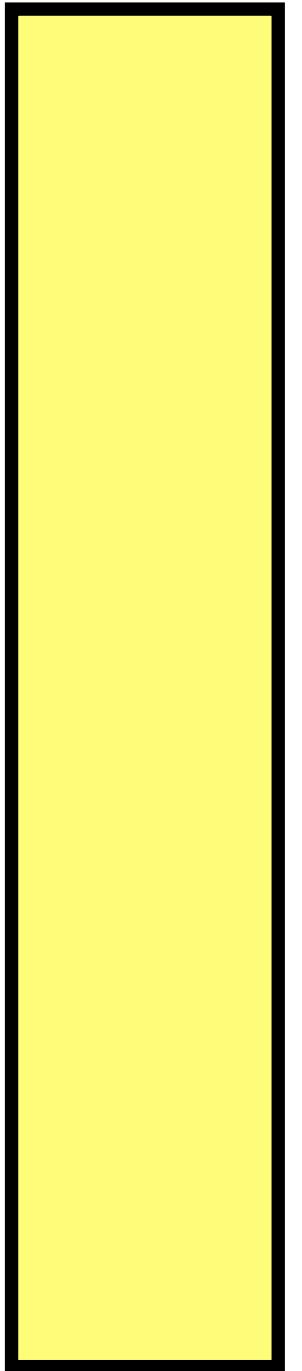
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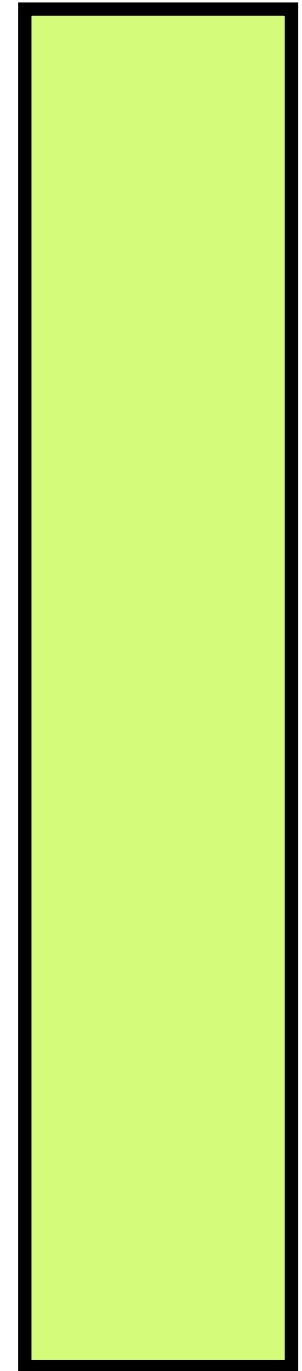
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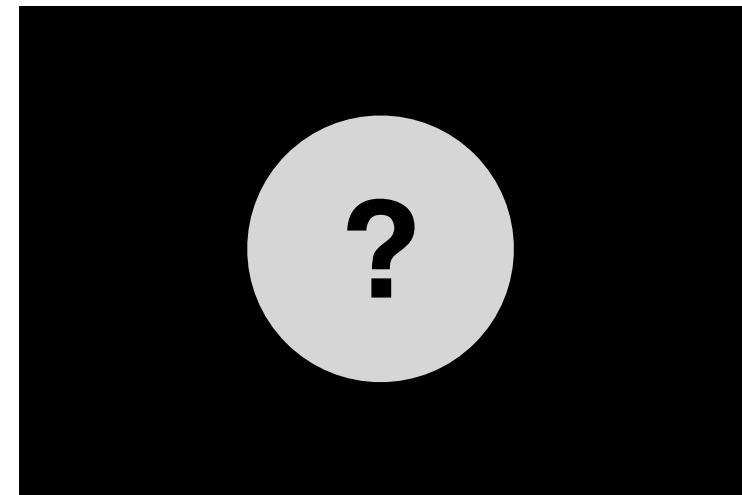
Layer 2



Layer 3

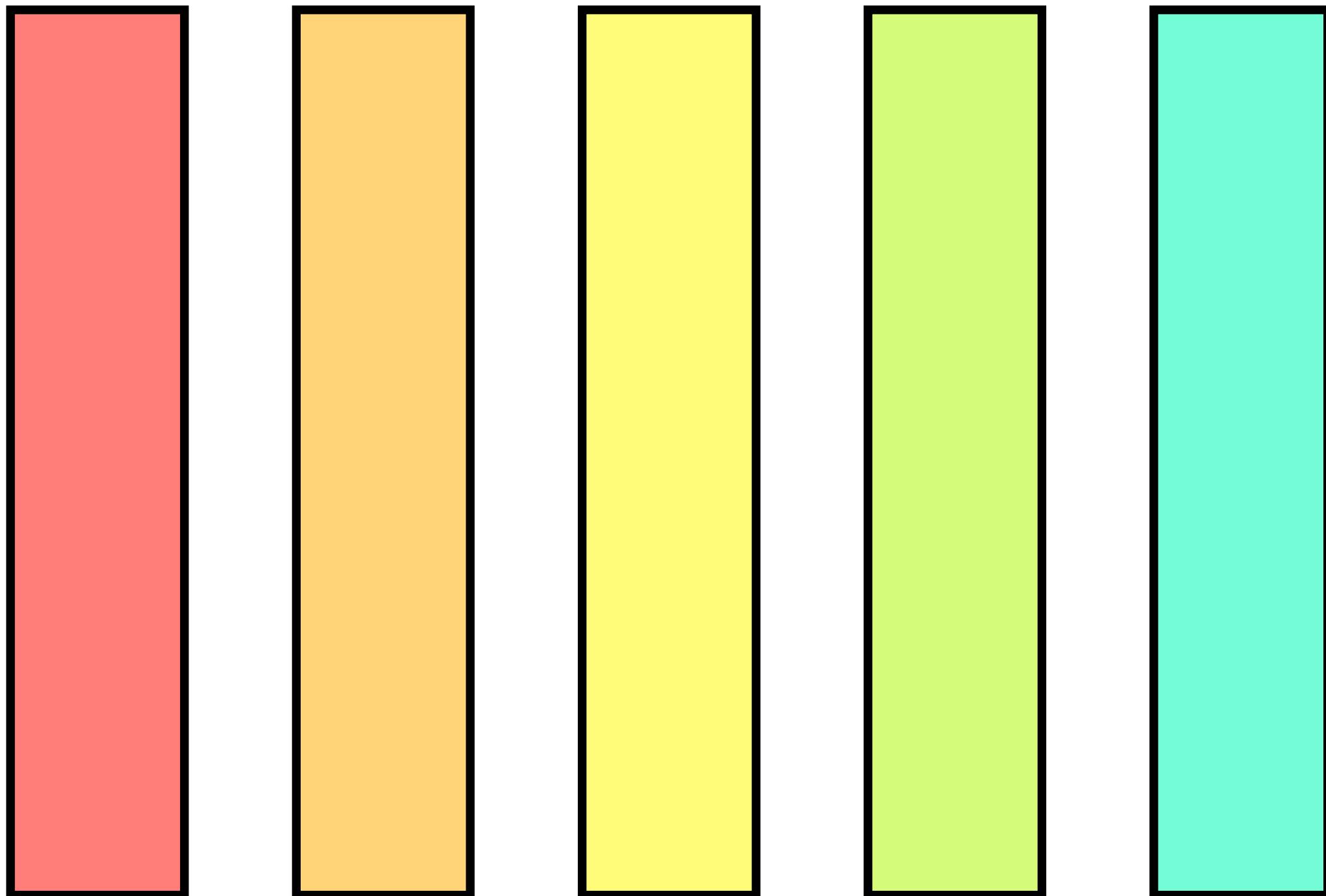


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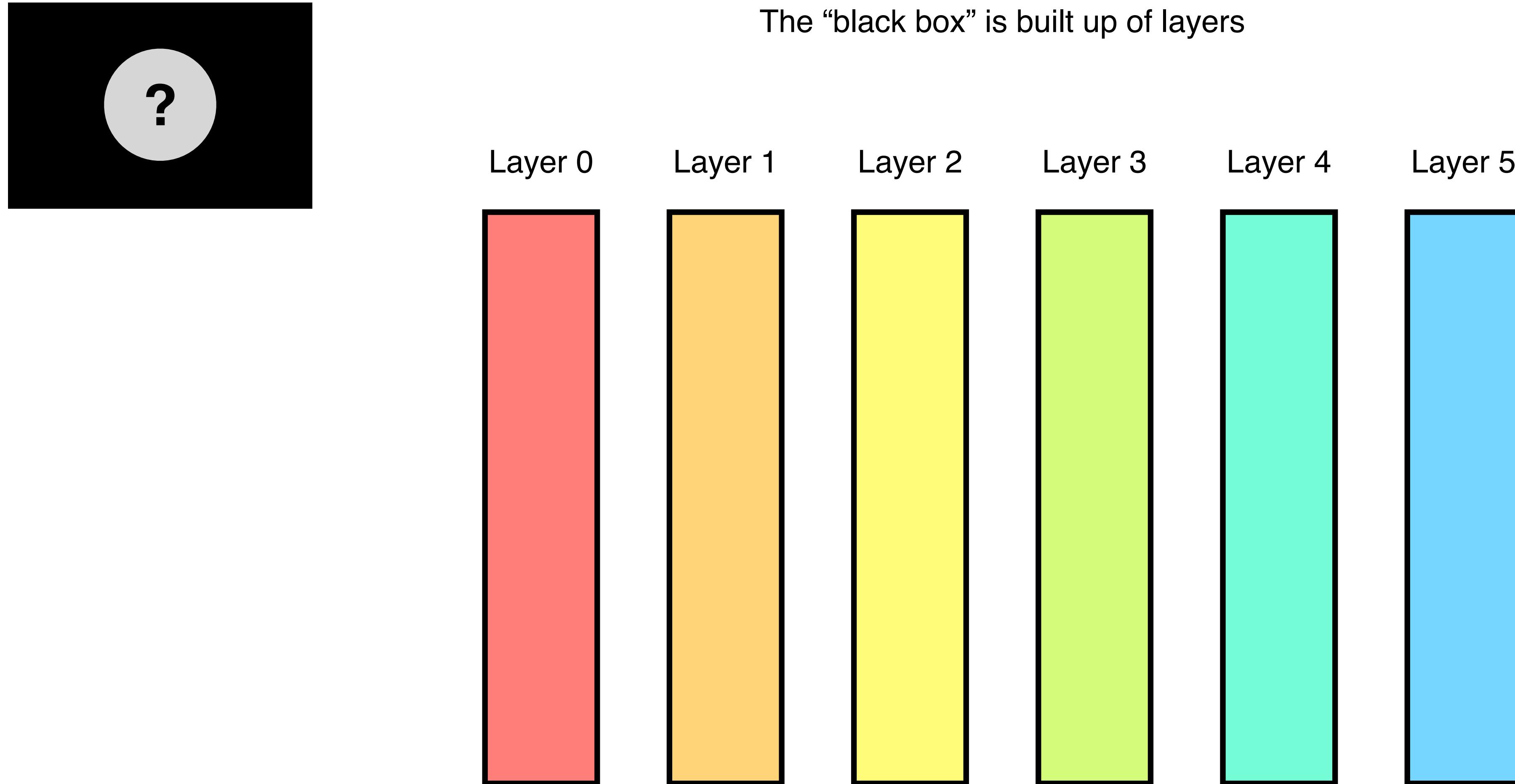


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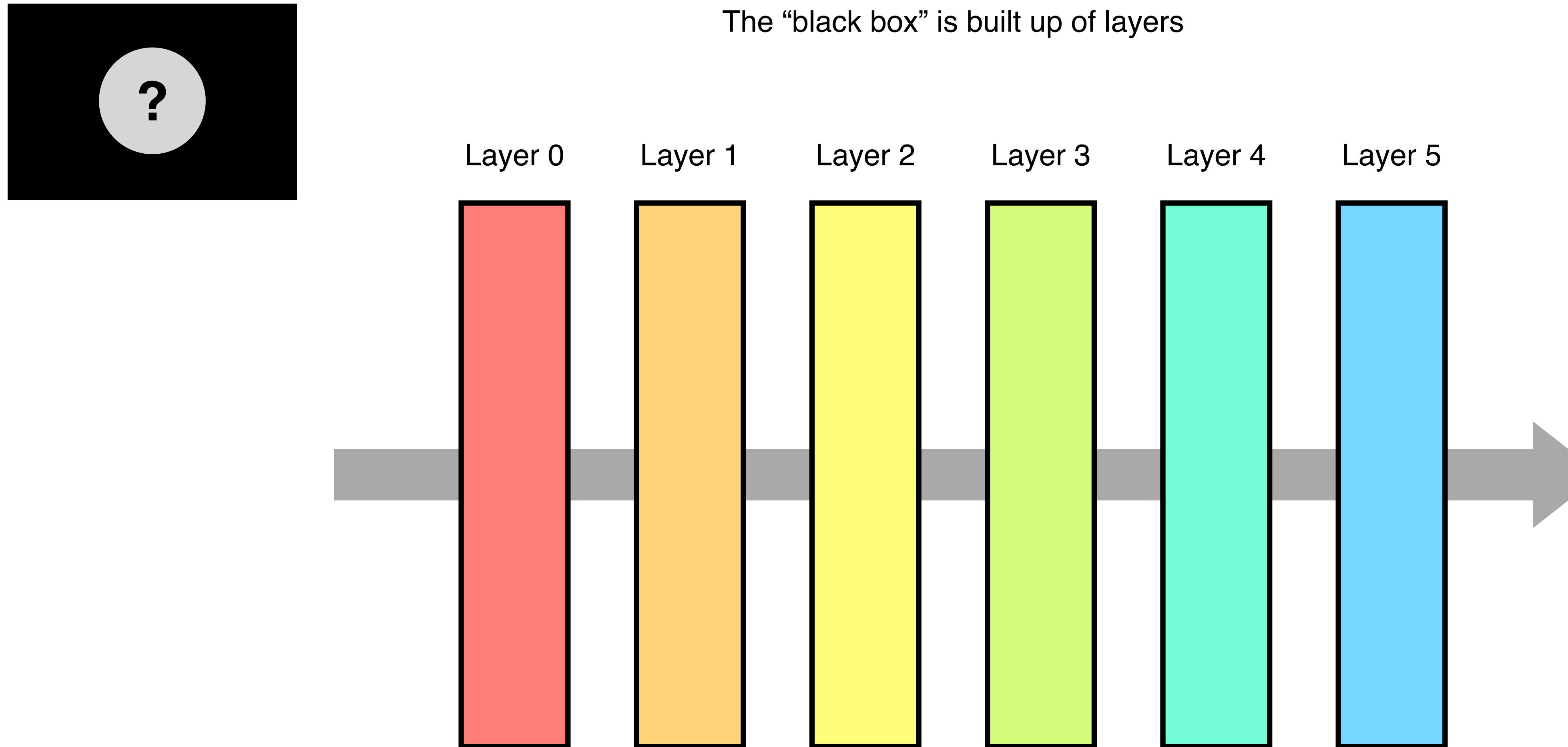
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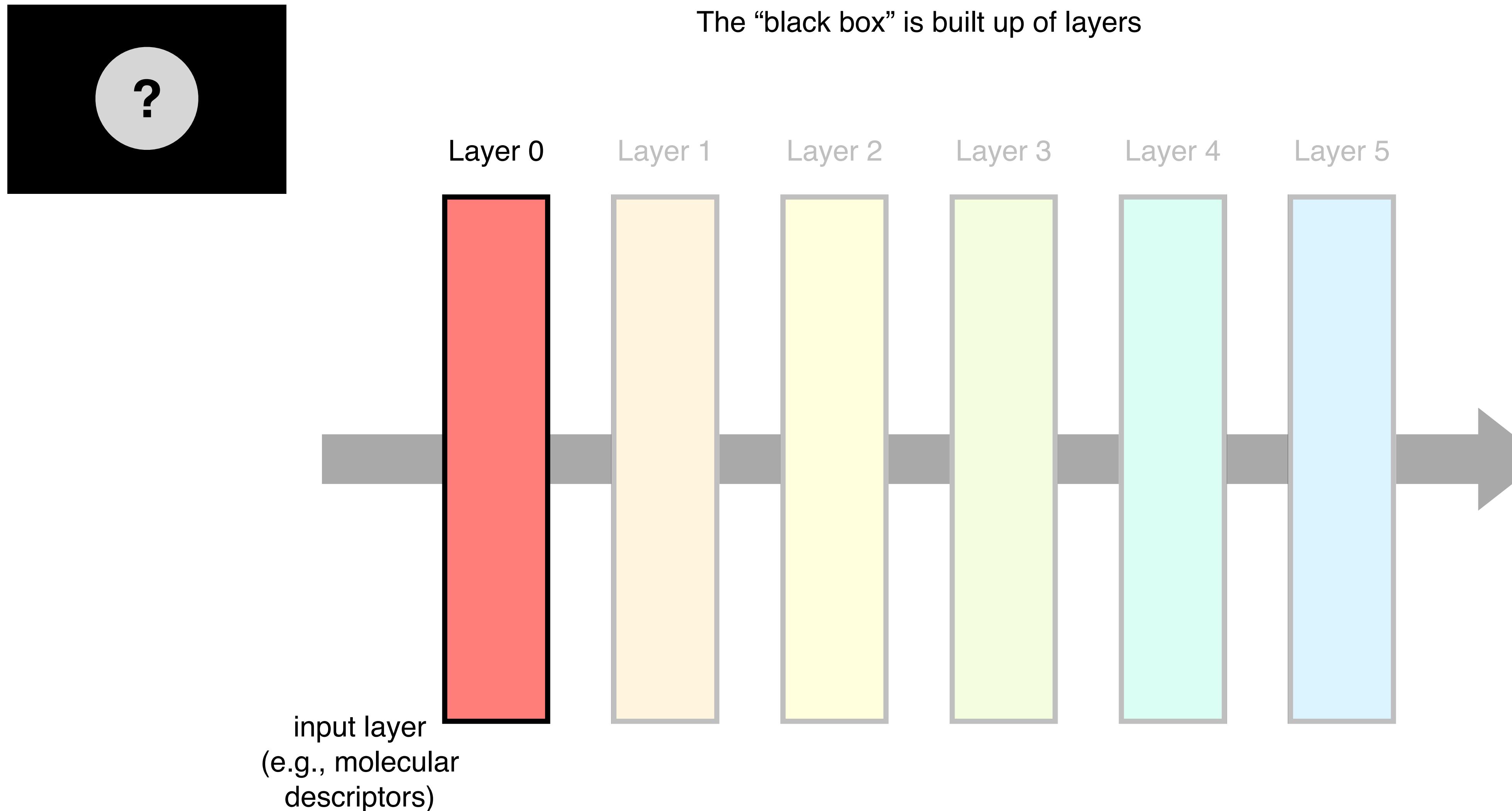
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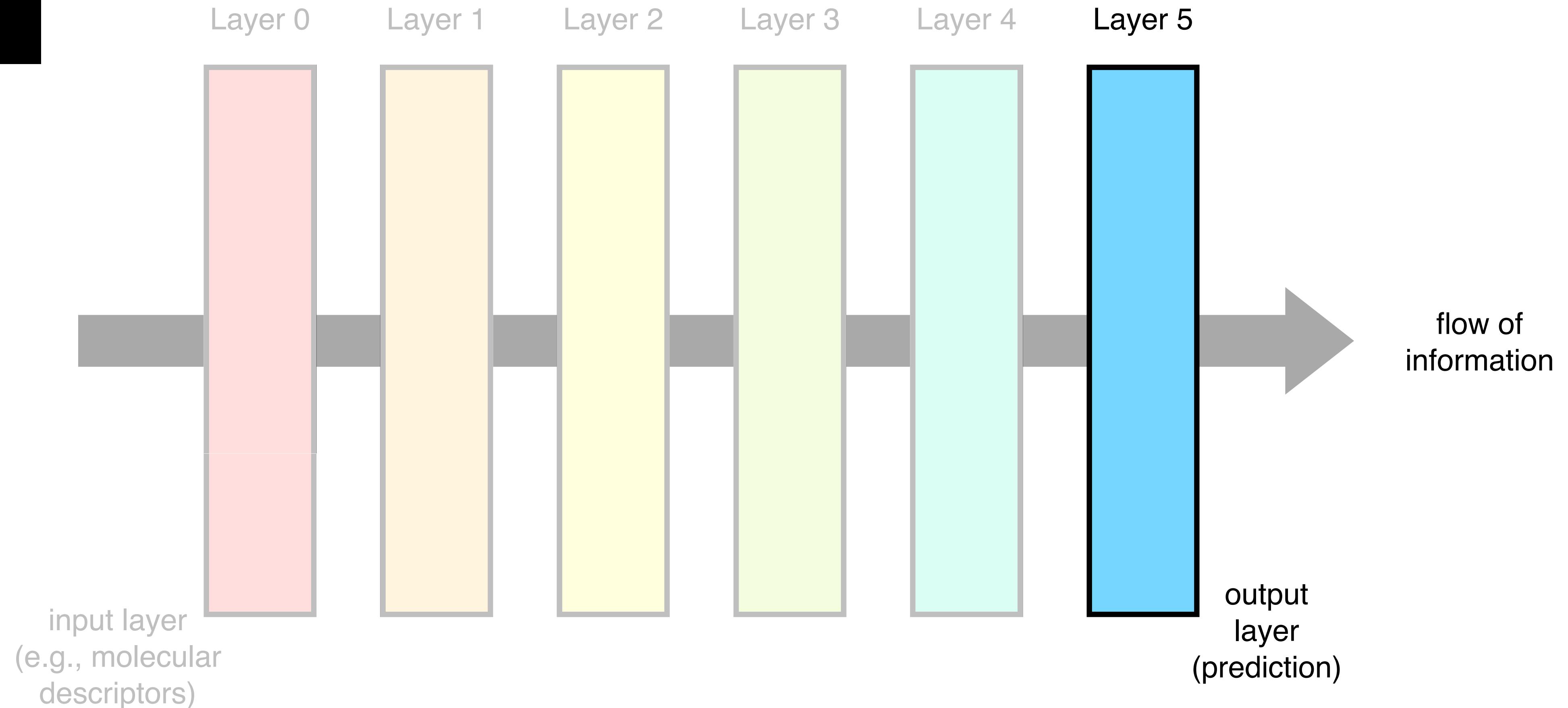
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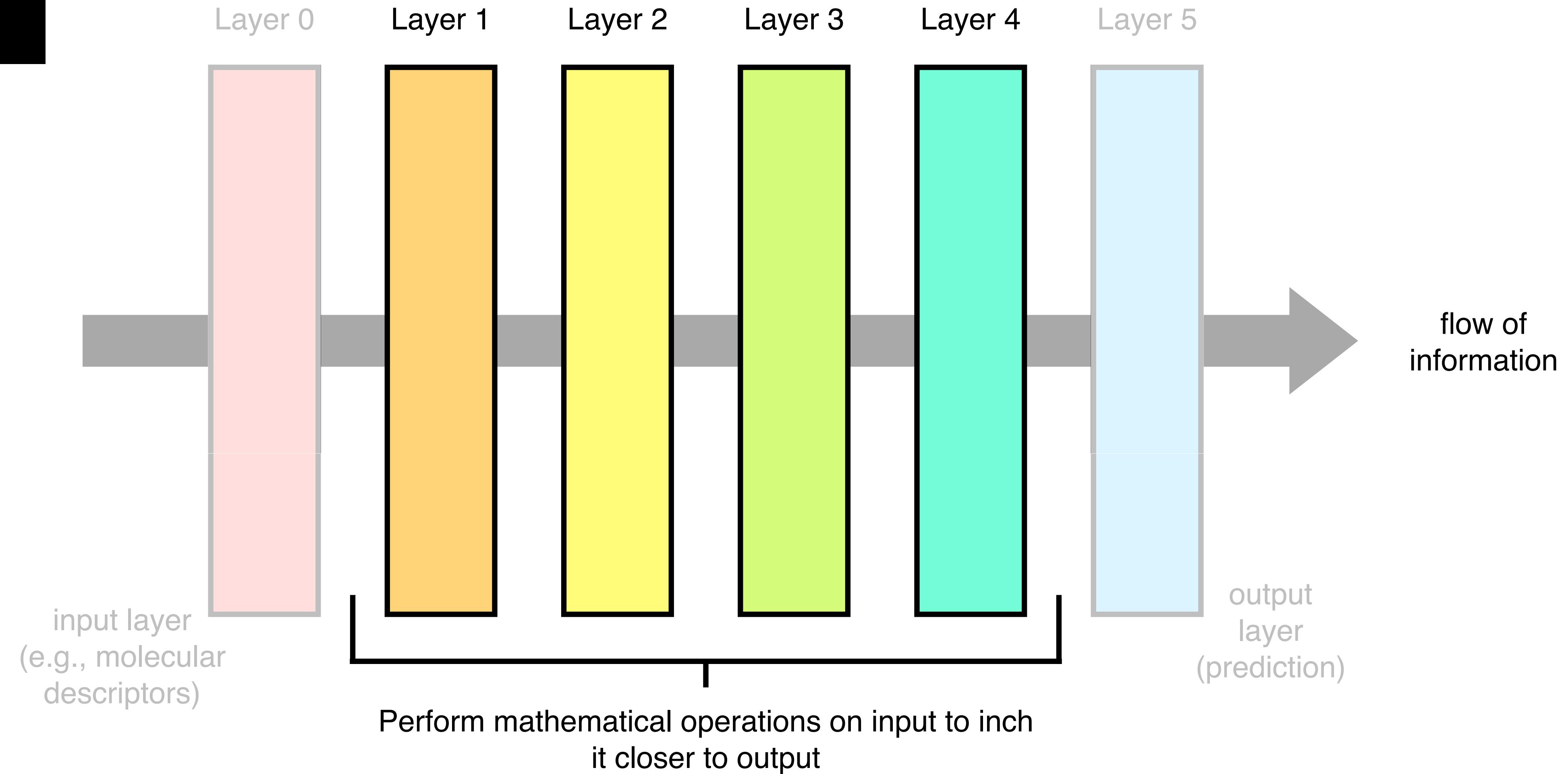
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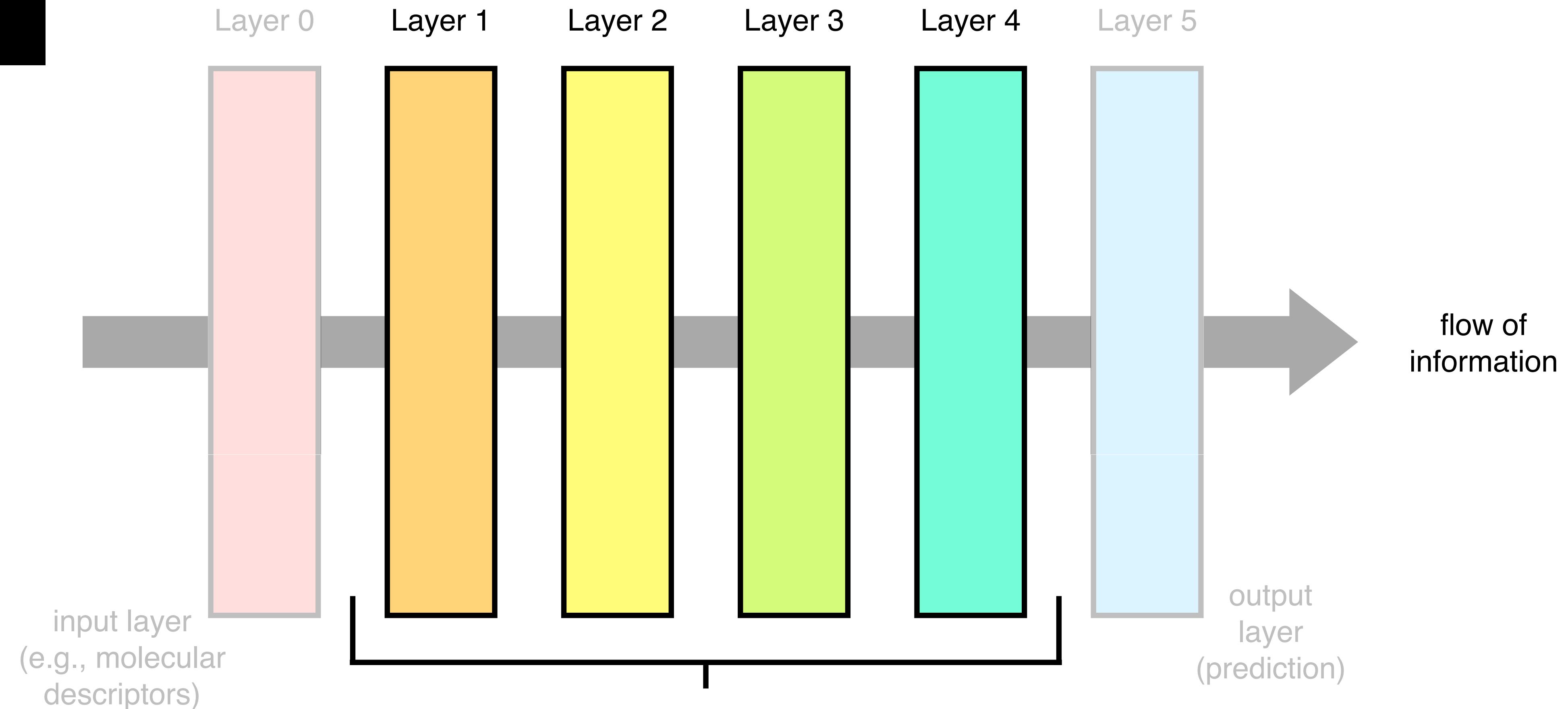
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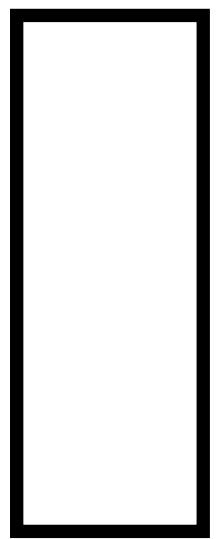


The “black box” is built up of layers



The robot is trying to find a way to relate  
molecular features with molecular properties.

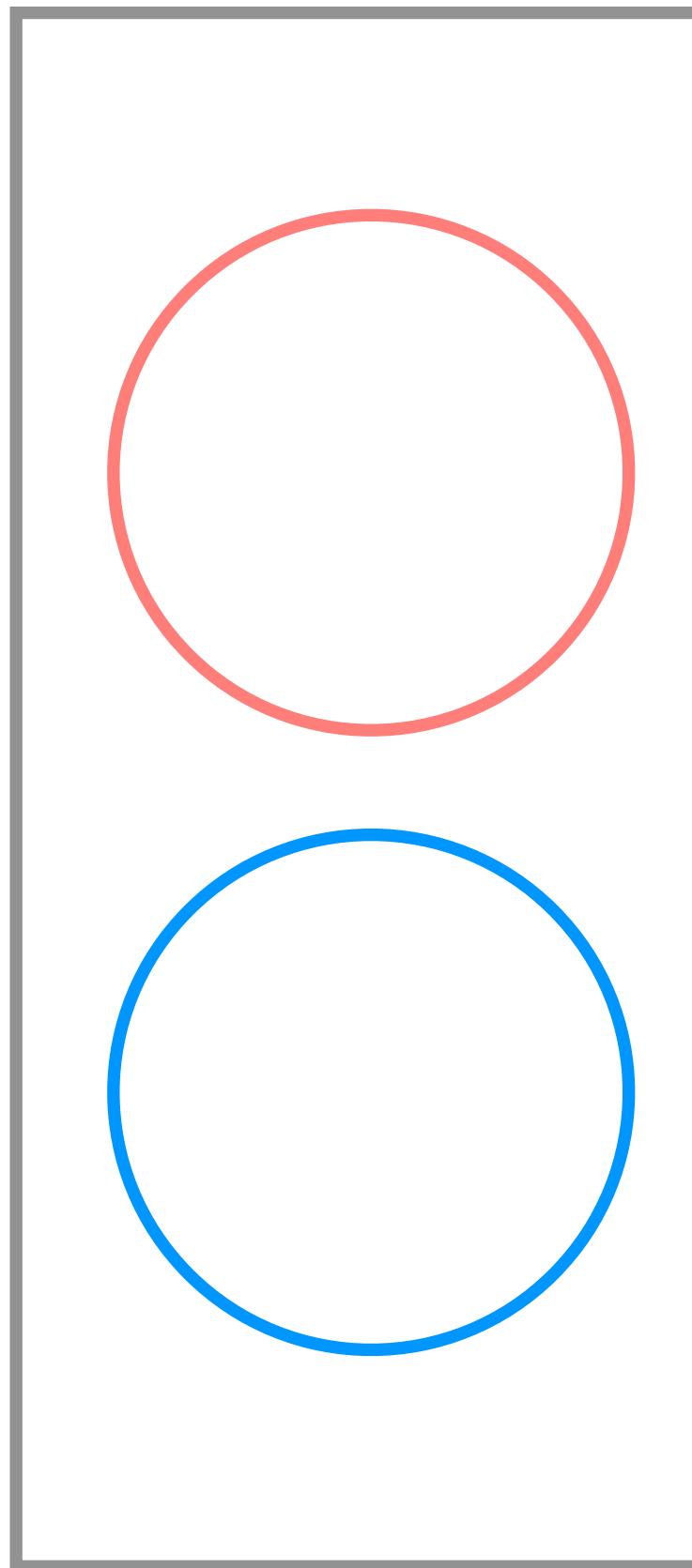
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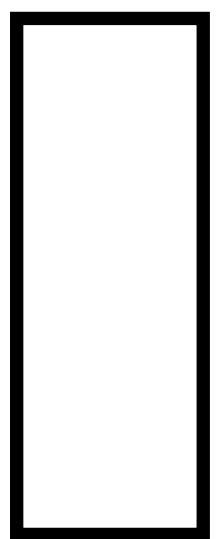
Every layer is built up of nodes (artificial neurons).

Nodes store numbers (information).

Nodes pass information onto new nodes in layers further down.



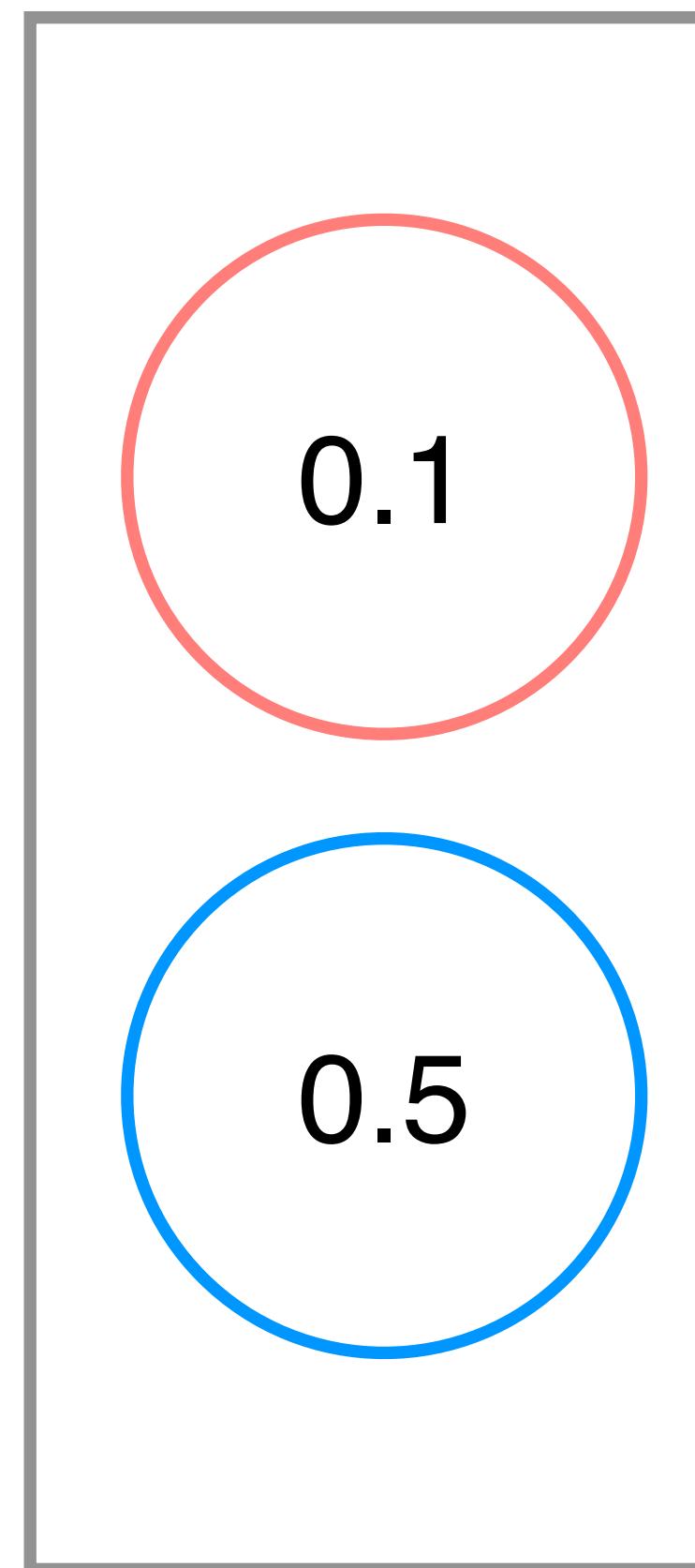
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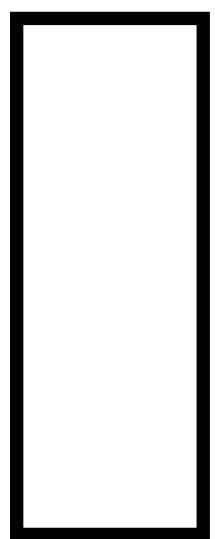
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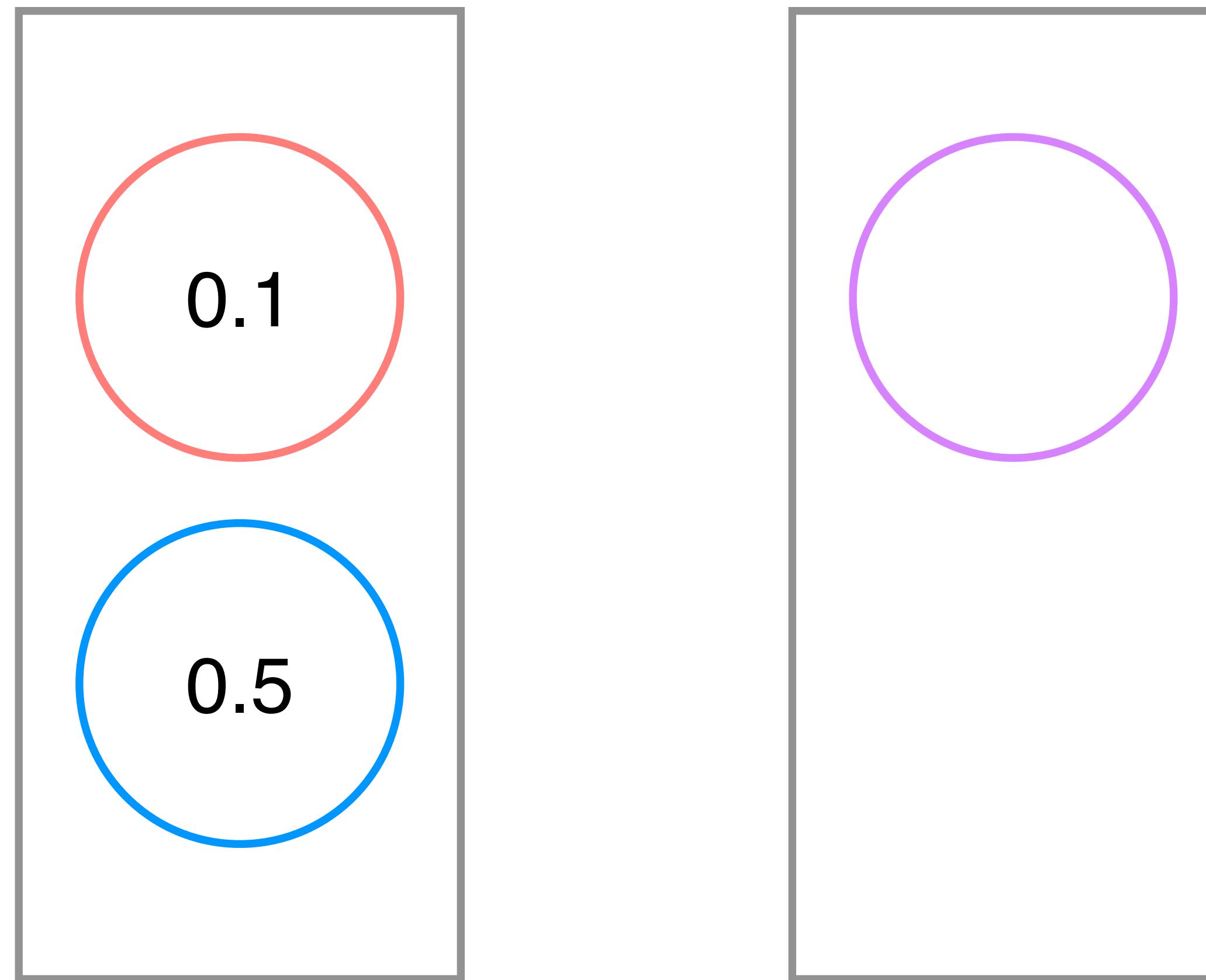
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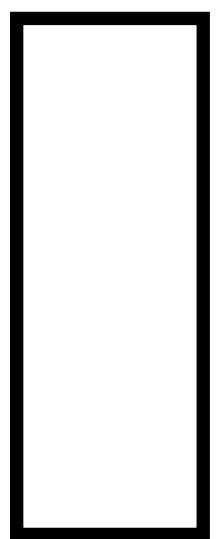
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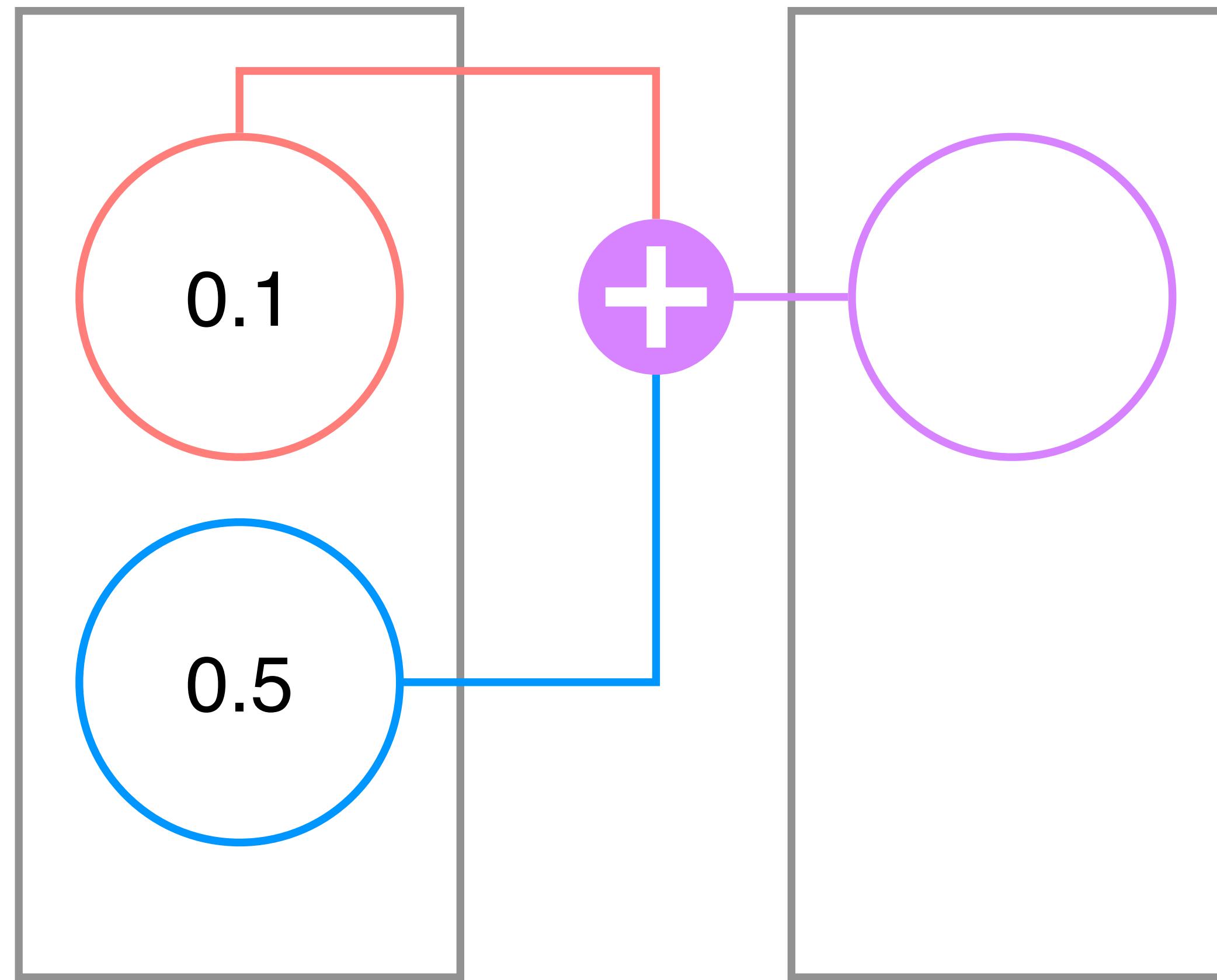
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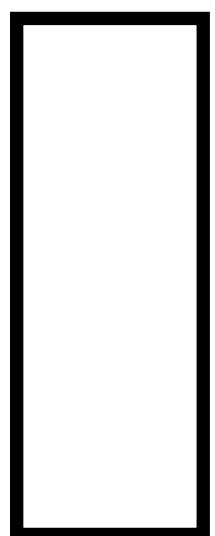
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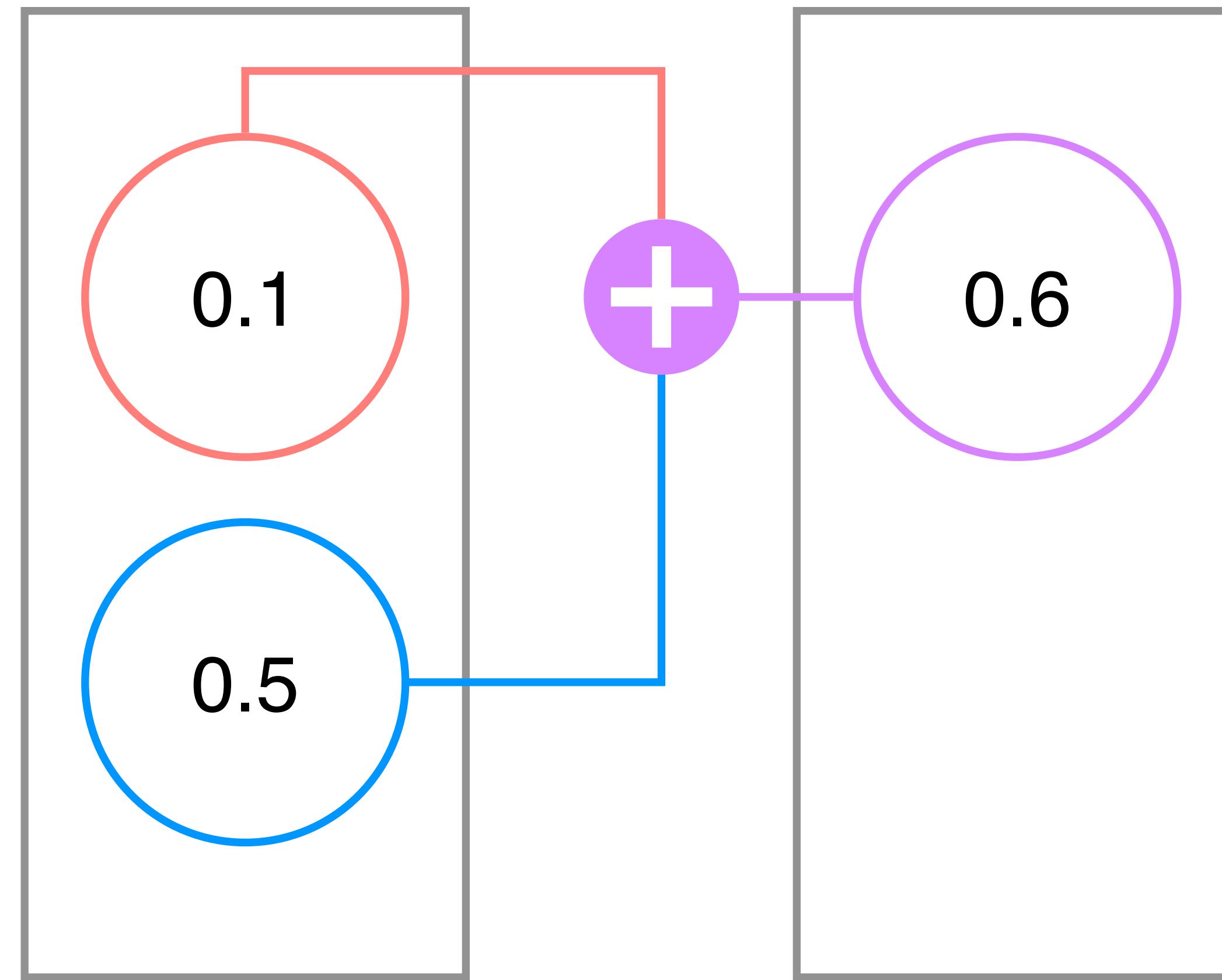
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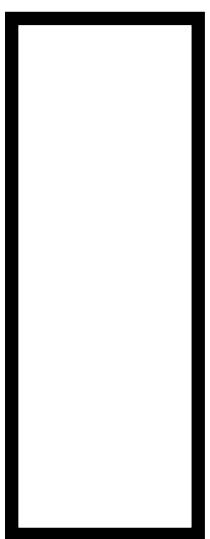
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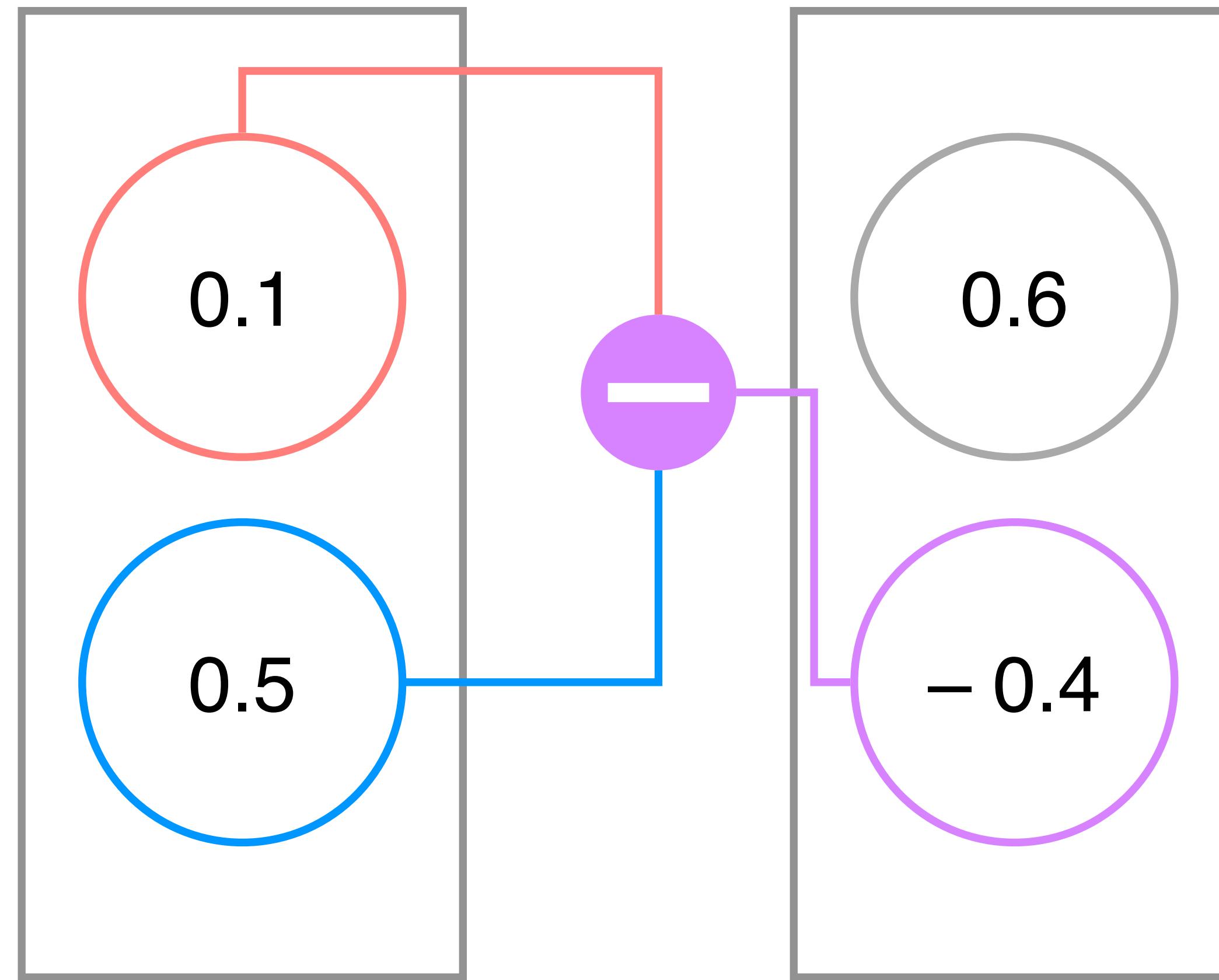
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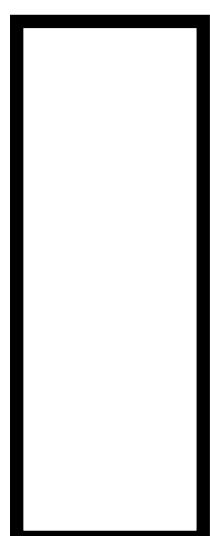
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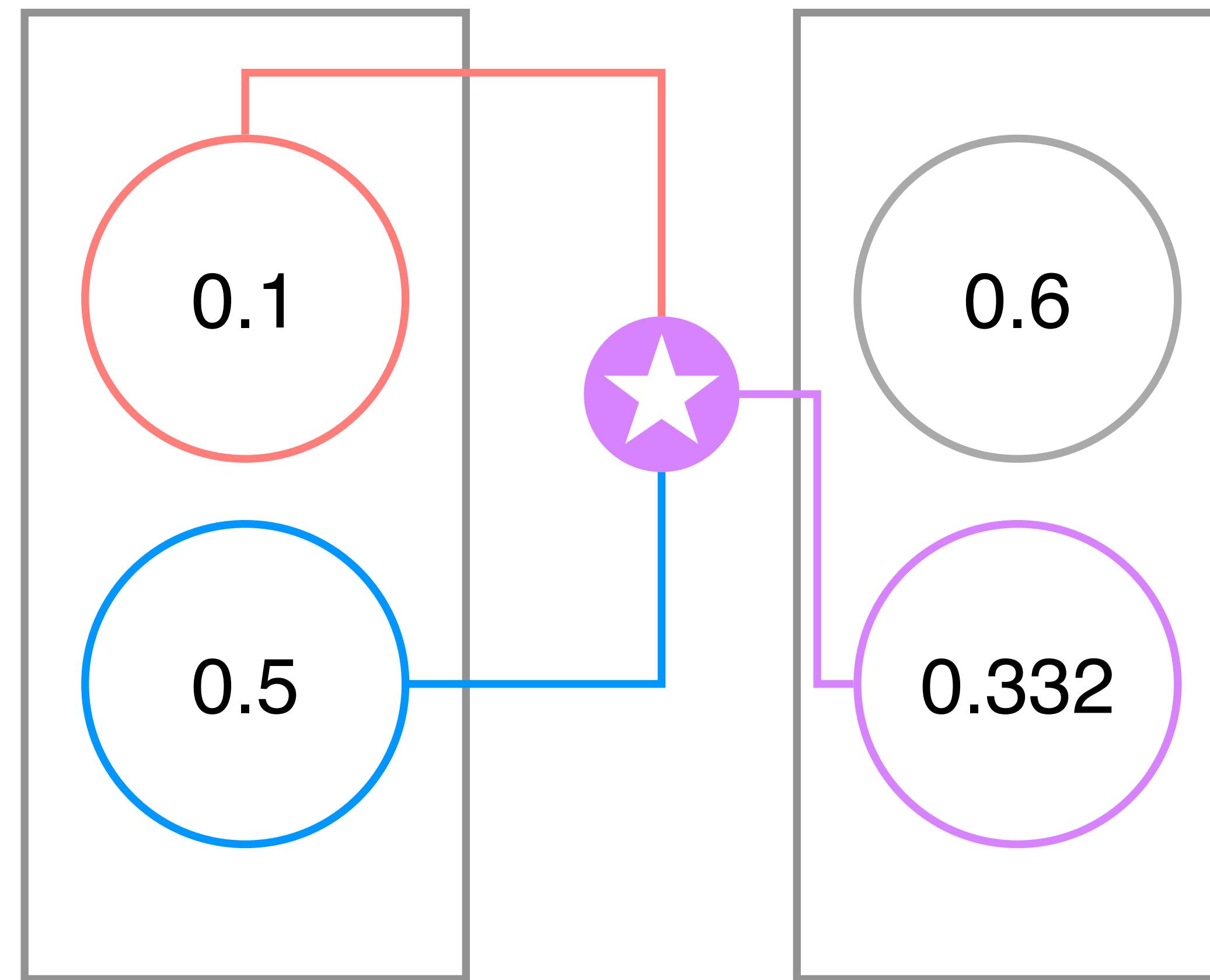
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$$\star = \frac{1}{1 + e^{2 \cdot (0.1) + 1 \cdot (0.5)}}$$

# Types of Outputs



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Is this a cat?



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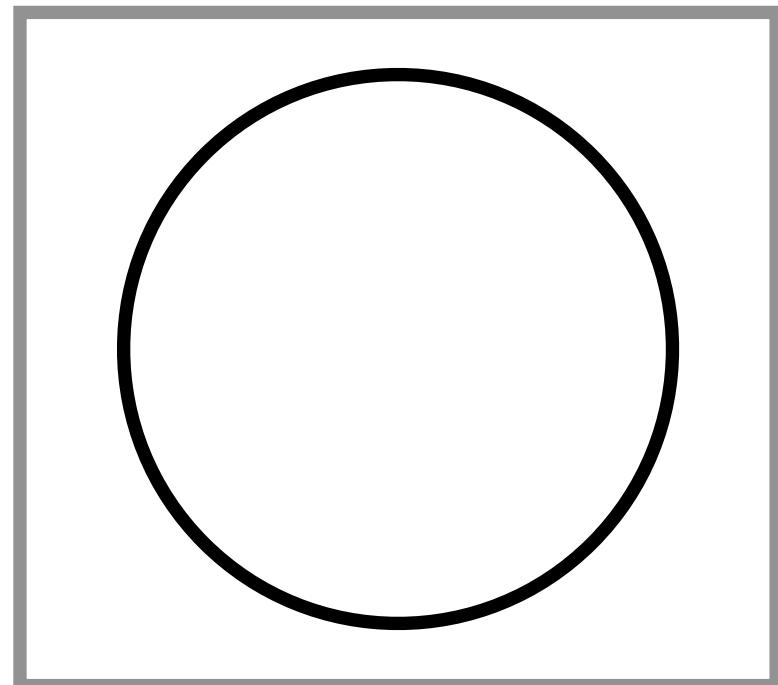


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Output layer = one node



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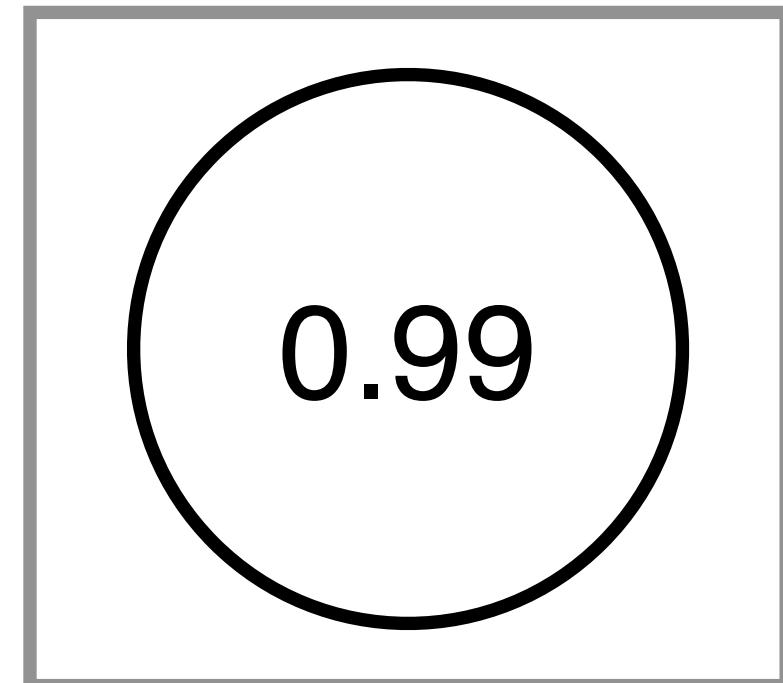


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Is this a cat?



Output layer = one node



I give 99% odds that this is a cat.

I classify this as a **cat**.

# Types of Outputs

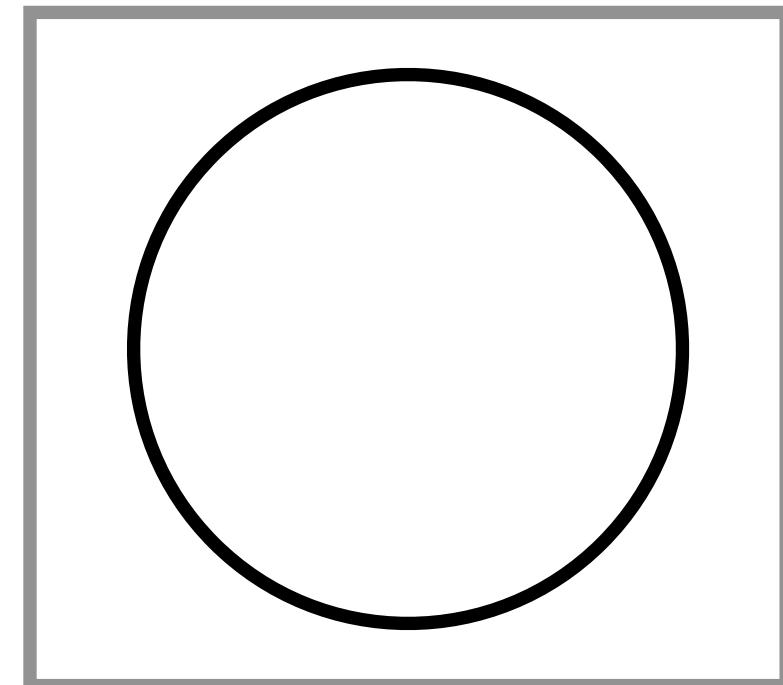


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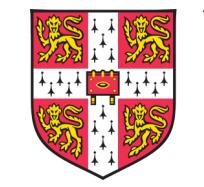
Is this a cat?



Output layer = one node



# Types of Outputs

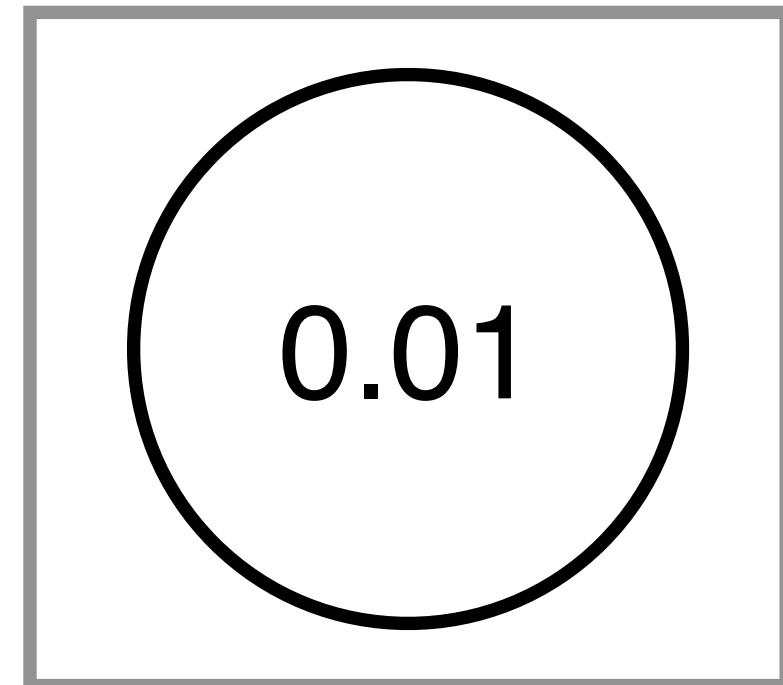


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Is this a cat?



Output layer = one node



I give 1% odds that this is a cat.

# Types of Outputs

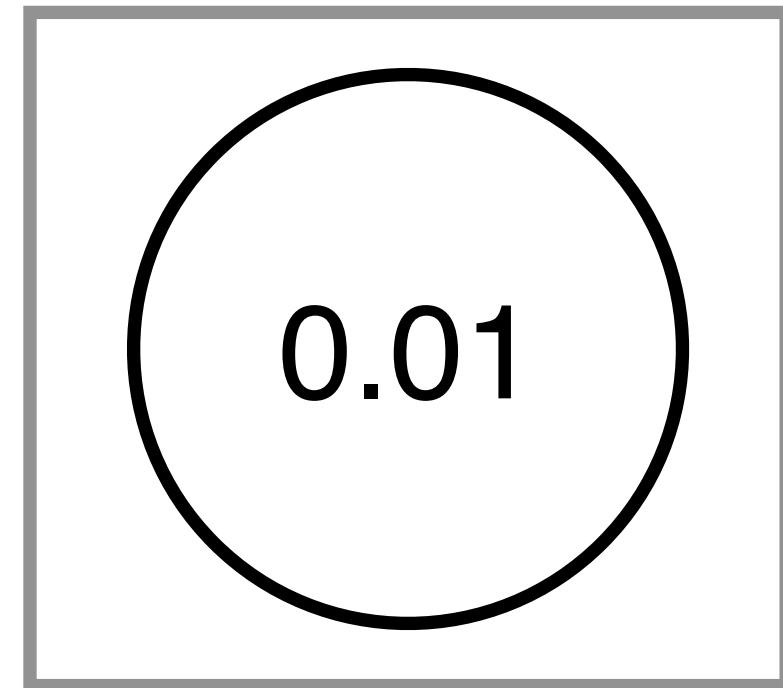


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Is this a cat?



Output layer = one node



I give 1% odds that this is a cat.

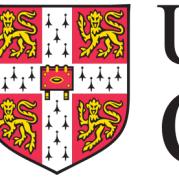
I give 99% odds that this is **not a cat**.

I classify this as a **not a cat**.

# Types of Outputs

What type of animal is this? Cat, Dog, or Owl?

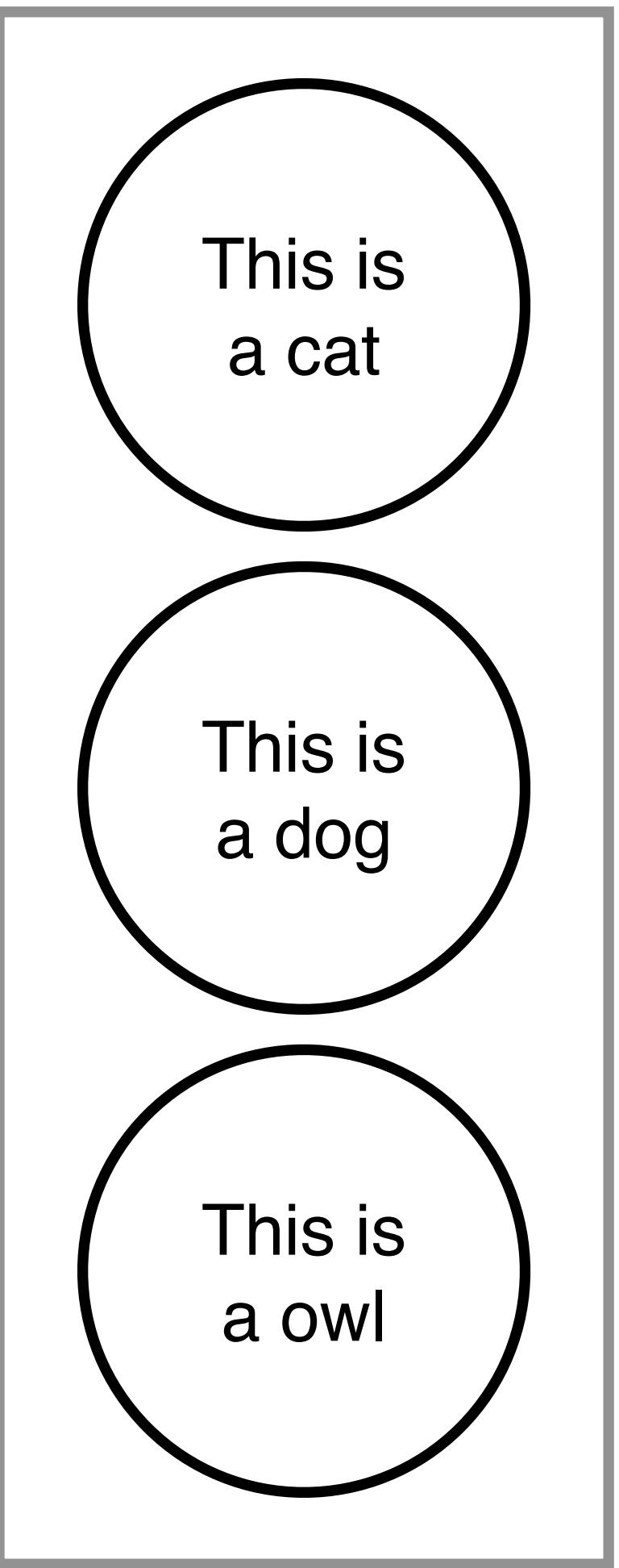
# Types of Outputs



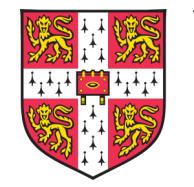
UNIVERSITY OF  
CAMBRIDGE

What type of animal is this? Cat, Dog, or Owl?

Output layer = 3 nodes



# Types of Outputs

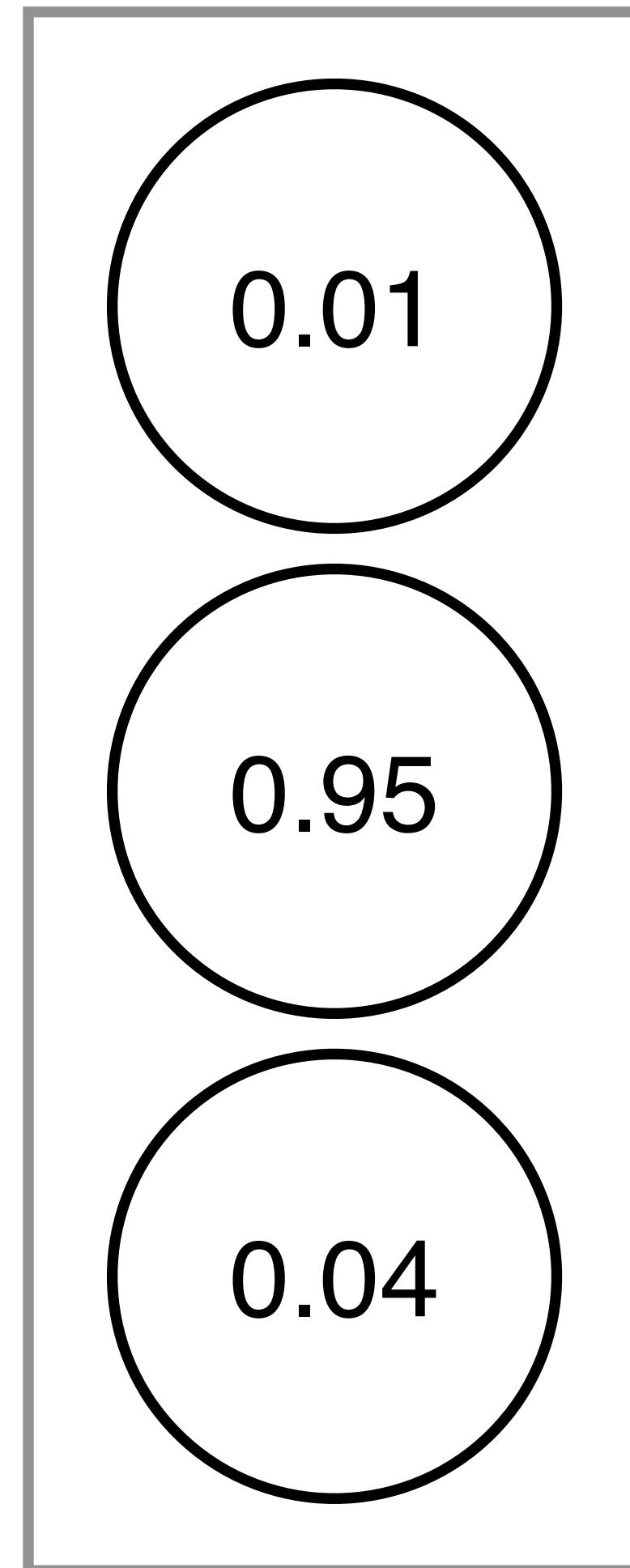


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What type of animal is this? Cat, Dog, or Owl?



Output layer = 3 nodes



# Types of Outputs

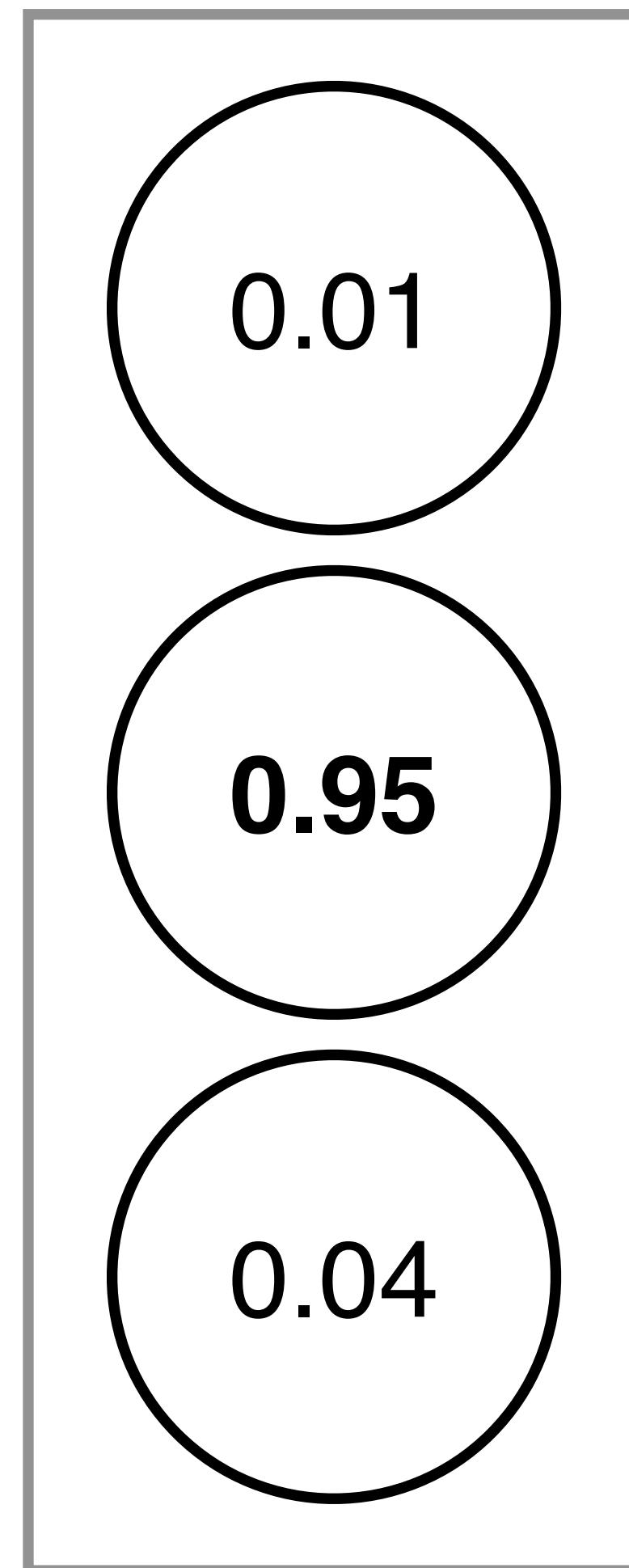
What type of animal is this? Cat, Dog, or Owl?



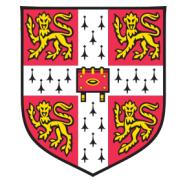
I give **95%** odds that this is a dog.

I classify this **as a dog**.

Output layer = 3 nodes



# Types of Outputs



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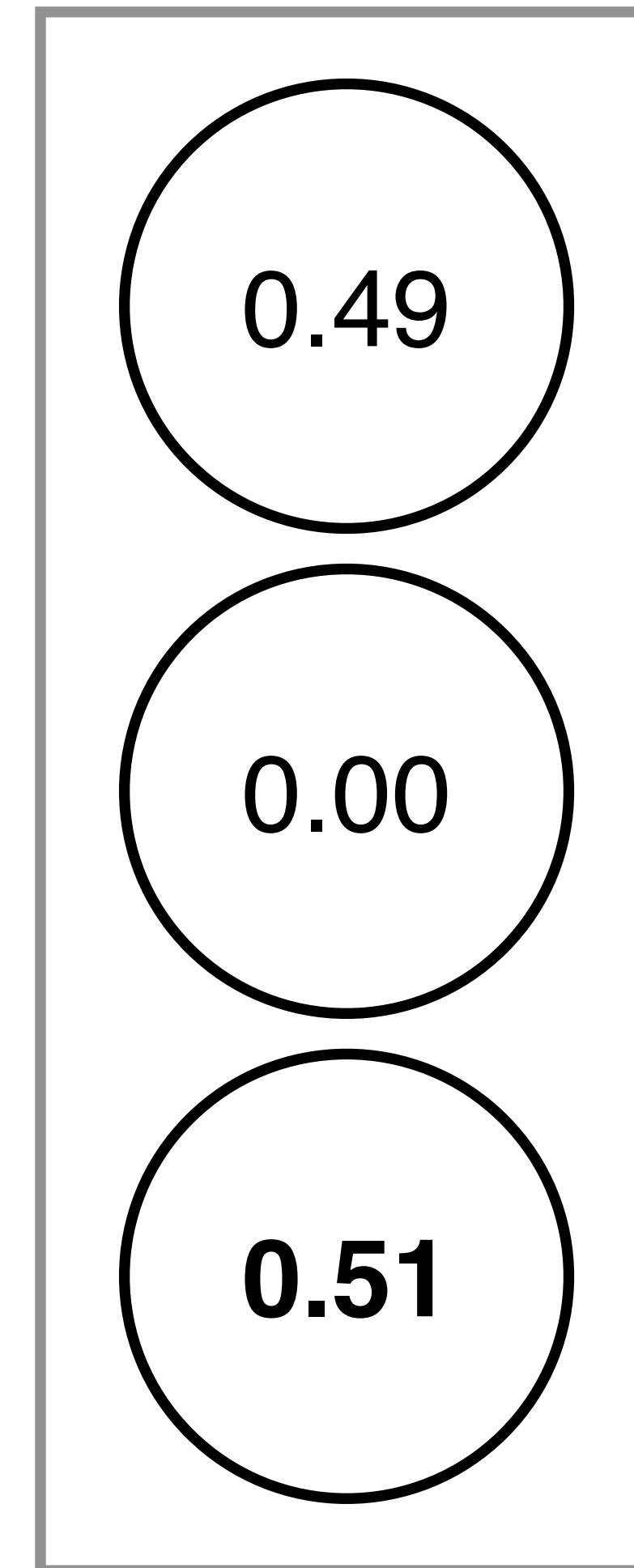
What type of animal is this? Cat, Dog, or Owl?



I give **51%** odds that this is an owl.

I classify this **as an owl**.

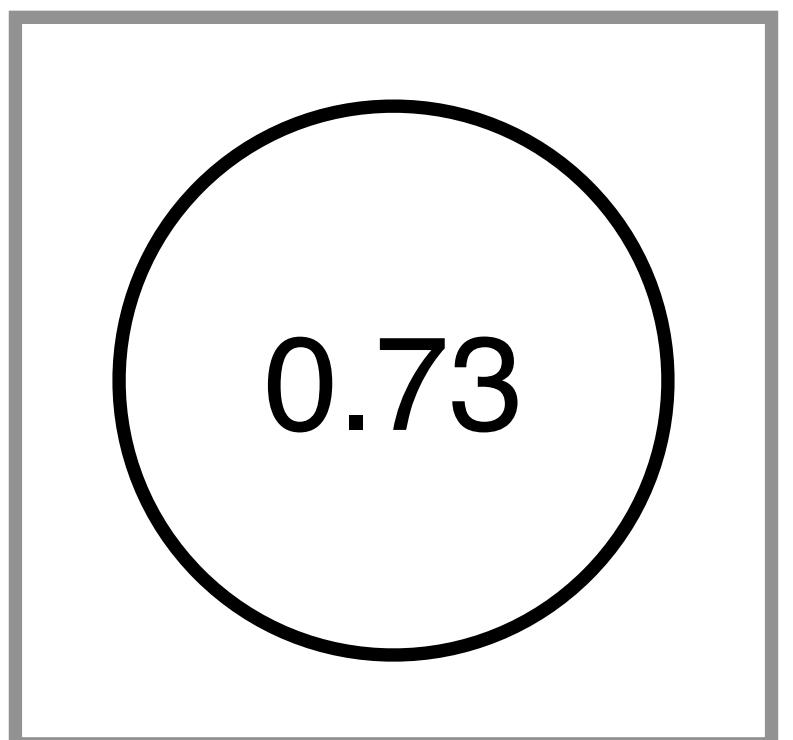
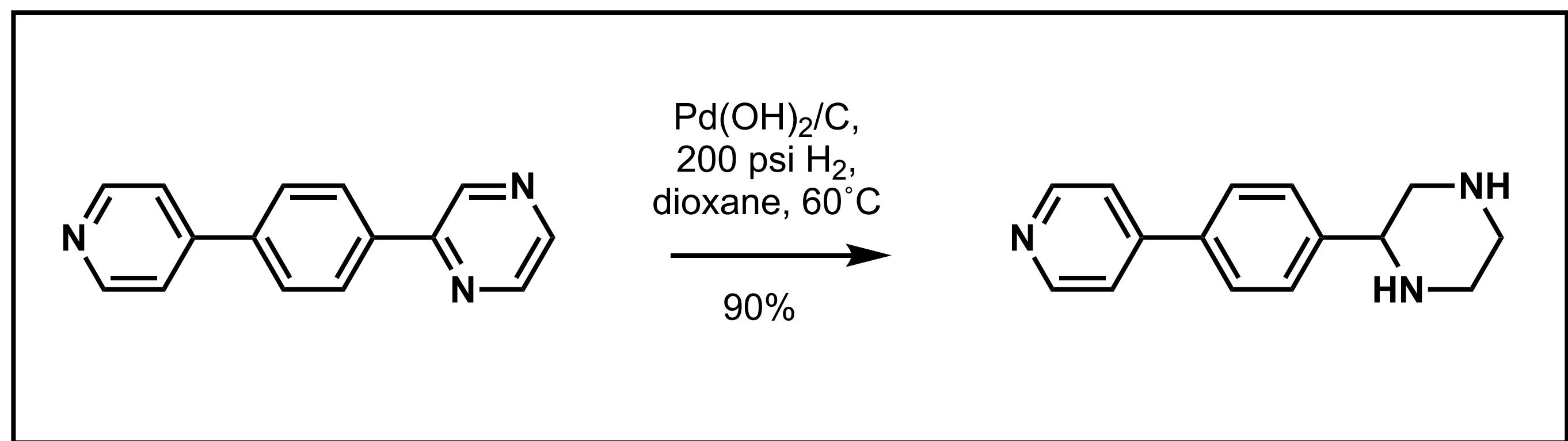
Output layer = 3 nodes



# Types of Outputs

What is the yield of this reaction?

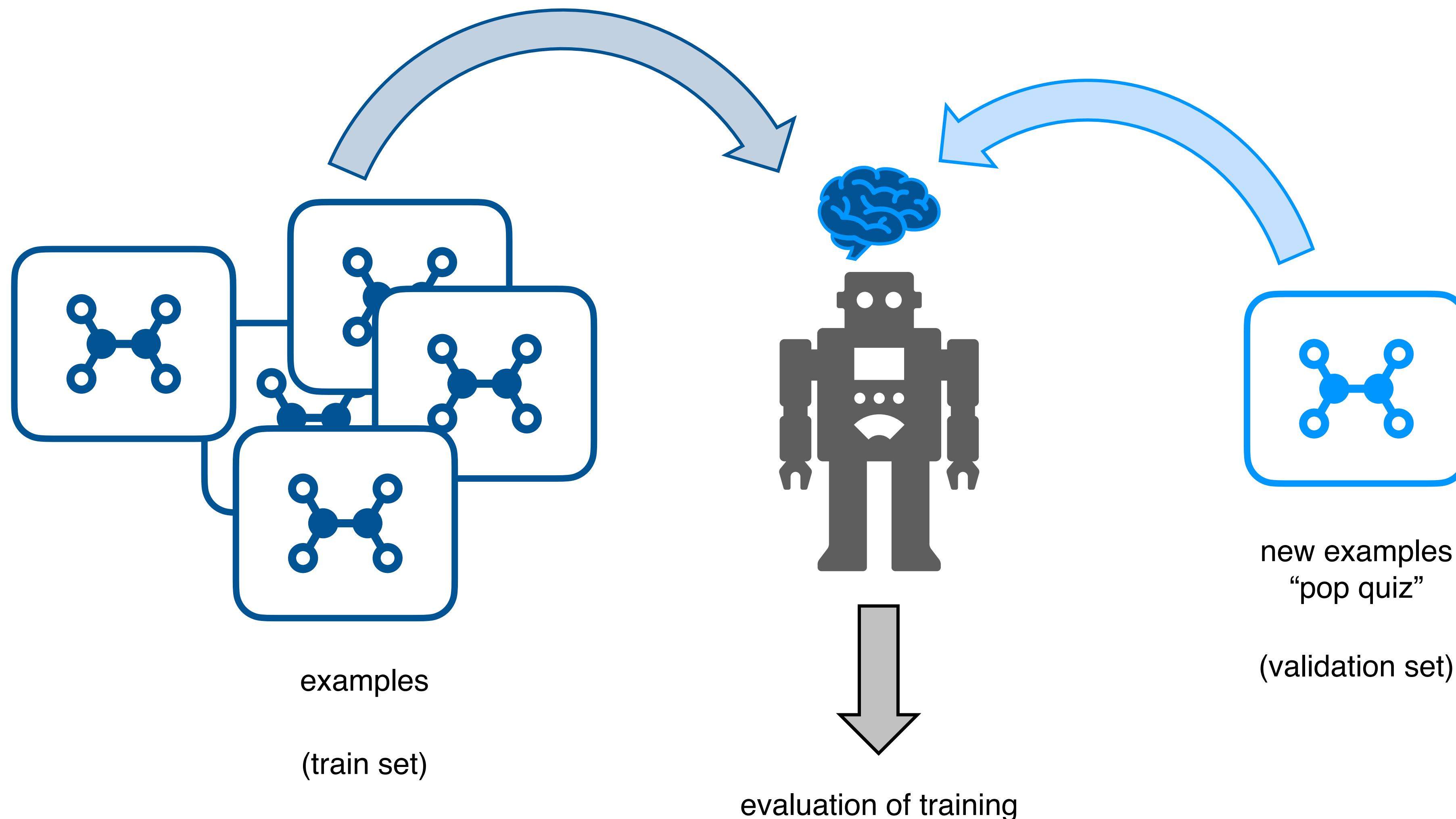
Output layer = 1 node



I predict the yield will be 73%

# Beware: Overfitting!

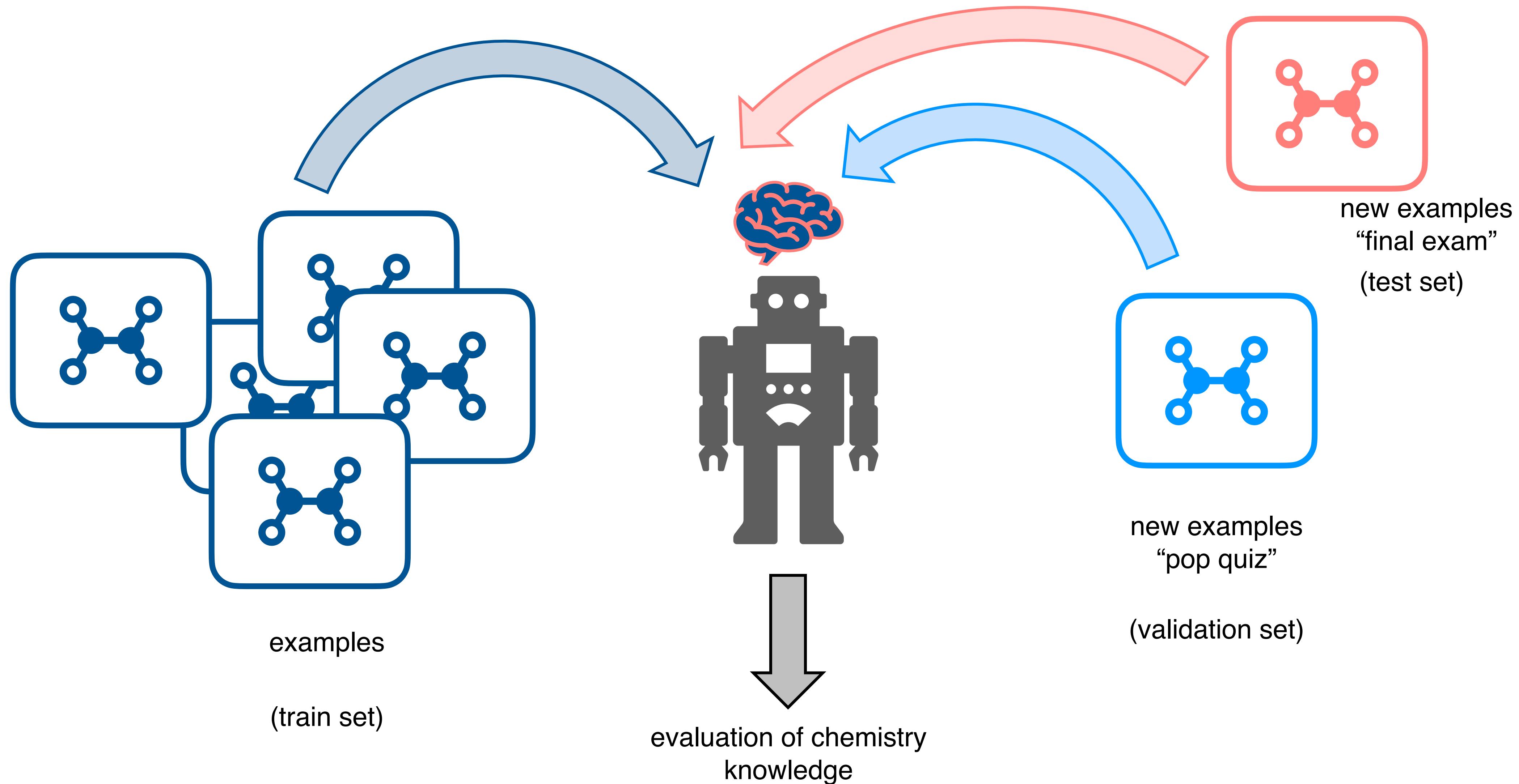
A common complaint - the network just memorizes the answers to the training questions!



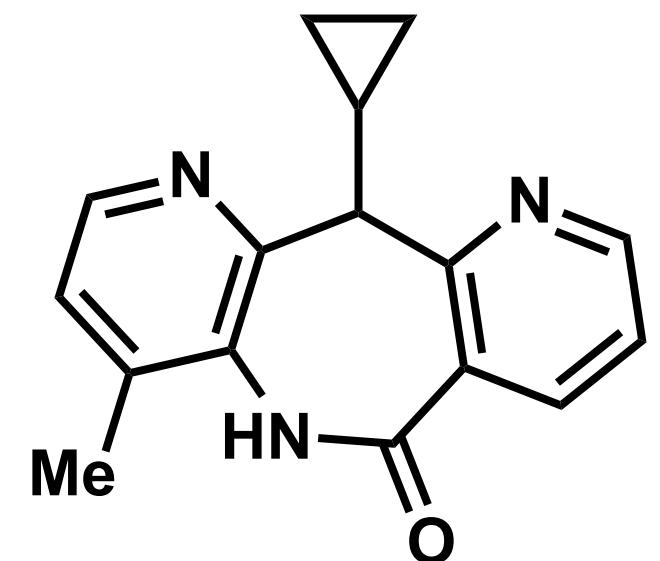
# Beware: Overfitting!



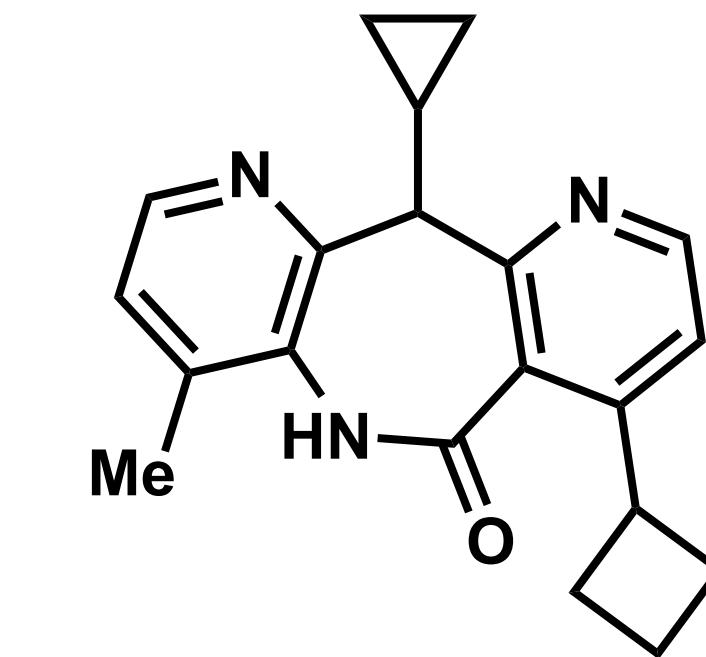
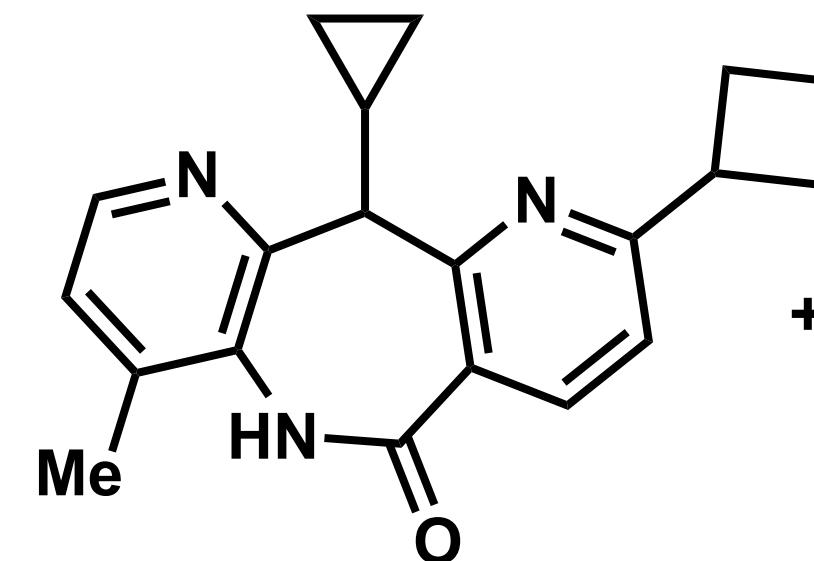
A common complaint - the network just memorizes the answers to  
the training questions!



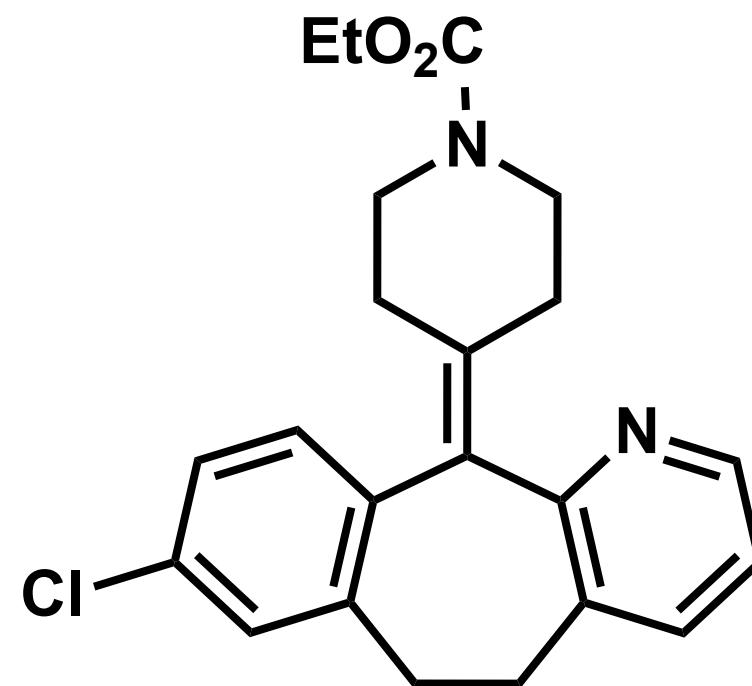
*Minisci*



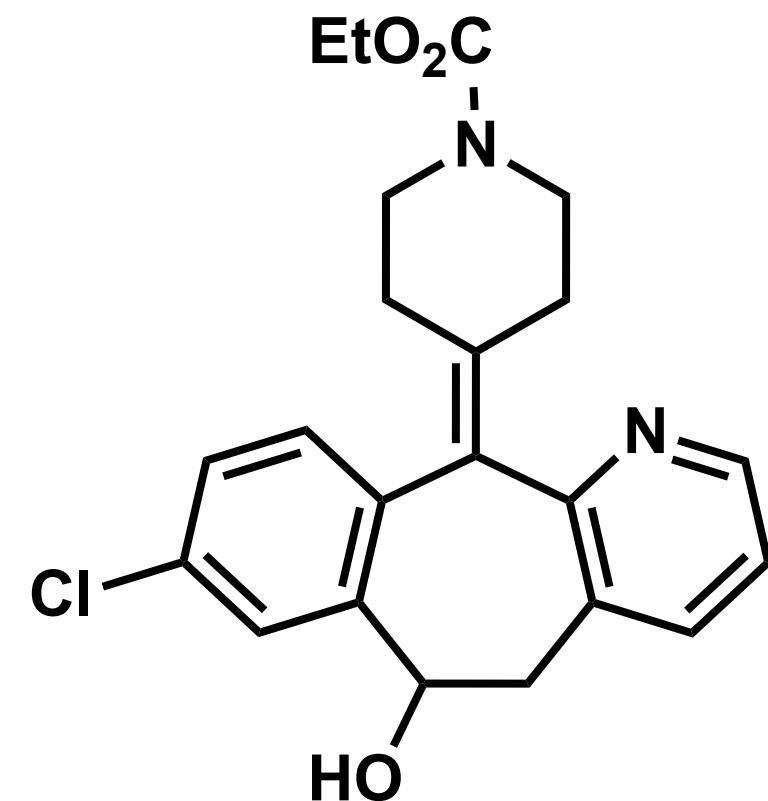
cBuBF<sub>3</sub>K,  
Mn(OAc)<sub>3</sub>,  
AcOH, AcOH/H<sub>2</sub>O



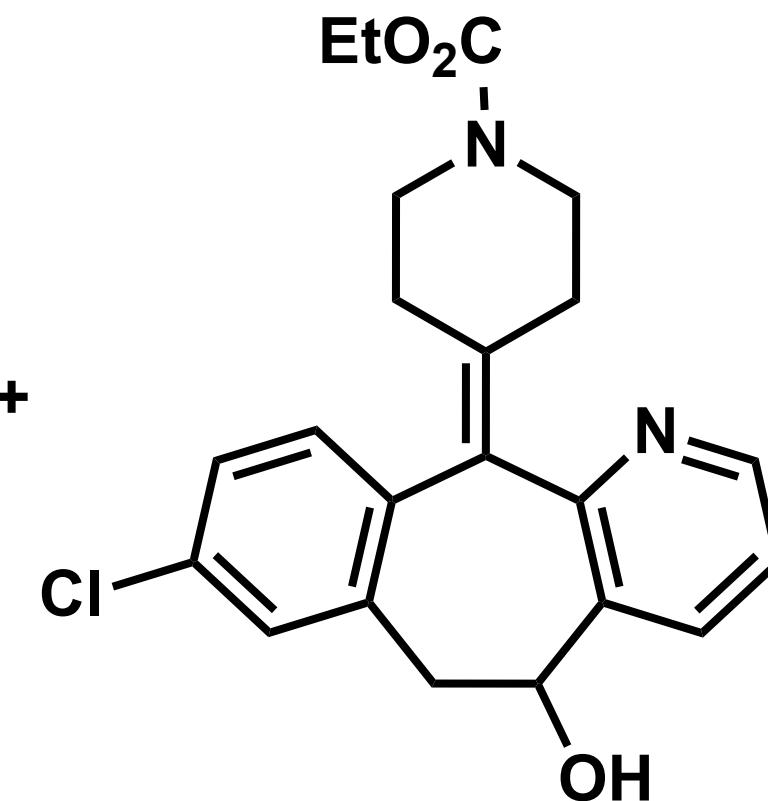
*P450 Ox.*



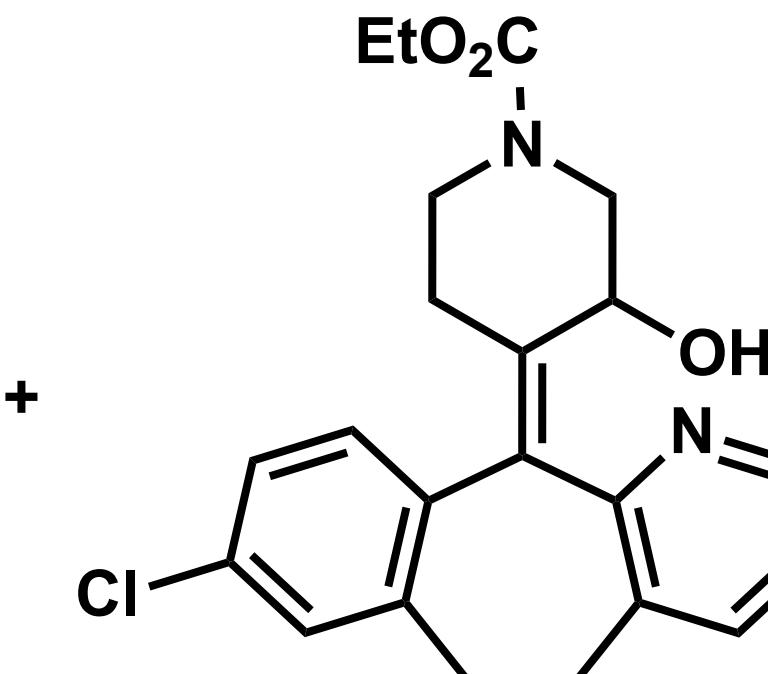
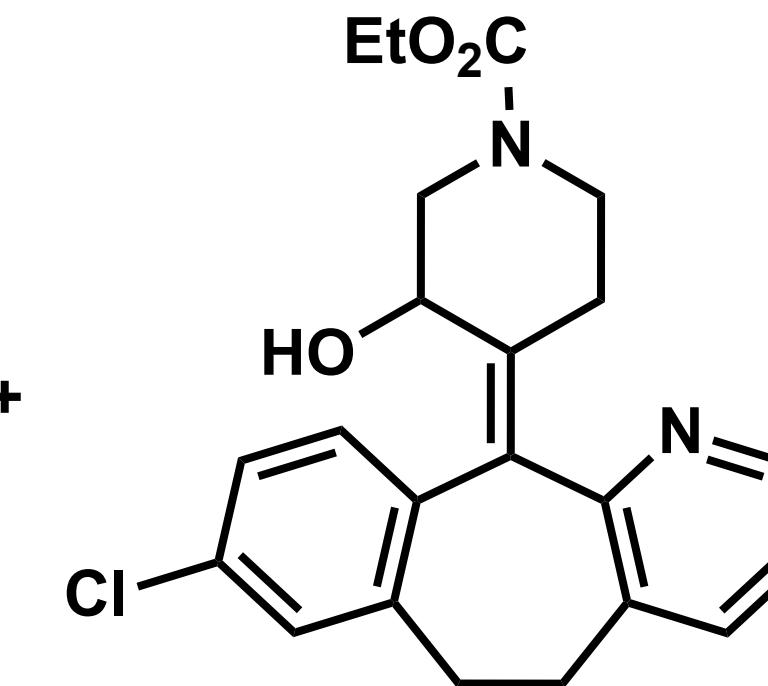
cBuBF<sub>3</sub>K,  
Mn(OAc)<sub>3</sub>,  
AcOH, AcOH/H<sub>2</sub>O



+

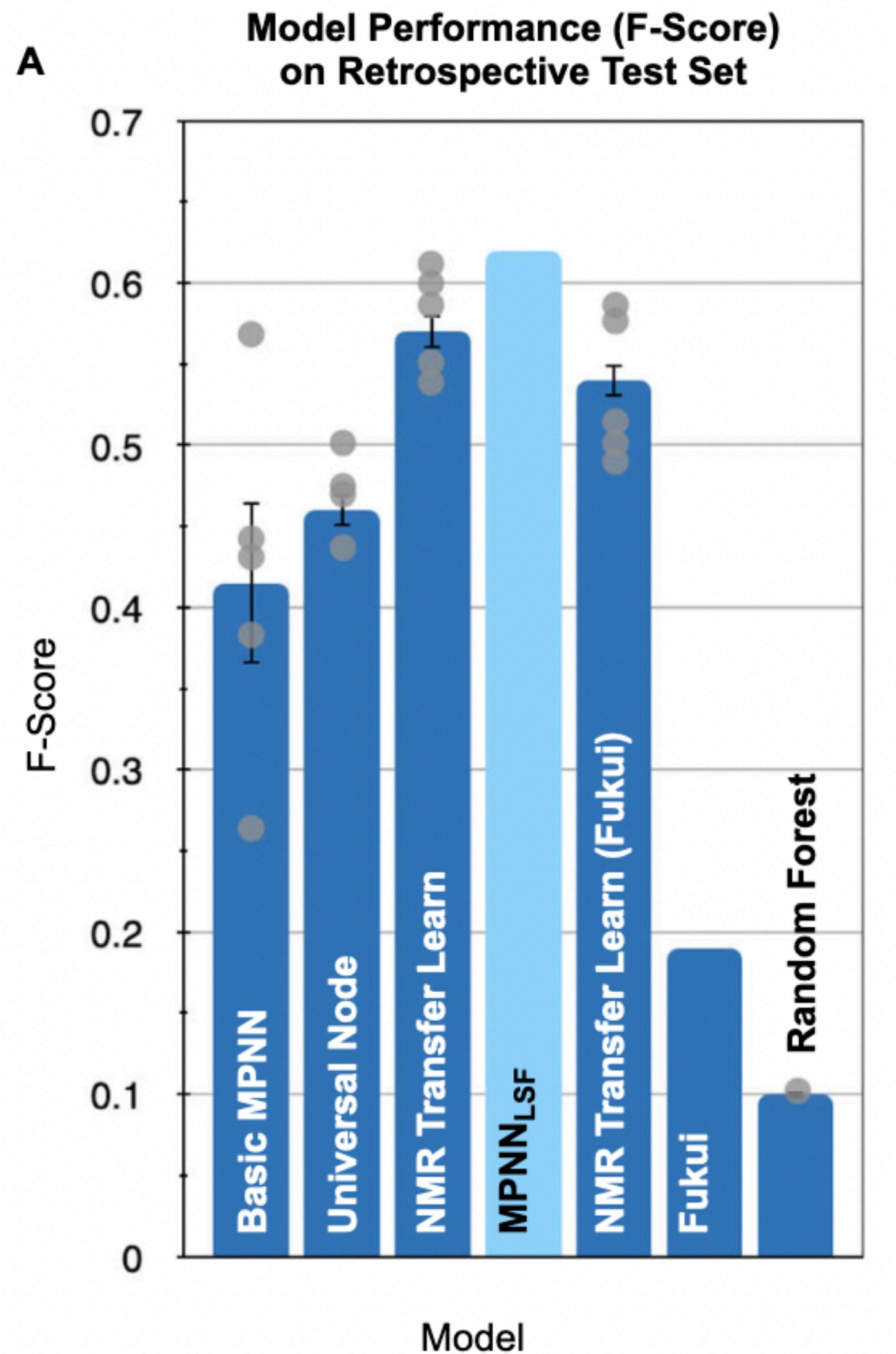


+

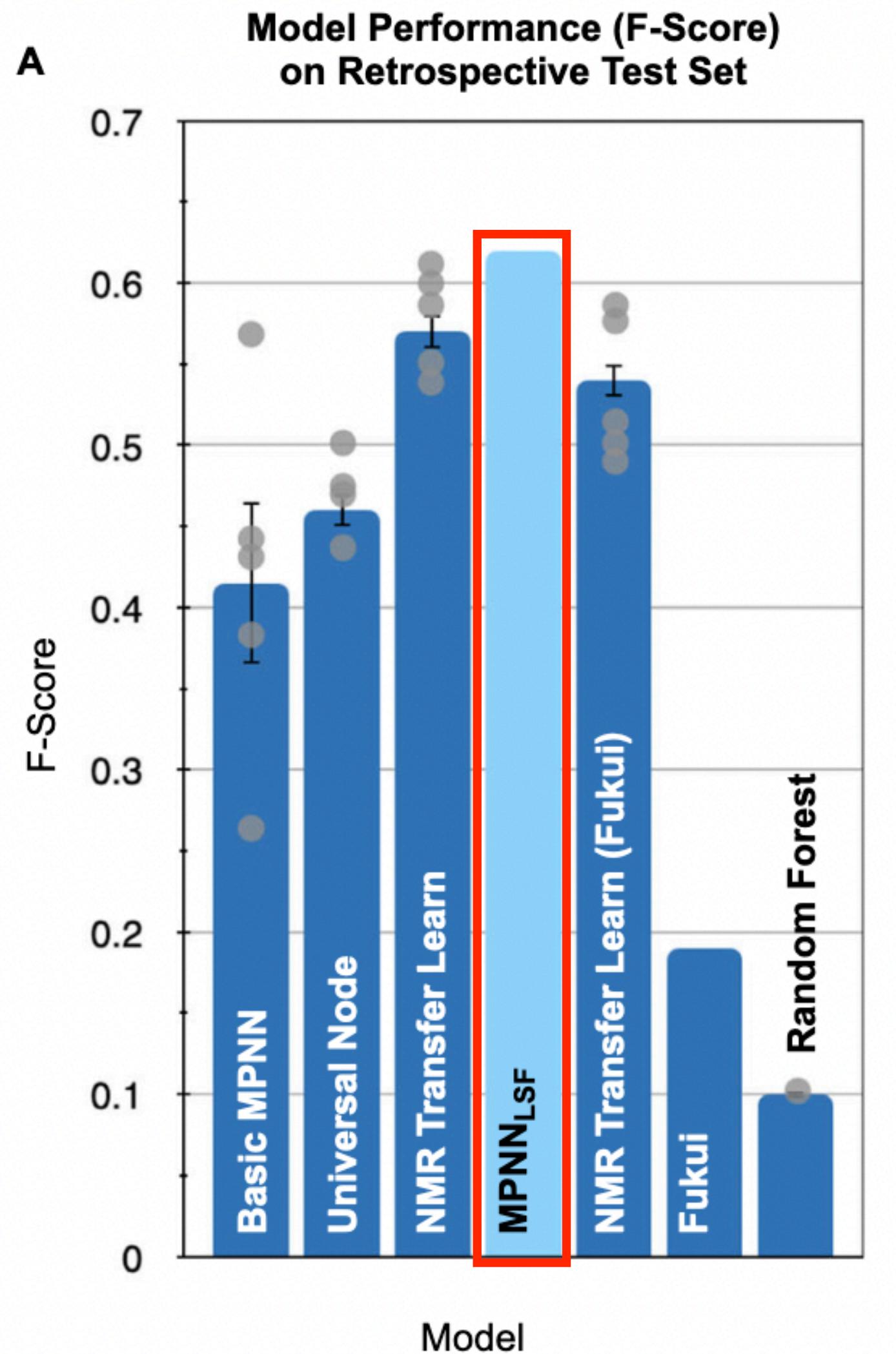


Predict regiochemical outcomes?

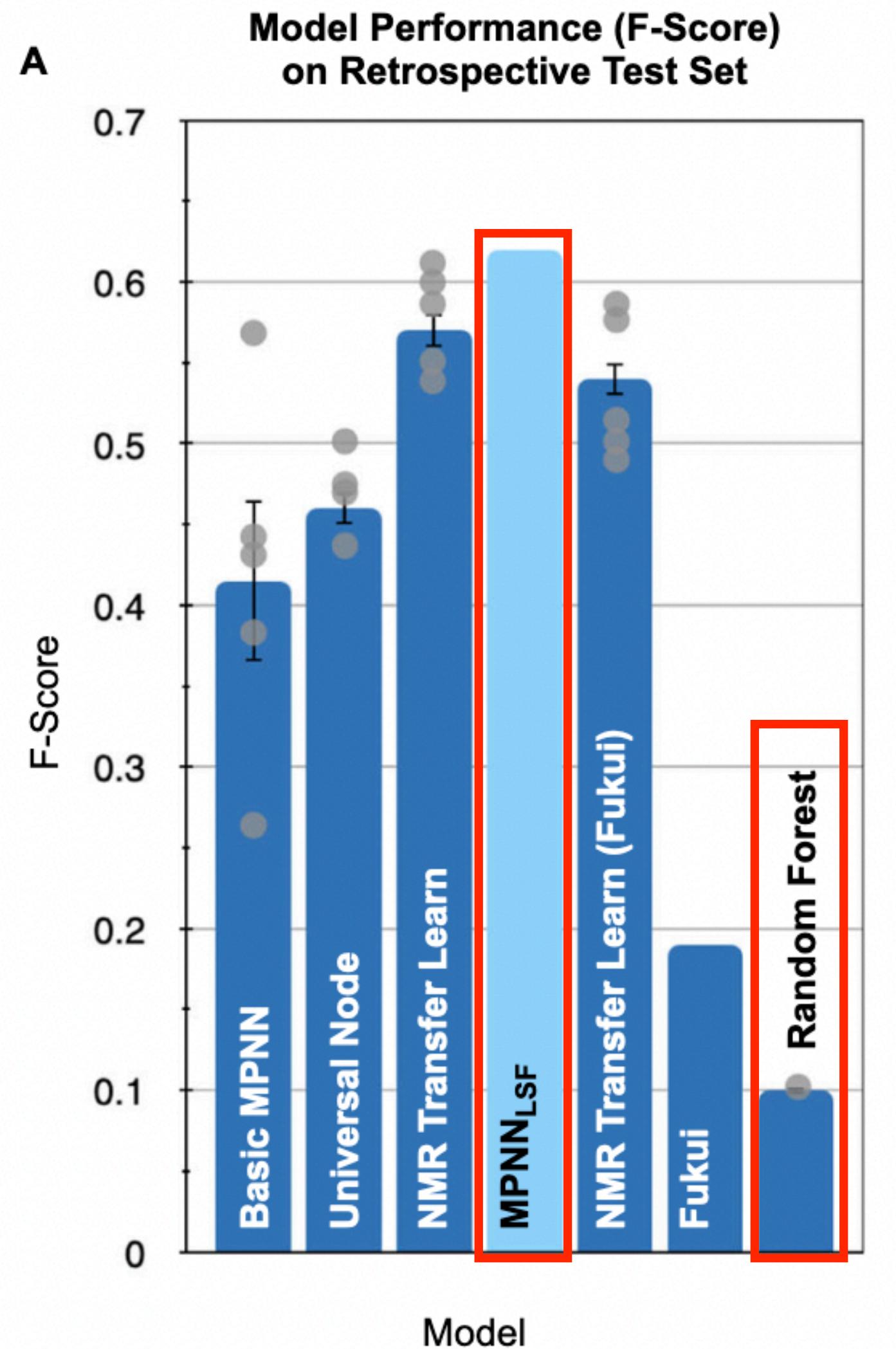
# Some Real World Examples of Neural Networks



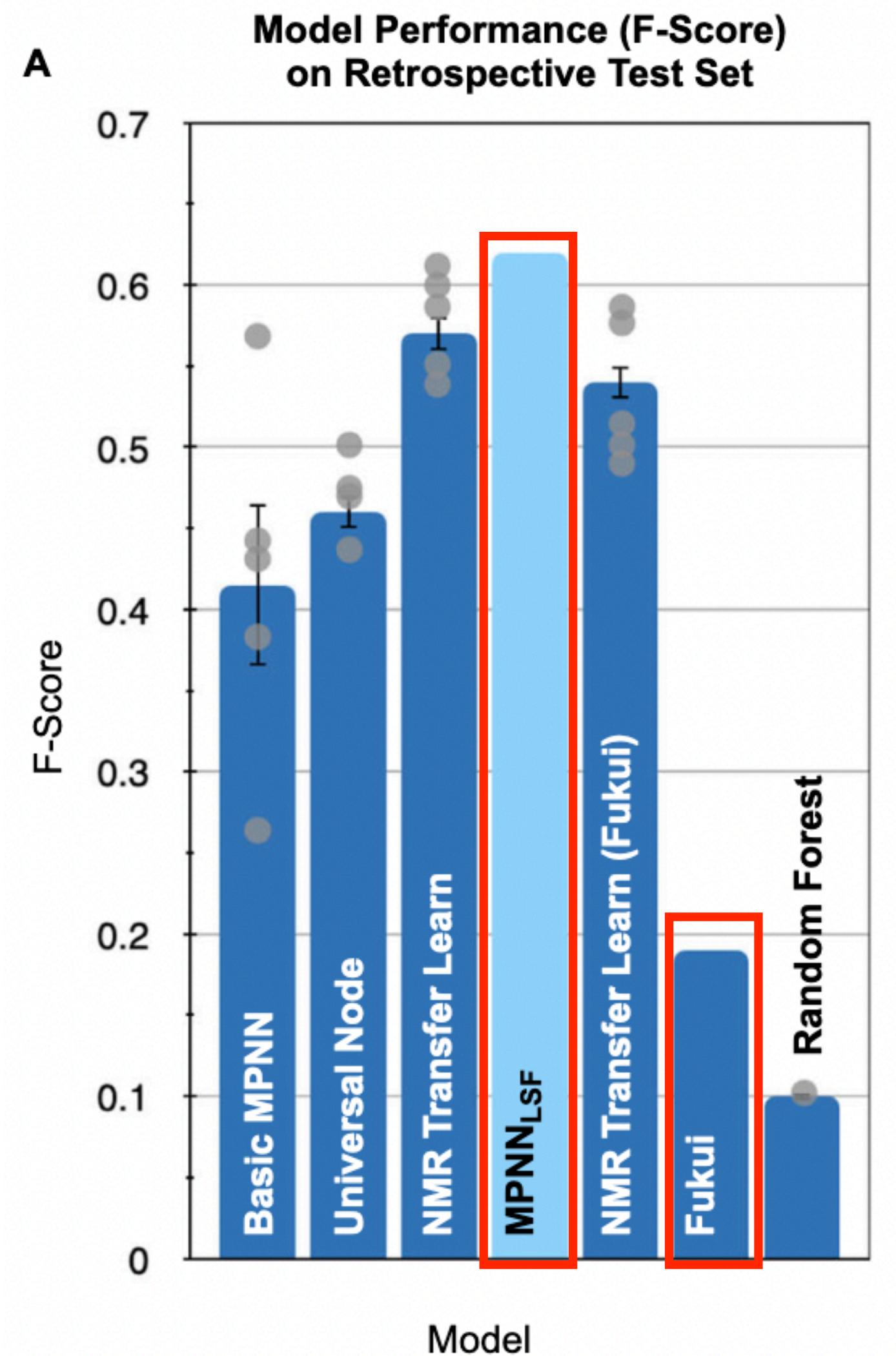
# Some Real World Examples of Neural Networks



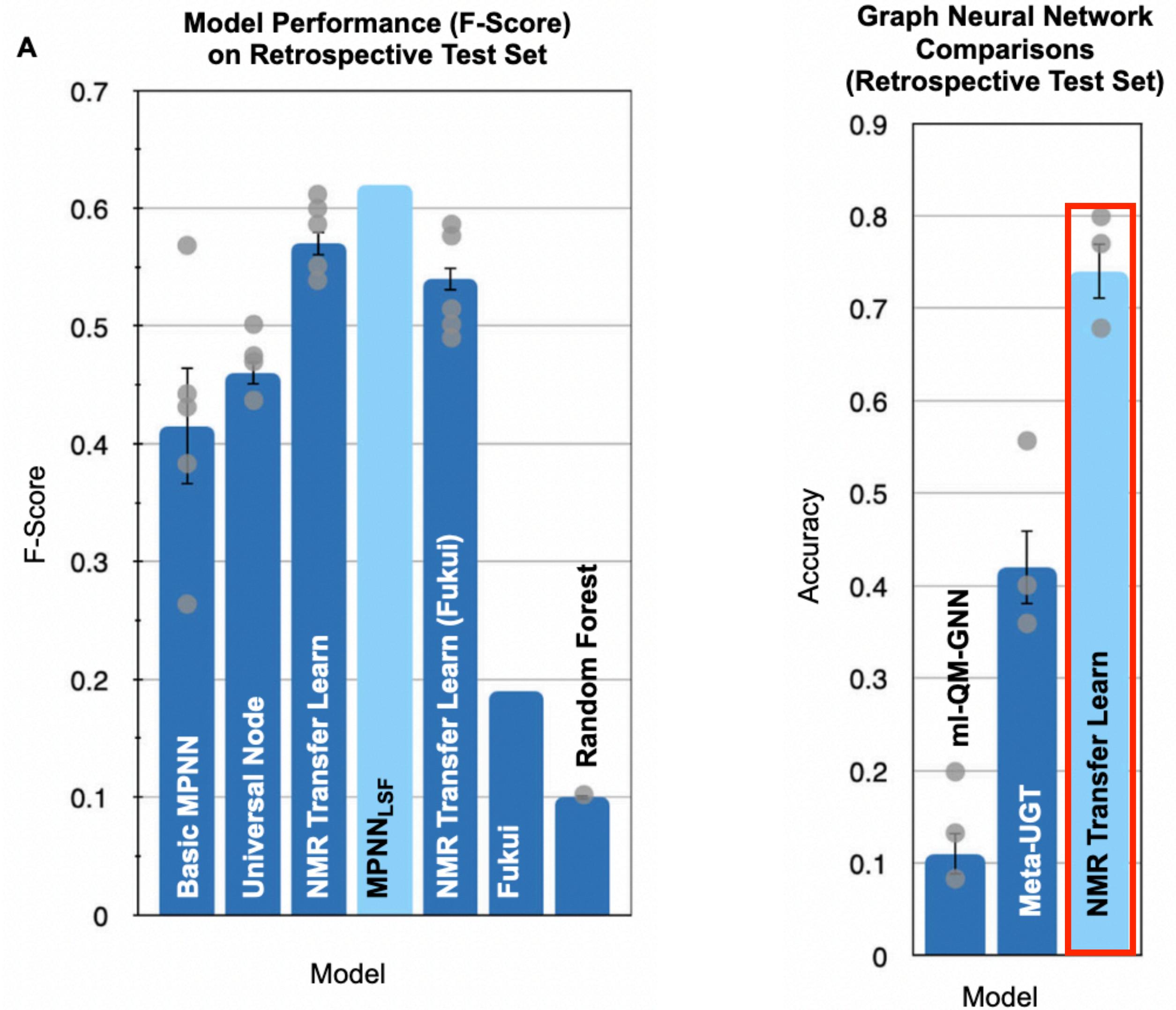
# Some Real World Examples of Neural Networks



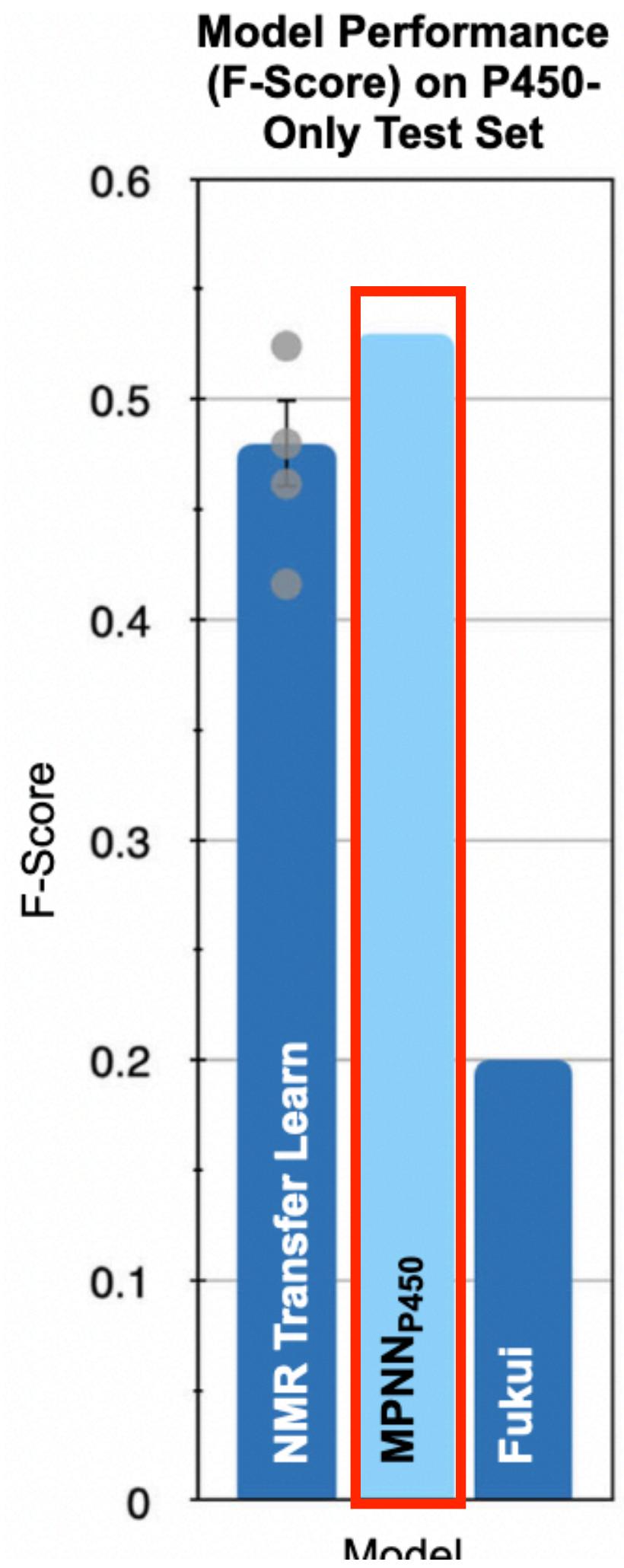
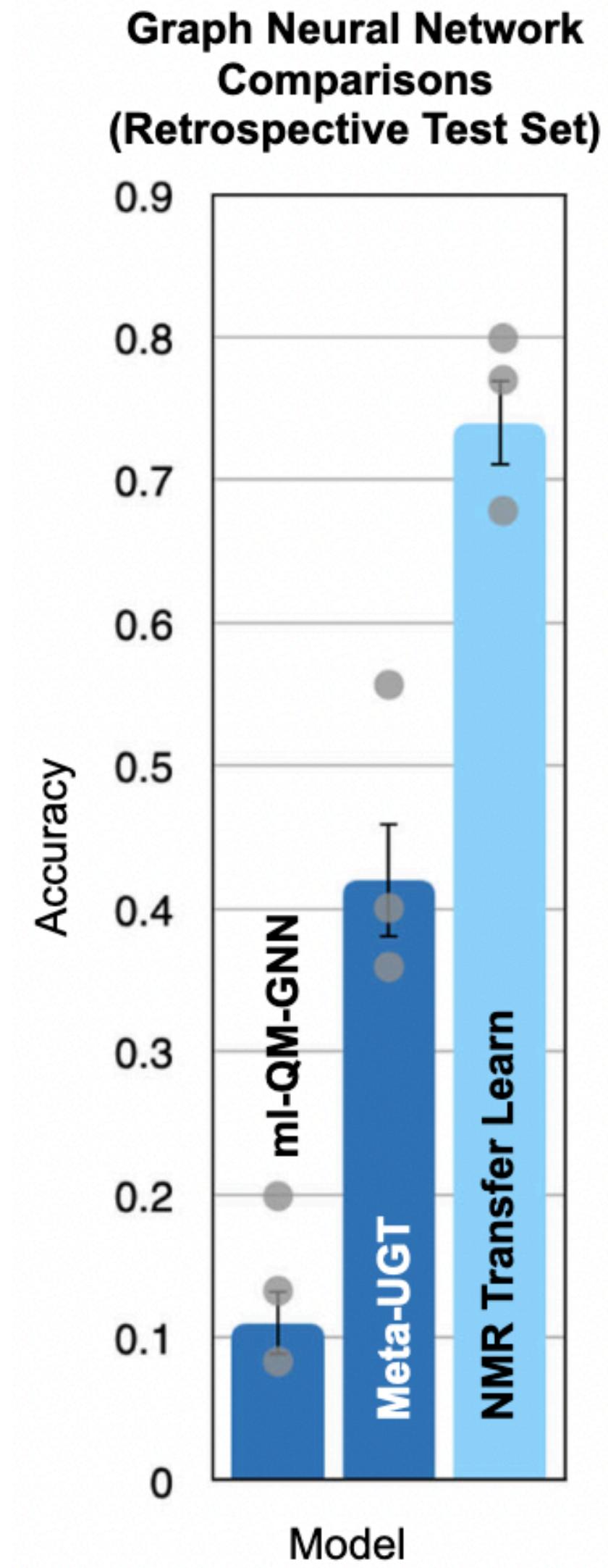
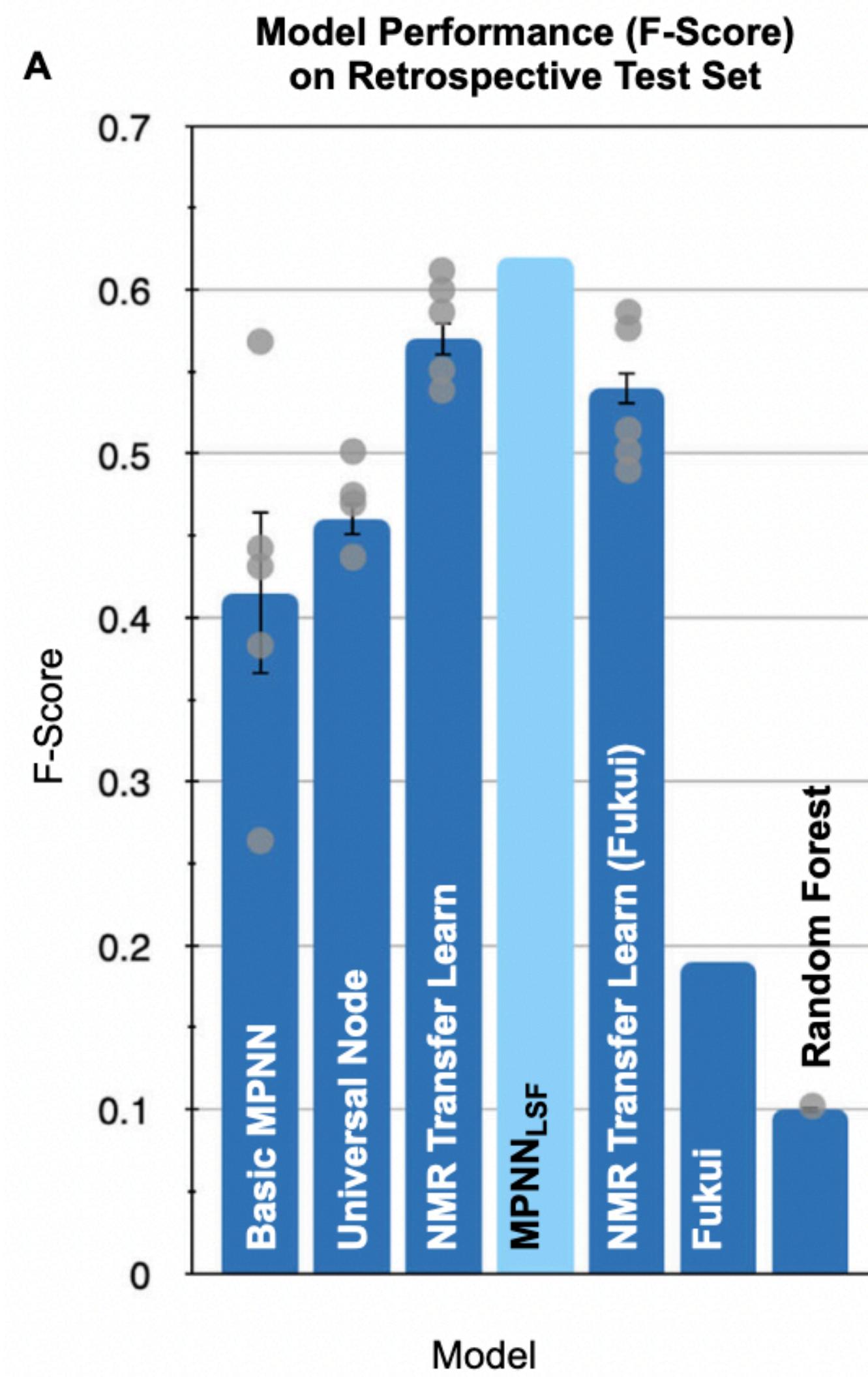
# Some Real World Examples of Neural Networks



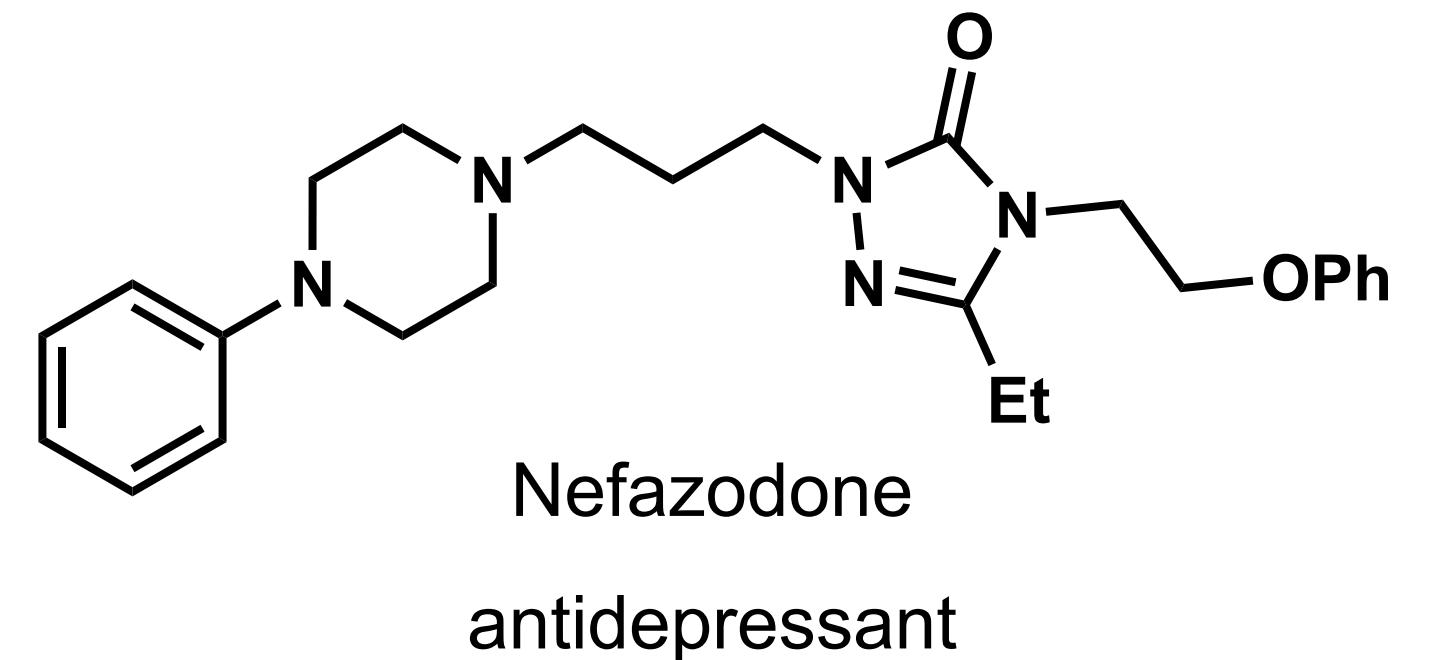
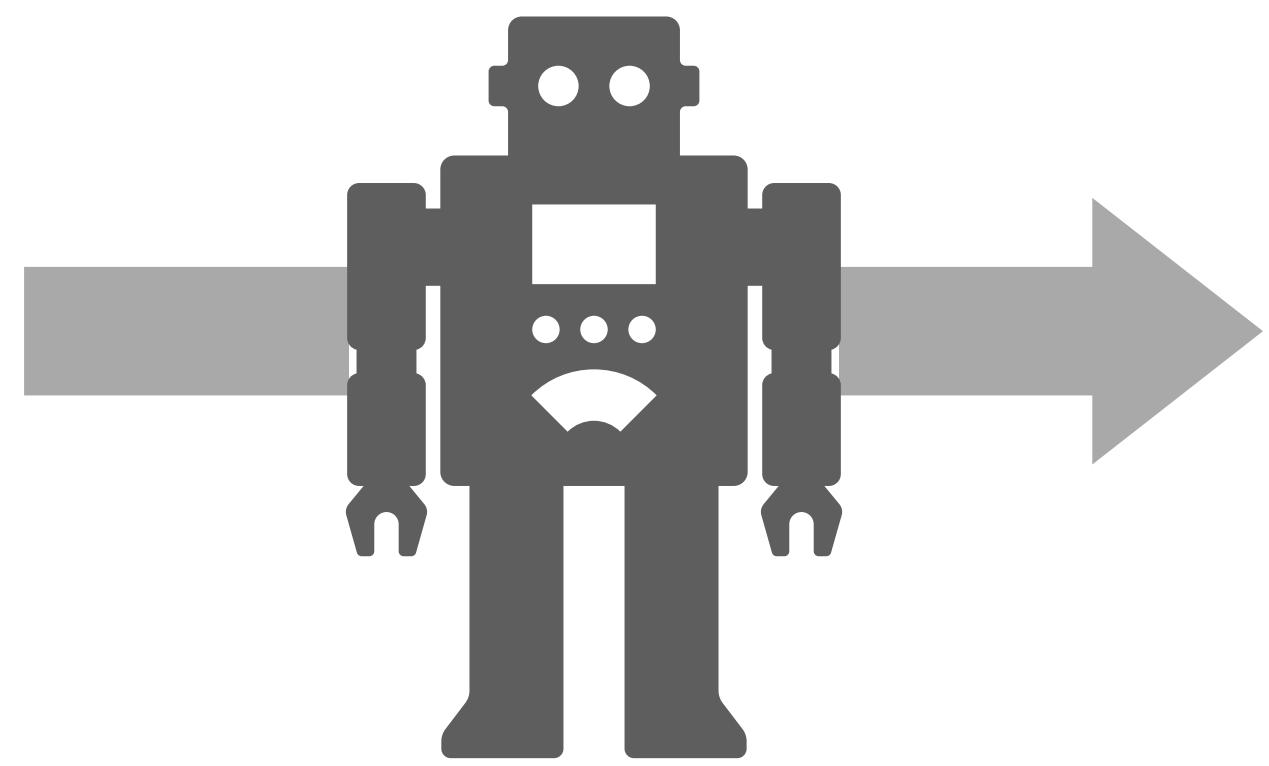
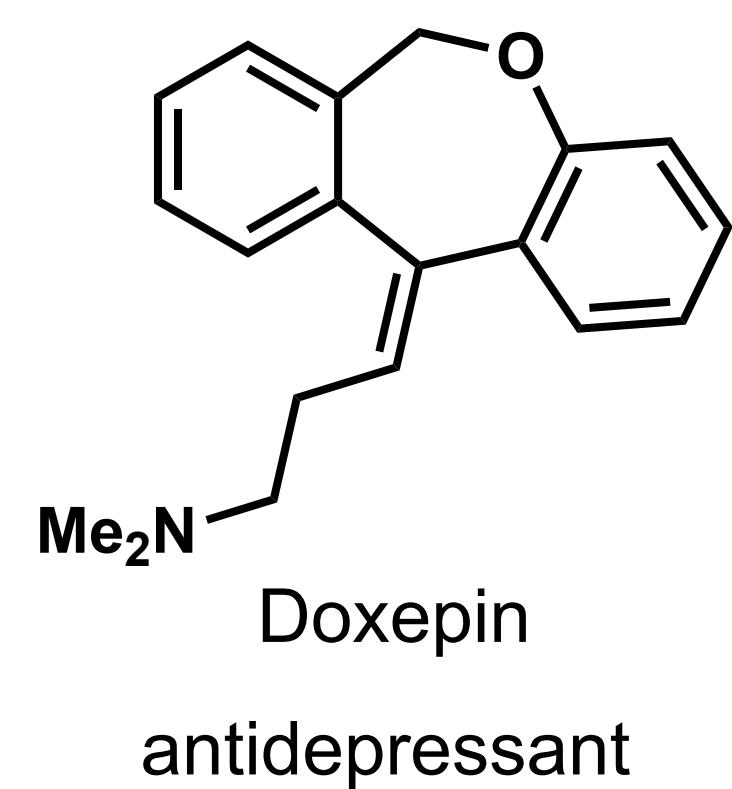
# Some Real World Examples of Neural Networks



# Some Real World Examples of Neural Networks

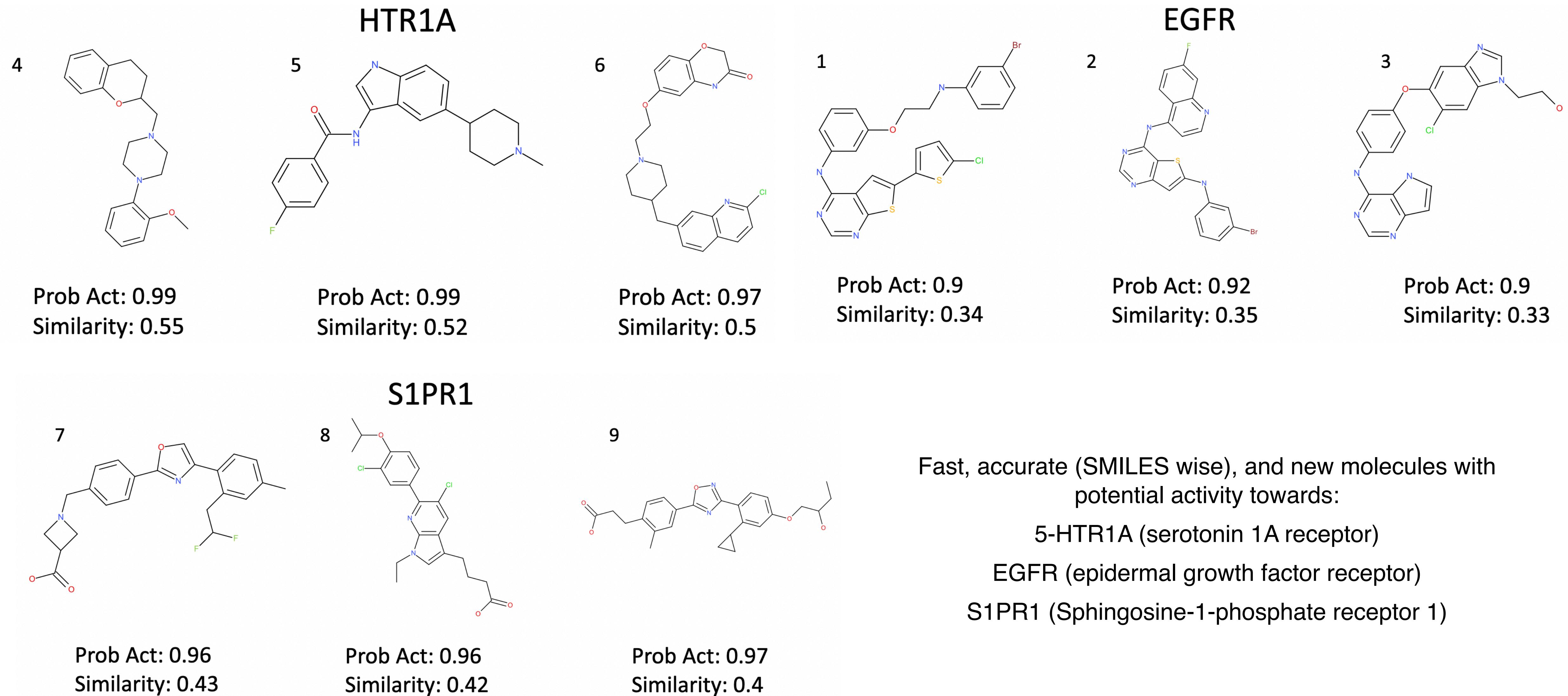


## Molecular Generators:



Same function, wildly different structure?

# Some Real World Examples of Neural Networks





<b>PCA   SVM   GP   RF</b>		<b>Feed Forward NNs</b>
No   Yes   Yes   Yes	Classification?	Yes
No   Yes   Yes   Yes	Regression?	Yes
No   No   Yes   No	Uncertainties?	Yes
None	Data assumptions?	None
Yes*   No   No   Yes	Interpretability?	No
Very beginner friendly	User friendliness?	Easier to screw up
Low-mid amount of data	Data Regime?	High amount of data
Not usually	Generalizability?	More able to



# Thank You!